Homomorphism Tensors and Linear Equations

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Abstract

Lovász (1967) showed that two graphs $G$ and $H$ are isomorphic if and only if they are homomorphism indistinguishable over the class of all graphs, i.e. for every graph $F$, the number of homomorphisms from $F$ to $G$ equals the number of homomorphisms from $F$ to $H$. Recently, homomorphism indistinguishability over restricted classes of graphs such as bounded treewidth, bounded treedepth and planar graphs, has emerged as a surprisingly powerful framework for capturing diverse equivalence relations on graphs arising from logical equivalence and algebraic equation systems.

In this paper, we provide a unified algebraic framework for such results by examining the linear-algebraic and representation-theoretic structure of tensors counting homomorphisms from labelled graphs. The existence of certain linear transformations between such homomorphism tensor subspaces can be interpreted both as homomorphism indistinguishability over a graph class and as feasibility of an equational system. Following this framework, we obtain characterisations of homomorphism indistinguishability over several natural graph classes, namely trees of bounded degree, graphs of bounded pathwidth (answering a question of Dell et al. (2018)), and graphs of bounded treedepth.

Keywords: graph homomorphisms, homomorphism indistinguishability, labelled graphs, treewidth, pathwidth, treedepth, linear equations, Sherali–Adams relaxation, Specht–Wiegmann Theorem, Weisfeiler–Leman

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1 Introduction

Representations in terms of homomorphism counts provide a surprisingly rich view on graphs and their properties. Homomorphism counts have direct connections to logic [17, 22, 34], category theory [14, 42], the graph isomorphism problem [16, 17, 34], algebraic characterisations of graphs [16], and quantum groups [39]. Counting subgraph patterns in graphs has a wide range of applications, for example in graph kernels (see [30]) and motif counting (see [2, 40]). Homomorphism counts can be used as a flexible basis for counting all kinds of substructures [13], and their complexity has been studied in great detail (e.g. [10, 11, 13, 50]). It has been argued in [24] that homomorphism counts are well-suited as a theoretical foundation for analysing graph embeddings and machine learning techniques on graphs, both indirectly through their connection with graph neural networks via the Weisfeiler–Leman algorithm [17, 43, 57] and directly as features for machine learning on graphs. The latter has also been confirmed experimentally [5, 31, 45].

The starting point of the theory is an old result due to Lovász [34]: two graphs $G$, $H$ are isomorphic if and only if for every graph $F$, the number $\text{hom}(F, G)$ of homomorphisms from $F$ to $G$ equals $\text{hom}(F, H)$. For a class $\mathcal{F}$ of graphs, we say that $G$ and $H$ are homomorphism indistinguishable over $\mathcal{F}$ if and only if $\text{hom}(F, G) = \text{hom}(F, H)$ for all $F \in \mathcal{F}$. A beautiful picture that has only emerged in the last few years shows that homomorphism indistinguishability over natural graph classes, such as paths, trees, or planar graphs, characterises a variety of natural equivalence relations on graphs.

Broadly speaking, there are two types of such results, the first relating homomorphism indistinguishability to logical equivalence, and the second giving algebraic characterisations of homomorphism equivalence derived from systems of linear (in)equalities for graph isomorphism. Examples of logical characterisations of homomorphism equivalence are the characterisation of homomorphism indistinguishability over graphs of treewidth at most $k$ in terms of the $(k+1)$-variable fragment of first-order logic with counting [17] and the characterisation of homomorphism indistinguishability over graphs of treedepth at most $k$ in terms of the quantifier-rank-$k$ fragment of first-order logic with counting [22]. Results of this type have also been described in a general category-theoretic framework [14, 42]. Examples of equational characterisations are the characterisation of homomorphism indistinguishability over trees in terms of fractional isomorphism [16, 17, 55], which may be viewed as the LP relaxation of a natural ILP for graph isomorphism, and a generalisation to homomorphism indistinguishability over graph of bounded treewidth in terms of the Sherali–Adams hierarchy over that ILP [4, 16, 26, 17, 38]. Further examples include a characterisation of homomorphism indistinguishability over paths in terms of the same system of equalities by dropping the non-negativity constraints of fractional isomorphism [16], and a characterisation of homomorphism indistinguishability over planar graphs in terms of quantum isomorphism [39]. Remarkably, quantum isomorphism is derived from interpreting the same system of linear equations over C*-algebras [3].

1.1 Results

Two questions that remained open in [16] are (1) whether the equational characterisation of homomorphism indistinguishability over paths can be generalised to graphs of bounded
pathwidth in a similar way as the characterisation of homomorphism indistinguishability over trees can be generalised to graphs of bounded treewidth, and (2) whether homomorphism indistinguishability over graphs of bounded degree suffices to characterise graphs up to isomorphism. In this paper, we answer the first question affirmatively.

**Theorem 1.1.** For every $k \geq 1$, the following are equivalent for $n$-vertex graphs $G$ and $H$:

1. $G$ and $H$ are homomorphism indistinguishable over the graphs of pathwidth at most $k$,
2. the level-$(k+1)$ relaxation $L_{iso}^{k+1}(G, H)$ of the standard ILP for graph isomorphism has a rational solution.

The detailed description of the system $L_{iso}^{k+1}(G, H)$ is provided in Section 2.7. In fact, we also devise an alternative system of linear equations $PW^{k+1}(G, H)$ characterising homomorphism indistinguishability over graphs of pathwidth at most $k$. The definition of this system turns out to be very natural from the perspective of homomorphism counting, and as we explain later, it forms a fruitful instantiation of a more general representation-theoretic framework for homomorphism indistinguishability.

Moreover, we obtain an equational characterisation of homomorphism indistinguishability over graphs of bounded treedepth. The resulting system $TD^k(G, H)$ is very similar to $L_{iso}^k(G, H)$ and $PW^k(G, H)$, except that variables are indexed by (ordered) $k$-tuples of variables rather than sets of at most $k$ variables, which reflects the order induced by the recursive definition of treedepth.

**Theorem 1.2.** For every $k \geq 1$, the following are equivalent for $n$-vertex graphs $G$ and $H$:

1. $G$ and $H$ are homomorphism indistinguishable over the graphs of treedepth at most $k$,
2. the linear systems of equations $TD^k(G, H)$ has a non-negative rational solution,
3. the linear systems of equations $TD^k(G, H)$ has a rational solution.

Along with [22], the above theorem implies that the logical equivalence of two graphs $G$ and $H$ over the quantifier-rank-$k$ fragment of first-order logic with counting can be characterised by the feasibility of the system $TD^k(G, H)$ of linear equations.

We cannot answer the second open question from [16], but we prove a partial negative result: homomorphism indistinguishability over trees of bounded degree is strictly weaker than homomorphism indistinguishability over all trees.

**Theorem 1.3.** For every integer $d \geq 1$, there exist graphs $G$ and $H$ such that $G$ and $H$ are homomorphism indistinguishable over trees of degree at most $d$, but $G$ and $H$ are not homomorphism indistinguishable over the class of all trees.

In conjunction with [16], the above theorem yields the following corollary: counting homomorphisms from trees of bounded degree is strictly less powerful than the classical Colour Refinement algorithm [25], in terms of their ability to distinguish non-isomorphic graphs.

To prove these results, we develop a general theory that enables us to derive some of the existing results as well as the new results in a unified algebraic framework exploiting a duality between algebraic varieties of “tensor maps” derived from homomorphism counts over families of rooted graphs and equationally defined equivalence relations, which are based on transformations of graphs in terms of unitary/orthogonal or, more often, pseudo-stochastic
or doubly-stochastic matrices. (We call a matrix over the complex numbers pseudo-stochastic if its row and column sums are all 1, and we call it doubly-stochastic if it is pseudo-stochastic and all its entries are non-negative reals.) The foundations of this theory have been laid in [16] and, mainly, [39]. Some ideas can also be traced back to the work on homomorphism functions and connection matrices [18, 35, 36, 51], and a similar duality, called Galois connection there, that is underlying the algebraic theory of constraint satisfaction problems [8, 9, 53, 58].

1.2 Techniques

To explain our core new ideas, let us start from a simple and well-known result: two symmetric real matrices $A, B$ are co-spectral if and only if for every $k \geq 1$ the matrices $A^k$ and $B^k$ have the same trace. If $A, B$ are the adjacency matrices of two graph $G, H$, the latter can be phrased graph theoretically as: for every $k$, $G$ and $H$ have the same number of closed walks of length $k$, or equivalently, the numbers of homomorphisms from a cycle $C_k$ of length $k$ to $G$ and to $H$ are the same. Thus, $G$ and $H$ are homomorphism indistinguishable over the class of all cycles if and only if they are co-spectral. Note next that the graphs, or their adjacency matrices $A, B$, are co-spectral if and only if there is an orthogonal matrix $U$ such that $UA = BU$.

Now, in [16] it was proved that $G, H$ are homomorphism indistinguishable over the class of all paths if and only if there is a pseudo-stochastic matrix $X$ such that $XA = BX$, and they are homomorphism indistinguishable over the class of all trees if and only if there is a doubly-stochastic matrix $X$ such that $XA = BX$. From an algebraic perspective, the transition from an orthogonal matrix in the cycle result to a pseudo-stochastic in the path result is puzzling: where orthogonal matrices are very natural, pseudo-stochastic matrices are much less so from an algebraic point of view. Moving on to the tree result, we suddenly add non-negativity constraints—where do they come from? Our theory presented in Section 5 provides a uniform and very transparent explanation for the three results. It also allows us to analyse homomorphism indistinguishability over $d$-ary trees, for every $d \geq 1$, and to prove that it yields a strict hierarchy of increasingly finer equivalence relations.

Now suppose we want to extend these results to edge coloured graphs. Each edge-coloured graph corresponds to a family of matrices, one for each colour. Theorems due to Specht [52] and Wiegmann [56] characterise families of matrices that are simultaneously equivalent with respect to a unitary transformation. Interpreted over coloured graphs, the criterion provided by these theorems can be interpreted as homomorphism indistinguishability over coloured cycles. One of our main technical contributions (Theorems 3.3 and 3.8) are variants of these theorems that establishes a correspondence between simultaneous equivalence with respect to pseudo-stochastic (doubly-stochastic) transformations and homomorphism indistinguishability over coloured paths (trees). The proof is based on basic representation theory, in particular the character theory of semisimple algebras.

Interpreting graphs of bounded pathwidth in a “graph-grammar style” over coloured paths using graphs of bounded size as building blocks, we give an equational characterisation of homomorphism indistinguishability over graphs of pathwidth at most $k$. After further manipulations, we even obtain a characterisation in terms of a system of equations that are derived by lifting the basic equations for paths in a Sherali–Adams style. (The basic idea of these lifted equations goes back to [4].) This answers the open question from [16] stated above. In the same way, we can lift the characterisations of homomorphism indistinguishability over
trees to graphs of treewidth $k$, and we can also establish a characterisation of homomorphism indistinguishability over graphs of “cyclewidth” $k$, providing a uniform explanation for all these results. Finally, we combine these techniques to prove a characterisation of homomorphism indistinguishability over graphs of treedepth $k$ in terms of a novel system of linear equations.

2 Preliminaries

We write $\mathbb{N} = \{0, 1, 2, \ldots\}$ for the set of non-negative integers.

2.1 Linear Algebra

The vector spaces considered in this article are over the rationals $\mathbb{Q}$, the reals $\mathbb{R}$, or complex numbers $\mathbb{C}$ and finite-dimensional. Thus, they carry an inner-product denoted by $\langle \cdot, \cdot \rangle$. We write $\mathbb{K} \in \{\mathbb{Q}, \mathbb{R}, \mathbb{C}\}$ and $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ as place holders for any of the respective fields.

For a vector space $V$ of dimension $n$, write $\text{End}(V)$ for the vector space of endomorphisms of $V$, that is the set of linear maps $V \to V$. Let $\text{id}_V \in \text{End}(V)$ denote the identity map. By standard linear algebra, $\text{End}(V)$ can be identified with $\mathbb{K}^{n \times n}$. Any $A \in \text{End}(V)$ corresponds to a matrix $(a_{ij}) \in \mathbb{K}^{n \times n}$ and $\text{tr} A = \sum_{i=1}^{n} a_{ii}$ where $\text{tr} A$ denotes the trace of the endomorphism $A$. Note that the trace is a property of an endomorphism as it does not depend on the concrete basis chosen.

Contrarily, the sum-of-entries of a matrix $A = (a_{ij}) \in \mathbb{K}^{n \times n}$ denoted by $\text{soe}(a_{ij}) = \sum_{i} a_{ij}$ is not a property of the endomorphism encoded by $(a_{ij})$ but of the matrix itself. For example, $\text{soe}(B^{-1}AB) \neq \text{soe}(A)$ for $A = \begin{pmatrix} 3 & 0 \\ 0 & 2 \end{pmatrix}$ and $B = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. Nevertheless, the vector spaces considered in this article always have a “natural” basis since they arise as subspaces of $\mathbb{K}^I$ for some finite index set $I$.

Of particular interest are maps between vector spaces. Let $V$ and $W$ be $\mathbb{K}$-vector spaces. A map $U : V \to W$ is unitary if $U^* U = \text{id}_V$ and $UU^* = \text{id}_W$ for $U^* : W \to V$ the adjoint of $U$, cf. [33, p. 185]. For a matrix $A = (a_{ij}) \in \mathbb{K}^{n \times n}$, $A^*$ is the conjugate transpose of $A$ when the base field is $\mathbb{C}$ and the transpose of $A$ when it is $\mathbb{R}$ or $\mathbb{Q}$. In the latter case, we write $A^T$ for $A^*$ and call a unitary matrix orthogonal. Note that a map $U : V \to W$ is unitary if and only if $\langle Ux, Uy \rangle = \langle x, y \rangle$ for all $x, y \in V$, i.e. $U$ preserves the inner-product.

Let $I$ and $J$ be finite index sets. Fix vector spaces $V \leq \mathbb{K}^I$ and $W \leq \mathbb{K}^J$ such that the all-ones vectors $\mathbf{1}_I \in V$ and $\mathbf{1}_J \in W$. Then a map $X : V \to W$ is pseudo-stochastic if $X\mathbf{1}_I = \mathbf{1}_J$ and $X^*\mathbf{1}_J = \mathbf{1}_I$ for $X^*$ the adjoint of $X$.

The Gram–Schmidt orthogonalisation procedure is a well-known method in linear algebra [33, Theorem 2.1]. For the purpose of this article, a variant of it is required to construct unitary linear transformations between vector spaces spanned by possibly infinite sequences of vectors.

Lemma 2.1 (Gram–Schmidt Orthogonalisation). Let $I$ be a possibly infinite index set. Let $(v_i)_{i \in I}$, $(w_i)_{i \in I}$ be two sequences of vectors in a finite-dimensional $\mathbb{K}$-vector space. Write $V$, respectively $W$, for the space spanned by the $v_i$, respectively the $w_i$. Suppose that $\langle v_i, v_j \rangle = \langle w_i, w_j \rangle$ for all $i, j \in I$. Then there exists a unitary linear transformation $\Phi : V \to W$ such that $\Phi(v_i) = w_i$ for all $i \in I$.
Proof. The map \( U \) will be constructed by linearly extending \( v_i \mapsto w_i \). It has to be shown that this can be done in a well-defined manner.

Claim 1. For every finite \( I' \subseteq I \), the \( \{ v_i \mid i \in I' \} \) form a basis of \( V \) if and only if the \( \{ w_i \mid i \in I' \} \) form a basis of \( W \).

Proof of Claim. Suppose that \( \{ v_i \mid i \in I' \} \) forms a set of linearly independent vectors. For the sake of contradiction, suppose that there exist scalars \( a_i \in \mathbb{K} \) such that \( \sum_{i \in I'} a_i v_i = 0 \). Let \( k \in I \) be arbitrary. Then \( 0 = \sum_{i \in I'} a_i \langle w_k, w_i \rangle = \sum_{i \in I'} a_i \langle v_k, v_i \rangle \). This implies that \( \sum_{i \in I'} a_i v_i = 0 \) and thus \( a_i = 0 \) for all \( i \in I' \). In other words, the \( w_i, i \in I' \), are linearly independent.

Suppose that \( \{ v_i \mid i \in I' \} \) spans \( U \). Let \( k, j \in I \) be arbitrary. Then there exist scalars \( \beta_i \in \mathbb{K} \) such that \( v_k = \sum_{i \in I'} \beta_i v_i \). Furthermore, \( \langle w_j, w_k \rangle = \langle v_j, v_k \rangle = \sum_{i \in I'} \beta_i \langle v_j, v_i \rangle = \sum_{i \in I'} \beta_i \langle w_j, w_i \rangle \). Hence, \( w_k = \sum_{i \in I'} \beta_i w_i \). So the \( w_i, i \in I' \), span \( W \). The converse direction follows analogously.

Now choose \( I' \subseteq I \) such that \( \{ v_i \mid i \in I' \} \) forms a basis of \( V \). Define \( U : V \rightarrow W \) by letting \( Uv_i := w_i \) for \( i \in I' \). It remains to verify that \( U \) is unitary and maps \( v_i \) to \( w_j \) for all \( j \in I \). Let \( k, j \in I \) be arbitrary. Let \( v_k = \sum_{i \in I'} \gamma_i v_i \) for some \( \gamma_i \in \mathbb{K} \). Then

\[
\langle w_j, Uv_k \rangle = \sum_{i \in I'} \gamma_i \langle w_j, v_i \rangle = \sum_{i \in I'} \gamma_i \langle v_j, v_i \rangle = \langle v_j, v_k \rangle = \langle w_j, w_k \rangle.
\]

Hence, \( Uv_k = w_k \) for all \( k \in I \). This implies that \( U \) is unitary. Indeed, \( v_k^* U^* U v_j = v_k^* w_j = v_k^* v_j = v_k^* \text{id}_V v_j \) for all \( k, j \in I \). So \( U^* U = \text{id}_V \). That \( UU^* = \text{id}_W \) follows analogously. \( \square \)

A recurring theme in this article is the study of \( \mathbb{K} \)-vector spaces over a finite set \( I \). On such a space, the Schur product of two vectors \( v, w \in \mathbb{K}^I \) is defined via \( (v \odot w)(x) := v(x)w(x) \) for all \( x \in I \). Write furthermore \( v^{\otimes i}, i \in \mathbb{N}, \) for the \( i \)-fold Schur product of the vector \( v \in \mathbb{K}^I \) with itself. Conventionally, \( v^{\otimes 0} := 1_I \) where \( 1_I \) denotes the all-ones vector on \( I \). The following fact is classical:

**Fact 2.2** (Vandermonde Determinant [33, p. 155]). Let \( I \) be a finite set of size \( n \). If \( v \in \mathbb{K}^I \) has distinct entries then \( 1, v, v^{\otimes 2}, \ldots, v^{\otimes (v-1)} \) is a basis of \( \mathbb{K}^I \).

Fact 2.2 will be applied in the following form:

**Lemma 2.3** (Vandermonde Interpolation). Fix a finite set \( I \). Let \( V \subseteq \mathbb{K}^I \) be a vector space closed under Schur product that contains \( 1 \). Define an equivalence relation \( \sim \) on \( I \) by \( x \sim x' \) iff \( v(x) = v(x') \) for all \( v \in V \). Then the indicator vectors \( 1_{C_1}, \ldots, 1_{C_r} \) of the equivalence classes form a basis of \( V \).

Proof. Write \( W \) for the space spanned by the \( 1_{C_1}, \ldots, 1_{C_r} \). Clearly, \( V \subseteq W \). Conversely, fix an equivalence class indicator vector \( 1_C \). Then there exists \( v \in V \) such that \( v(i) \neq v(j) \) for some \( i \in C \) and \( j \in I \setminus C \). Furthermore, \( v \) is constant on \( C \). Let \( \ell \) denote the number of different values that \( v \) exhibits. Reduce \( v \) to a length-\( \ell \) vector \( v' \) keeping only one entry for every occurring value. The space spanned by \( 1, v', v'^{\otimes 2}, \ldots, v'^{\otimes (\ell-1)} \) is \( \ell \)-dimensional by Fact 2.2. Hence, every length-\( \ell \) vector is a linear combination of iterated Schur products of \( v' \). Lifting the reduced vectors by replicating entries, shows that \( 1_C \) is in the space spanned by iterated Schur products of \( v \). Hence \( W \subseteq V \). \( \square \)
For the sake of completeness, we give a proof of the following lemma on doubly-stochastic matrices. Recall that a matrix $X \in \mathbb{R}^{I \times I}$ is doubly-stochastic if it is pseudo-stochastic and its entries are non-negative.

**Lemma 2.4** ([54, Lemma 1]). Let $I$ and $J$ be finite sets. Let $v \in \mathbb{R}^I$ and $w \in \mathbb{R}^I$. If $X \in \mathbb{R}^{I \times I}$ is doubly-stochastic such that $Xv = w$ and $X^Tw = v$ then $v(i) = w(j)$ for all $i \in I$ and $j \in J$ such that $X(j,i) > 0$.

**Proof.** In virtue of a classical theorem of Hardy, Littlewood, and Polya [41, Theorem 1a], $Xv = w$ and $X^Tw = v$ imply that $v$ and $w$ have the same multisets of entries.

Let $A \subseteq I$, respectively $B \subseteq J$, denote the set of tuples on which $v$, respectively $w$, assumes its least value $r$. It is claimed that if $i \in I \setminus A$ and $j \in B$ or if $i \in A$ and $j \in J \setminus B$ then $X(j,i) = 0$. By induction on the number of different values in $v$ and $w$, this yields the claim. First observed that for $j \in B$,

$$r = w(j) = (Xv)(j) = r \sum_{i \in A} X(j,i) + \sum_{i \in I \setminus A} X(j,i)v(i) \geq r \sum_{i \in I} X(j,i) = r(X1)(j) = r.$$

Hence, equality holds throughout. This implies that $\sum_{i \in I \setminus A} X(j,i) = 0$ as $v(i) > r$ for all $i \in I \setminus A$. It follows that $X(j,i) = 0$ for $j \in B$ and $i \in I \setminus A$. The same holds when $i \in A$ and $j \in J \setminus B$. \hfill \Box

### 2.2 Representation Theory of Involution Monoids

A **monoid** $\Gamma$ is a possibly infinite set equipped with an associative binary operation and an identity element denoted by $1_\Gamma$. An example for a monoid is the **endomorphism monoid** $\text{End} \ V$ for a vector space $V$ over $\mathbb{K}$ with composition as binary operation and $\text{id}_V$ as identity element. A **monoid representation** of $\Gamma$ is a map $\varphi: \Gamma \rightarrow \text{End} \ V$ such that $\varphi(1_\Gamma) = \text{id}_V$ and $\varphi(gh) = \varphi(g)\varphi(h)$ for all $g, h \in \Gamma$. The representation is **finite-dimensional** if $V$ is finite-dimensional. For every monoid $\Gamma$, there exists a representation, for example the **trivial representation** $\Gamma \rightarrow \text{End}\{0\}$ given by $g \mapsto \text{id}_{\{0\}}$.

Let $\varphi: \Gamma \rightarrow \text{End}(V)$ and $\psi: \Gamma \rightarrow \text{End}(W)$ be two representations over $\mathbb{K}$. Then $\varphi$ and $\psi$ are **equivalent** if there exists a $\mathbb{K}$-vector space isomorphism $X: V \rightarrow W$ such that $X\varphi(g) = \psi(g)X$ for all $g \in \Gamma$. Moreover, $\varphi$ is a **subrepresentation** of $\psi$ if $V \leq W$ and $\psi(g)$ restricted to $V$ equals $\varphi(g)$ for all $g \in \Gamma$. A representation $\varphi$ is **simple** if its only subrepresentations are the trivial representation and $\varphi$ itself. The **direct sum** of $\varphi$ and $\psi$ denoted by $\varphi \oplus \psi: \Gamma \rightarrow \text{End}(V \oplus W)$ is the representation that maps $g \in \Gamma$ to $\varphi(g) \oplus \psi(g) \in \text{End}(V) \oplus \text{End}(W) \leq \text{End}(V \oplus W)$. A representation $\varphi$ is **semisimple** if it is the direct sum of simple representations.

Let $\varphi: \Gamma \rightarrow \text{End} \ V$ be a representation with subrepresentations $\psi': \Gamma \rightarrow \text{End} \ V'$ and $\psi'': \Gamma \rightarrow \text{End} \ V''$. Then the restriction of $\varphi$ to $V' \cap V''$ is a representation as well, called the **intersection** of $\psi'$ and $\psi''$. For a set $S \subseteq V$, define the **subrepresentation** of $\varphi$ generated by $S$ as the intersection of all subrepresentations $\psi': \Gamma \rightarrow \text{End} \ V'$ of $\varphi$ such that $S \subseteq V'$.

The **character** of a representation $\varphi$ is the map $\chi_\varphi: \Gamma \rightarrow \mathbb{K}$ defined as $g \mapsto \text{tr}(\varphi(g))$. Its significance stems from the following theorem, which can be traced back to Frobenius and Schur [19]. For a contemporary proof, consult [32, Theorem 7.19].
Theorem 2.5 (Frobenius–Schur [19]). Let \( \Gamma \) be a monoid. Let \( \varphi : \Gamma \to \text{End}(V) \) and \( \psi : \Gamma \to \text{End}(W) \) be finite-dimensional semisimple representations over \( K \). Then \( \varphi \) and \( \psi \) are equivalent if and only if \( \chi_\varphi = \chi_\psi \).

The monoids studied in this work are equipped with an additional structure which ensures that their finite-dimensional representations are always semisimple: An involution monoid is a monoid \( \Gamma \) with a unary operation \( ^* : \Gamma \to \Gamma \) such that

\[
(gh)^* = h^*g^* \quad \text{and} \quad (g^*)^* = g \quad \text{for all } g, h \in \Gamma.
\]

(1)

Note that \( \text{End} \ V \) is an involution monoid with the adjoint operation \( X \mapsto X^* \). Representations of involution monoids must preserve the involution operations. Thereby, they correspond to representations of \(*\)-algebras.

Lemma 2.6. Every finite-dimensional representation of an involution monoid \( \Gamma \) over \( K \) is semisimple.

Proof. Let \( \varphi : \Gamma \to \text{End} \ V \) be a finite-dimensional representation of \( \Gamma \). It suffices to show that for every subrepresentation \( \psi : \Gamma \to \text{End} \ W \) of \( \varphi \) there exists a subrepresentation \( \psi' : \Gamma \to \text{End} \ W' \) of \( \varphi \) such that \( \varphi = \psi \oplus \psi' \), i.e. \( \varphi \) acts as \( \psi \) on \( W \) and as \( \psi' \) on \( W' \). Set \( W' \) to be the orthogonal complement of \( W \) in \( V \). It has to be shown that \( \varphi(g) \in \text{End} \ V \) for every \( g \in \Gamma \) can be restricted to an endomorphism of \( W' \). Let \( w \in W \) and \( w' \in W' \) be arbitrary. Then \( \langle \varphi(g)w', w \rangle = \langle w', \varphi(g)^*w \rangle = \langle w', \varphi(g^*)w \rangle = 0 \) since \( \varphi(g^*) \) maps \( W \to W \) and \( W \perp W' \). Hence, the image of \( W' \) under \( \varphi(g) \) is contained in the orthogonal complement of \( W \), which equals \( W' \). Clearly, \( \varphi = \psi \oplus \psi' \). \( \square \)

2.3 Tensors, Tensor Maps, and Algebraic Operations

Fix \( K \in \{ Q, \mathbb{R}, C \} \). For a set \( V \) and \( k, \ell \in \mathbb{N} \), the set of all functions \( X : V^k \times V^\ell \to K \) forms a \( K \)-vector space denoted by \( K^{V^k \times V^\ell} \). We call the elements of \( K^{V^k \times V^\ell} \) the \(( k, \ell )\)-dimensional tensors over \( V \). We abbreviate \(( k, 0 )\)-dimensional and \(( 0, k )\)-dimensional by \( k \)-dimensional.

We identify 0-dimensional tensors with scalars, i.e. \( K^{V^0} = K \). Furthermore, 1-dimensional tensors are vectors in \( K^V \), \(( 1, 1 )\)-dimensional tensors are matrices in \( K^{V \times V} \), et cetera.

A \(( k, \ell )\)-dimensional tensor map on graphs is a function \( \varphi \) that maps graphs \( G \) to \(( k, \ell )\)-dimensional tensors \( \varphi_G \in C^{V(G)^k \times V(G)^\ell} \). A \(( k, \ell )\)-dimensional tensor map \( \varphi \) is equivariant if for all isomorphic graphs \( G \) and \( H \), all isomorphisms \( f \) from \( G \) to \( H \), and all \( v \in V(G)^k \) and \( u \in V(G)^\ell \) it holds that \( \varphi_G(v, u) = \varphi_H(f(v), f(u)) \) where \( f \) acts entry-wise on tuples. We write \( \mathfrak{g}(k, \ell) \) for the set of all \(( k, \ell )\)-dimensional equivariant tensor maps on graphs. We consider the following operations on equivariant tensor maps. In each case, it is straightforward to check that the resulting maps are equivariant.

The set \( \mathfrak{g}(k, \ell) \) forms a \( K \)-vector space under point-wise operations, i.e. for \( \varphi, \psi \in \mathfrak{g}(k, \ell) \) and \( a, b \in K \), \( (a\varphi + b\psi)_G(u, v) := a\varphi_G(u, v) + b\psi_G(u, v) \) for every graph \( G \) and \( v \in V(G)^k \) and \( u \in V(G)^\ell \).

The sum-of-entries of \( \varphi \in \mathfrak{g}(k, \ell) \) is the \(( 0, 0 )\)-dimensional tensor map \( \text{soe} \varphi \) defined via \( (\text{soe} \varphi)_G := \sum_{u \in V(G)^k, v \in V(G)^\ell} \varphi_G(u, v) \) for every graph \( G \). The trace of \( \varphi \in \mathfrak{g}(k, k) \) is the \(( 0, 0 )\)-dimensional tensor map \( \text{tr} \varphi \) defined via \( (\text{tr} \varphi)_G := \sum_{u \in V(G)^k} \varphi_G(u, u) \) for every graph \( G \).

The tensor product \( \varphi \otimes \psi \in \mathfrak{g}(k_1 + k_2, \ell_1 + \ell_2) \) for two tensor maps \( \varphi \in \mathfrak{g}(k_1, \ell_1), \psi \in \mathfrak{g}(k_2, \ell_2) \) where \( k_1, k_2, \ell_1, \ell_2 \in \mathbb{N} \) is defined by the equation \( (\varphi \otimes \psi)_G(uu', vv') := \varphi_G(u, v)\psi_G(u', v') \) for every graph \( G \) and \( u \in V(G)^{k_1}, u' \in V(G)^{k_2}, v \in V(G)^{\ell_1}, v' \in V(G)^{\ell_2} \).
We henceforth tacitly assume that all graphs are simple.

2.5 Homomorphism Tensors and Homomorphism Tensor Maps
denote the number of homomorphisms $h$ of homomorphisms $F$ the disjoint union of $F$ and $G$ and $v \in V(G)^k$. Analogously, the matrix product of $\varphi \in \mathcal{F}(k, \ell)$ and $\psi \in \mathcal{F}(\ell, m)$ for $m \in \mathbb{N}$ denoted by $\varphi \cdot \psi \in \mathcal{F}(k, m^\dagger)$ is defined as $(\varphi \cdot \psi)(v, u) := \sum_{w \in V(G)^k} \varphi(v, w)\psi(w, u)$ for every graph $G$ and $v \in V(G)^k$ and $u \in V(G)^m$.

The Schur product of $\varphi, \psi \in \mathcal{F}(k)$ is defined as $(\varphi \odot \psi)(v) := \varphi(v)\psi(v)$ for every graph $G$ and $v \in V(G)^k$. The inner-product of $\varphi, \psi \in \mathcal{F}(k)$ is defined as $(\varphi, \psi)_G = (\varphi_G, \psi_G)$ for every graph $G$.

2.4 Bilabelled Graphs and Combinatorial Operations
For $\ell \in \mathbb{N}$, an $\ell$-labelled graph $F$ is a tuple $F = (F, v)$ where $F$ is a graph and $v \in V(F)^\ell$. The vertices in $v$ are not necessarily distinct, i.e. vertices may have several labels. Write $G(\ell)$ for the class of all $\ell$-labelled graphs.

The operation of gluing two $\ell$-labelled graphs $F = (F, u)$ and $F' = (F', u')$ yields the $\ell$-labelled graph $F \circ F'$ obtained by taking the disjoint union of $F$ and $F'$ and pairwise identifying the vertices $u_i$ and $v_i$ to become the $i$-th labelled vertex, for $i \in [\ell]$, and removing any multiedges in the process. In fact, since we consider homomorphisms into simple graphs, multiedges can always be omitted. Likewise, self-loops can also be disregarded since the number of homomorphisms $F \to G$ where $F$ has a self-loop and $G$ does not is always zero. We henceforth tacitly assume that all graphs are simple.

For $\ell_1, \ell_2 \in \mathbb{N}$, an $(\ell_1, \ell_2)$-bilabelled graph $F$ is a tuple $(F, u, v)$ for $u \in V(F)^{\ell_1}$, $v \in V(F)^{\ell_2}$. If $u = (u_1, \ldots, u_{\ell_1})$ and $v = (v_1, \ldots, v_{\ell_2})$, it is usual to say that the vertex $u_i$, resp. $v_i$, is labelled with the $i$-th in-label, resp. out-label. Write $G(\ell_1, \ell_2)$ for the class of all $(\ell_1, \ell_2)$-bilabelled graphs.

The reverse of an $(\ell_1, \ell_2)$-bilabelled graph $F = (F, u, v)$ is defined to be the $(\ell_2, \ell_1)$-bilabelled graph $F^* = (F, v, u)$ with roles of in- and out-labels interchanged. The concatenation or series composition of an $(\ell_1, \ell_2)$-bilabelled graph $F = (F, u, v)$ and an $(\ell_2, \ell_3)$-bilabelled graph $F' = (F', u', v')$, $\ell_3 \in \mathbb{N}$, denoted by $F \cdot F'$ is the $(\ell_1, \ell_3)$-bilabelled graph obtained by taking the disjoint union of $F$ and $F'$ and identifying for all $i \in [\ell_2]$ the vertices $v_i$ and $u'_i$. The in-labels of $F \cdot F'$ lie on $u$ while its out-labels are positioned on $v'$. The parallel composition of $(\ell_1, \ell_2)$-bilabelled graphs $F = (F, u, v)$ and $F' = (F', v', u')$ denoted by $F \odot F'$ is obtained by taking the disjoint union of $F$ and $F'$ and identifying $u_i$ with $u'_i$, and $v_j$ with with $v'_j$ for $i \in [\ell_1]$ and $j \in [\ell_2]$.

2.5 Homomorphism Tensors and Homomorphism Tensor Maps
For graphs $F$ and $G$, let $\text{hom}(F, G)$ denote the number of homomorphisms from $F$ to $G$, i.e. the number of mappings $h: V(F) \to V(G)$ such that $v_1v_2 \in E(F)$ implies $h(v_1)h(v_2) \in E(G)$. For a graph class $\mathcal{F}$ and graphs $G$ and $H$, write $G \equiv_{\mathcal{F}} H$ if $G$ and $H$ are homomorphism indistinguishable over $\mathcal{F}$, i.e. $\text{hom}(F, G) = \text{hom}(F, H)$ for all $F \in \mathcal{F}$.

For an $\ell$-labelled graph $F = (F, v)$ and $w \in V(G)^\ell$, let $\text{hom}(F, G, w)$ denote the number of homomorphisms $h$ from $F$ to $G$ such that $h(v_i) = w_i$ for all $i \in [\ell]$. Analogously, for an $(\ell_1, \ell_2)$-bilabelled graph $F' = (F', u, v)$ and $x \in V(G)^{\ell_1}$, $y \in V(G)^{\ell_2}$, let $\text{hom}(F', G, x, y)$ denote the number of homomorphisms $h: F' \to G$ such that $h(u_i) = x_i$ and $h(v_i) = y_j$ for all $i \in [\ell_1], j \in [\ell_2]$. More succinctly, we write $F_G \in \mathbb{N}^{V(G)^\ell}$ for the homomorphism tensor defined
As outlined in Section 2.6 Algebraic and Combinatorial Operations on Homomorphism Tensor Maps

As outlined in Section 2.3, tensor maps naturally admit a plenitude of algebraic operations. Crucially, many operations when applied to homomorphism tensor maps correspond to operations on (bi)labelled graphs. This observation due to [37, 39] is illustrated by the following examples.

**Sum-of-Entries and dropping labels** Given a $k$-labelled graph $F = (F,u)$, let $\text{soe}(F)$ denote the 0-labelled graph $(F,())$. Then, for every graph $G$, $\text{soe}(F)_G = \text{hom}(F,G) = \sum_{v \in V(G)} F_G(v) =: \text{soe}(F_G)$. For an example, see Figure 2c.

**Matrix Product and series composition** Let an $(\ell_1, \ell_2)$-bilabelled graph $F = (F, u, v)$ and an $(\ell_2, \ell_3)$-bilabelled graph $F' = (F', u', v')$ be given. Then for every graph $G$, vertices $x \in V(G)^{\ell_1}$ and $y \in V(G)^{\ell_2}$, $(F \cdot F'_G)(x,y) = \sum_{w \in V(G)^{\ell_2}} F_G(x,w)F'_G(w,y) =: (F_G \cdot F'_G)(x,y)$. A similar operation corresponds to the matrix-vector product, where $F'$ is assumed to be $\ell_2$-labelled. For an example, see Figure 2a.

**Schur Product and gluing** The gluing product $F \odot F'$ of two $k$-labelled graphs $F = (F, u)$ and $F' = (F', u')$ corresponds to the Schur product of the homomorphism tensors. That is, for
every graph $G$ and $v \in V(G)^k$, $(F \odot F)_G(v) = F_G(v)F'_G(v) =: (F_G \odot F'_G)(v)$. Moreover, the inner-product of $\ell$-labelled graphs $F, F'$ can be defined by $\langle F, F' \rangle := \text{soe}(F \odot F')$. It corresponds to the standard inner-product on the tensor space.

**Tensor product and disjoint union** For a $k$-labelled graph $F = (F, (u_1, \ldots, u_k))$ and an $\ell$-rooted graph $F' = (F', (v_1, \ldots, v_\ell))$, the tensor map $F \otimes F'$ is the homomorphism tensor map corresponding to the $k$-labelled graph $(F \otimes F', (u_1, \ldots, u_k, v_1, \ldots, v_\ell))$, where $F \otimes F'$ is the disjoint union of $F$ and $F'$.

**Traces and identifying and dropping labels** Given a $(k,k)$-bilabelled graph $F = (F, u, v)$, let $\text{tr}(F)$ denote the 0-labelled graph obtained from $F$ by identifying $u_i$ with $v_i$ for $i \in [k]$ and dropping the labels. Then, for every graph $G$, $\text{tr}(F)_G = \text{hom}(\text{tr} F, G) = \sum_{v \in V(G)^k} F_G(v, v)$. For an example, see Figure 2b.

### 2.7 Linear Programming Relaxations for Graph Isomorphism

Let $G$ and $H$ be graphs. The standard LP relaxation for the graph isomorphism problem [54], denoted by $F_{\text{iso}}(G, H)$, is defined as follows. Its variables are $X_{vw}$ for every $v \in V(G)$ and $w \in V(H)$.

\[
F_{\text{iso}}(G, H) = \begin{array}{ll}
\sum_{v \in V(G)} X_{vw} = 1 & \text{for all } w \in V(H), \\
\sum_{w \in V(H)} X_{vw} = 1 & \text{for all } v \in V(G), \\
\sum_{v' \in V(G)} X_{v'w} A_G(v', v) - \sum_{w' \in V(H)} A_H(w, w') X_{w'w} = 0 & \text{for all } v \in V(G) \text{ and } w \in V(H).
\end{array}
\]

The last equation can be concisely stated as a matrix equation $X A_G = A_H X$, where $A_G$ and $A_H$ are the adjacency matrices of $G$ and $H$ respectively.

The existence of a solution of $F_{\text{iso}}(G, H)$ over $\{0,1\}$ is equivalent to $G$ and $H$ being isomorphic. The existence of a non-negative rational solution in turn is equivalent to 1-WL indistinguishability [54].

The system of equations $F^k_{\text{iso}}(G, H)$ is described next. Instead of variables $X_{vw}$ for vertices $v \in V(G)$, $w \in V(H)$, as in the system $F_{\text{iso}}(G, H)$, the new system has variables $X_\pi$ for $\pi \subseteq V(H) \times V(G)$ of size $|\pi| \leq k$. We call $\pi = \{(w_1, v_1), \ldots, (w_\ell, v_\ell)\} \subseteq V(H) \times V(G)$ a partial bijection if $v_i = v_j \iff w_i = w_j$ for all $i,j$, and we call it a partial isomorphism if in addition $v_i,v_j \in E(G) \iff w_iw_j \in E(H)$. Now consider the following system of linear equations.
The graph $F$

We recall the well-known notion of a tree decomposition in the following slightly more formal form.

**Definition 2.8.** Let $F$ be a graph. An $F$-decomposition of a graph $G$ is a pair $(F, \beta)$ and $\beta$ is a map $V(F) \rightarrow 2^{V(G)}$ such that
1. the union of the $\beta(v)$ for $v \in V(F)$ is equal to $V(G)$,
2. for every edge $e \in E(G)$ there exists $v \in V(F)$ such that $e \subseteq \beta(v)$,
3. for every vertex $u \in V(G)$ the set of vertices $v \in V(F)$ such that $u \in \beta(v)$ is connected in $F$.

The sets $\beta(v)$ for $v \in V(F)$ are called the bags of $(F, \beta)$. The width of $(F, \beta)$ is the maximum over all $|\beta(v)| - 1$ for $v \in V(F)$. An $F$-decomposition is called a tree decomposition if $F$ is a tree, a path decomposition if $F$ is a path, and a cycle decomposition if $F$ is a cycle. The tree-/path-/ cyclewidth of a graph $G$ is the minimum width of a tree/path/cycle decomposition of $G$. The following Lemma 2.9 generalises [6, Lemma 8].

**Lemma 2.9.** Let $k \geq 1$ and $F$ be a connected graph. If a graph $G$ has an $F$-decomposition of width at most $k$ and $|V(G)| \geq k + 1$ then there is an $F'$-decomposition $\beta : F' \rightarrow 2^{V(G)}$ of $G$ such that
1. $|\beta(t)| = k + 1$ for all $t \in V(F')$, and
2. $|\beta(s) \cap \beta(t)| = k$ for all $st \in E(F')$.

The graph $F'$ can be obtained from $F$ by contracting and/or subdividing edges.

**Proof.** If $|V(G)| = k + 1$ then $F'$ can be taken to be the single vertex graph. If $|V(G)| > k + 1$ then $F$ must contain at least one edge. Let $\beta : F \rightarrow 2^{V(G)}$ be the $F$-decomposition of width at most $k$. We repeatedly apply the following steps:

---

$^{1}$For convenience, we regard the cliques $K_1$ and $K_2$ as cycles.
We first recall the classical Specht–Wiegmann Theorem, which applies to the fields $\mathbb{R}$ and $\mathbb{C}$. Let $A = (A_i)_{i \in M}$ be a sequence of matrices in $\mathbb{K}^{I \times I}$ for some finite index set $I$. For a word $w \in \Gamma_M$, let $w_A$ denote the matrix obtained by substituting $x_i \mapsto A_i$ and $y_i \mapsto A_i^*$ for all $i \in M$ and evaluating the matrix product. Furthermore, $e_A$ is set to be the identity matrix in $\mathbb{K}^{I \times I}$. Crucially, the words in $\Gamma_M$ are finite despite that the underlying alphabet is infinite. Hence, this map is well-defined. The substitution $w \mapsto w_A$ is an involution monoid representation of $\Gamma_M$.

3.1 Unitary and Orthogonal Similarity

We first recall the classical Specht–Wiegmann Theorem, which applies to the fields $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$. See also [28, 20] for a more recent account.
Theorem 3.1 (Specht [52], Wiegmann [56]). Let \( I \) and \( J \) be finite index sets. Let \( M \) be any set. Let \( A = (A_i)_{i \in M} \) and \( B = (B_i)_{i \in M} \) be two sequences of matrices such that \( A_i \in \mathbb{F}^{1 \times 1} \) and \( B_i \in \mathbb{F}^{1 \times 1} \) for all \( i \in M \). Then the following are equivalent:

1. there exists a unitary \( U \in \mathbb{F}^{1 \times 1} \) such that \( UA_i = B_i U \) and \( UA_i^* = B_i^* U \) for every \( i \in M \),
2. for every word \( w \in \Gamma_M \), \( \text{tr}(w_A) = \text{tr}(w_B) \).

Proof. As observed above, the maps \( w \mapsto w_A \) and \( w \mapsto w_B \) yield two representations of the involution monoid \( \Gamma_M \). By Lemma 2.6, these representations are semisimple. If \( \text{tr}(w_A) = \text{tr}(w_B) \) for every word \( w \in \Gamma_M \), these two representations have the same character, and hence, by Theorem 2.5, they are equivalent. Therefore, there exists an invertible matrix \( X \) such that \( X^{-1} w_B X = w_A \) for every word \( w \in \Gamma_M \).

The desired unitary matrix \( U \) can then be recovered from the polar decomposition of \( X = HU \), where \( H \) is positive definite, cf. [33, p. 292] and [28, Corollary 2.3]. Since \( XX^* \) commutes with \( B_i \) for every \( i \in M \), so does \( H \) and hence, \( X^{-1} B_i X = U^* (H^{-1} B_i H) U = U^* B_i U = A_i \) for every \( i \in M \).

In fact, it suffices to compare traces from finitely many words in \( \Gamma_M \) to establish the assertions of Theorem 3.1. The following result is due to [47]. Tighter bounds are known [46], a linear bound is conjectured. We include the following proof for completeness.

Theorem 3.2 ([47, Theorem 1]). Writing \( n := |I| = |J| \), the conditions of Theorem 3.1 are equivalent to the following: For every word \( w \in \Gamma_M \) of length at most \( 2n^2 - 1 \), \( \text{tr}(w_A) = \text{tr}(w_B) \).

Proof. To ease notation, we suppose wlog that \( I \) and \( J \) are disjoint. For a word \( w \in \Gamma_M \), define the block matrix \( w_{A \oplus B} := \begin{pmatrix} w_A & 0 \\ 0 & w_B \end{pmatrix} \in \mathbb{F}^{(|I|) \times (|J|)} \). Observe that \( w \mapsto w_{A \oplus B} \) is an involution monoid representation. In particular, \((xy)_{A \oplus B} = x_{A \oplus B} y_{A \oplus B} \) and \((x^*)_{A \oplus B} = (x_{A \oplus B})^* \) for all \( x, y \in \Gamma_M \).

Let \( S_{A \oplus B}^{\leq \ell} \leq \mathbb{F}^{(|I|) \times (|J|)} \) denote the vector space spanned by the \( w_{A \oplus B} \) for \( w \in \Gamma_M \). Clearly, \( S_{A \oplus B} \) has dimension at most \( 2n^2 \). Furthermore, for \( \ell \geq 0 \), write \( S_{A \oplus B}^{\leq \ell} \subseteq S_{A \oplus B} \) for the vector space spanned by the \( w_{A \oplus B} \) for words \( w \in \Gamma_M \) of length at most \( \ell \). The space \( S_{A \oplus B}^{\leq 0} \) containing the identity matrix, has dimension 1.

Claim 2. If \( S_{A \oplus B}^{\leq \ell} = S_{A \oplus B}^{\leq \ell+1} \) for some \( \ell \in \mathbb{N} \) then \( S_{A \oplus B} = S_{A \oplus B}^{\leq \ell} \). In particular, \( S_{A \oplus B}^{2n^2-1} = S_{A \oplus B} \).

Proof of Claim. By induction on \( j \geq 1 \), it is shown that \( S_{A \oplus B}^{\leq \ell+j} \subset S_{A \oplus B}^{\leq \ell} \). The base case \( j = 1 \) holds by assumption. Let \( x \in \Gamma_M \) be a word of length \( \ell + i + 1 \). Let \( y \) denote the first character of \( x \) and write \( z \) for the length-(\( \ell + j \)) suffix of \( x \), i.e. \( x = yz \). By assumption, there exist words \( z^1, \ldots, z^r \) of length at most \( \ell \) and coefficients \( \alpha_1, \ldots, \alpha_r \in \mathbb{F} \) such that \( z_{A \oplus B} = \sum_{i=1}^{r} \alpha_i z^i_{A \oplus B} \). Hence, \( x_{A \oplus B} = y_{A \oplus B} z_{A \oplus B} = \sum_{i=1}^{r} \alpha_i y_{A \oplus B} z^i_{A \oplus B} = \sum_{i=1}^{r} \alpha_i (y z^i)_{A \oplus B} \in S_{A \oplus B}^{\leq \ell+1} \). Thus, \( S_{A \oplus B}^{\leq \ell+j} \subseteq S_{A \oplus B}^{\leq \ell+1} \subseteq S_{A \oplus B}^{\leq \ell} \), as desired.

Equipped with Claim 2, we prove the main claim. For a matrix \( C \in \mathbb{F}^{(|I|) \times (|J|)} \), write \( \text{tr}_A C := \sum_{i \in I} C(i,i) \) and analogously \( \text{tr}_B C := \sum_{j \in J} C(j,j) \). Let \( w \in \Gamma_M \) be arbitrary. By Claim 2, there exist \( w^1, \ldots, w^r \in \Gamma_M \) of length at most \( 2n^2 - 1 \) and coefficients \( \alpha_1, \ldots, \alpha_r \in \mathbb{F} \) such that \( w_{A \oplus B} = \sum_{i=1}^{r} \alpha_i w^i_{A \oplus B} \). Hence,

\[
\text{tr}(w_A) = \text{tr}_A (w_{A \oplus B}) = \sum \alpha_i \text{tr}_A (w^i_{A \oplus B}) = \sum \alpha_i \text{tr}(w^i_A) = \sum \alpha_i \text{tr}(w^i_B) = \text{tr}_B (w_{A \oplus B}) = \text{tr}(w_B).
\]

Thus, the assertion in Theorem 3.2 implies Item 2 of Theorem 3.3. \( \square \)
3.2 Pseudo-Stochastic Similarity

Our first variant of Theorem 3.1 establishes a criterion for simultaneous similarity w.r.t. a pseudo-stochastic matrix. In this case, instead of traces, sums-of-entries have to be considered. Theorem 3.3 applies to any base field $\mathbb{K} \in \{\mathbb{Q}, \mathbb{R}, \mathbb{C}\}$.

**Theorem 3.3.** Let $I$ and $J$ be finite index sets. Let $M$ be any set. Let $A = (A_i)_{i \in M}$ and $B = (B_i)_{i \in M}$ be two sequences of matrices such that $A_i \in \mathbb{K}^{I \times I}$ and $B_i \in \mathbb{K}^{I \times I}$ for $i \in M$. Then the following are equivalent:

1. there exists a pseudo-stochastic matrix $X \in \mathbb{K}^{I \times I}$ such that $XA_i = B_i X$ and $X A_i^* = B_i^* X$ for all $i \in M$.
2. for every word $w \in \Gamma_M$, $\text{soe}(w_A) = \text{soe}(w_B)$.

Theorem 3.3 is implied by Lemma 3.4, which provides a sum-of-entries analogue of Theorem 2.5. As it establishes a character-theoretic interpretation of the function $\text{soe}$, it may be of independent interest.

**Lemma 3.4.** Let $\Gamma$ be an involution monoid. Let $I$ and $J$ be finite index sets. Let $\varphi: \Gamma \to \mathbb{K}^{I \times I}$ and $\psi: \Gamma \to \mathbb{K}^{J \times J}$ be representations of $\Gamma$. Let $\varphi': \Gamma \to V$ and $\psi': \Gamma \to W$ denote the subrepresentations of $\varphi$ and of $\psi$ generated by $1_I$ and $1_J$, respectively. Then the following are equivalent:

1. for all $g \in \Gamma$, $\text{soe}(g \varphi) = \text{soe}(g \psi)$,
2. there exists a unitary pseudo-stochastic $U: V \to W$ such that $U \varphi'(g) = \psi'(g) U$ for all $g \in \Gamma$,
3. there exists a pseudo-stochastic $X \in \mathbb{K}^{I \times I}$ such that $X \varphi(g) = \psi(g) X$ for all $g \in \Gamma$.

**Proof.** Suppose that Item 1 holds. The space $V$ is spanned by the vectors $\varphi(g) 1_I$ for $g \in \Gamma$ while $W$ is spanned by the $\psi(g) 1_J$ for $g \in \Gamma$. For $g, h \in \Gamma$, it holds that

$$\langle \varphi(g) 1_I, \varphi(h) 1_I \rangle = \langle 1_I, \varphi(g^* h) 1_I \rangle = \text{soe}(g^* h) = \text{soe}(g^* h) = \langle \psi(g) 1_J, \psi(h) 1_J \rangle.$$ 

Hence, $V$ and $W$ are spanned by vectors whose pairwise inner-products are respectively the same. Thus, by Lemma 2.1, there exists a unitary $U: V \to W$ such that $U \varphi(g) 1_I = \psi(g) 1_J$ for all $g \in \Gamma$. This immediately implies that $U \varphi'(g) = \psi'(g) U$ for all $g \in \Gamma$. Furthermore, $U 1_I = U \varphi(1_I) 1_I = \varphi(1_I) 1_I = 1_I$ and $U^* 1_J = 1_J$ since $U$ is unitary. Thus, Item 2 holds.

Suppose now that Item 2 holds. By Lemma 2.6, write $\varphi = \varphi' \oplus \varphi''$ and $\psi = \psi' \oplus \psi''$. By assumption, there exists a unitary $U: V \to W$ such that $U \varphi'(g) = \psi'(g) U$ for all $g \in \Gamma$. Extend $U$ to $X$ by letting it annihilate $V^\perp$. Then $X \varphi(g) = (U \oplus 0)(\varphi' \oplus \varphi'')(g) = U \varphi'(g) \oplus 0 = \psi'(g) U \oplus 0 = \psi(g) X$ for all $g \in \Gamma$. Since $U$ is pseudo-stochastic and $1_I \in V$ and $1_J \in W$, $X$ is pseudo-stochastic as well. Hence, Item 3 holds. That Item 3 implies Item 1 is immediate. □

The following Theorem 3.5 parallels the polynomial bound from Theorem 3.2 on the length of the words which need to be inspected.

**Theorem 3.5.** Writing $n := |I| = |J|$, the conditions of Theorem 3.3 are equivalent to the following:
For every word $w \in \Gamma_M$ of length at most $2n - 1$, $\text{soe}(w_A) = \text{soe}(w_B)$.

**Proof.** Suppose wlog that $I$ and $J$ are disjoint. As in the proof of Theorem 3.2, write $w_{A \oplus B} := \begin{pmatrix} w_A & 0 \\ 0 & w_B \end{pmatrix} \in \mathbb{K}^{(I \cup J) \times (I \cup J)}$ for $w \in \Gamma_M$. Furthermore, write $1$ for the all-ones vector in $\mathbb{K}^{I \cup J}$. Write $V_{A \oplus B} \leq \mathbb{K}^{I \cup J}$ for the space spanned by the $w_{A \oplus B} 1$ for all $w \in \Gamma_M$. Write $V_{A \oplus B}^{\leq \ell} \leq V_{A \oplus B}^{\leq \ell}$ for $\ell \geq 0$ for the subspace spanned by the $w_{A \oplus B} 1$ for $w \in \Gamma_M$ of length $\leq \ell$. Clearly, $V_{A \oplus B}^{\leq 0}$ containing $1$ is one-dimensional. The space $V_{A \oplus B}$ is at most $2n$-dimensional.
Claim 3. If $V_{A \otimes B}^{< \ell} = V_{A \otimes B}^{< \ell+1}$ for some $\ell \in \mathbb{N}$ then $V_{A \otimes B} = V_{A \otimes B}^{< \ell}$. In particular, $V_{A \otimes B}^{< 2n-1} = V_{A \otimes B}$. 

Proof of Claim. By induction on $j \geq 1$, we show that $V_{A \otimes B}^{< \ell+j} \leq V_{A \otimes B}^{< \ell}$. The base case $j = 1$ holds by assumption. Let $x \in \Gamma_M$ be a word of length $\ell + j + 1$. Let $y$ denote the first character of $x$ and write $z$ for the length-$(\ell + j)$ suffix of $x$, i.e. $x = yz$. By assumption, there exist words $z^1, \ldots, z^r$ of length at most $\ell$ and coefficients $a_1, \ldots, a_r \in K$ such that $z_{A \otimes B} = \sum_{i=1}^r a_i z_{A \otimes B}^i$. Hence, $x_{A \otimes B} = y_{A \otimes B} z_{A \otimes B} = \sum_{i=1}^r a_i y_{A \otimes B} z_{A \otimes B}^i = \sum_{i=1}^r a_i (yz^i)_{A \otimes B} \in V_{A \otimes B}^{< \ell+1}$. Thus, $V_{A \otimes B}^{< \ell+j+1} \leq V_{A \otimes B}^{< \ell+1} \leq V_{A \otimes B}^{< \ell}$, as desired.

Let $w \in \Gamma_M$ be arbitrary. By Claim 3, there exist $w^i \in \Gamma_M$ of length at most $2n - 1$ and coefficients $a_i \in K$ such that $w_{A \otimes B} = \sum a_i w^i_{A \otimes B}$. Hence, writing $1_A$ and $1_B$ for the indicator vectors on $I$ and $J$ in $K^{l_I, l_J}$,

$$\text{soe}(w_A) = 1_A^T w_{A \otimes B} 1 = \sum a_i 1_A^T w^i_{A \otimes B} 1 = \sum a_i \text{soe}(w^i_A) = \sum a_i \text{soe}(w^i_B) = \text{soe}(w_B),$$

as desired. \qed

### 3.3 Doubly-Stochastic Similarity

Our second variant of the Specht–Wiegmann Theorem gives a criterion for simultaneous doubly-stochastic similarity. Recall that a real matrix is doubly-stochastic if it is pseudo-stochastic and has non-negative entries. Since doubly-stochasticity makes no sense over complex numbers, we restrict our attention to representations of involution monoids over real vector spaces. In contrast to Theorems 3.1 and 3.3, the criterion derived in this section does not involve words over some set of matrices but trees, defined as follows:

**Definition 3.6** (Trees over a monoid). Let $\Gamma$ be a monoid. A *tree over* $\Gamma$ is a tuple $t = (T, r, e)$ where $T$ is a finite tree, $r \in V(T)$, and $e : E(T) \to \Gamma$ is a map which assigns an element of $\Gamma$ to every edge of $T$. Write $T(\Gamma)$ for the set of trees over $\Gamma$. The set $T(\Gamma)$ forms a monoid under the operation $\odot$ of gluing two of its elements together at their roots.

Note that the elements of $T(\Gamma)$ can be constructed from the tree over $\Gamma$ with only one vertex by gluing and by attaching a new root $s$ to a tree $t = (T, r, e)$ and picking an element $g \in \Gamma$ to associate with the new edge $rs$.

**Definition 3.7**. Let $\Gamma$ be a monoid and $I$ a finite index set. A representation $\varphi : \Gamma \to \mathbb{R}^{l \times I}$ of $\Gamma$ induces a representation $\hat{\varphi} : T(\Gamma) \to \mathbb{R}^I$ of $T(\Gamma)$ defined inductively as follows:

1. $\hat{\varphi}(t) := 1_I$ if $t$ has only one vertex,
2. $\hat{\varphi}(t') := \hat{\varphi}(t') \odot \hat{\varphi}(t'')$ if $t := t' \odot t''$ for $t', t'' \in T(\Gamma)$ on more than one vertex,
3. $\hat{\varphi}(t) := \varphi(e(rs)) \cdot \hat{\varphi}(t')$ if $t = (T, r, e)$ is such that $r$ has only one child $s$. Here, $t' = (T', s, e') \in T(\Gamma)$ is obtained by deleting $r$ from $t$ and making $s$ the new root, i.e. $T' := T - r$ and $e' := e|_{V(T')}$. 

For the involution monoid $\Gamma_M$, we abbreviate the representation of $T(\Gamma_M)$ induced by $w \mapsto w_A$ as $t \mapsto t_A$. The main result of this section is the following:

**Theorem 3.8**. Let $I$ and $J$ be finite index sets. Let $M$ be any set. Let $A = (A_i)_{i \in M}$ and $B = (B_i)_{i \in M}$ be two sequences of matrices such that $A_i \in \mathbb{R}^{l \times I}$ and $B_i \in \mathbb{R}^{l \times J}$ for $i \in M$. Then the following are equivalent:

\[ V_{A \otimes B}^{< \ell} = V_{A \otimes B}^{< \ell+1} \text{ for some } \ell \in \mathbb{N} \Rightarrow \]
1. there exists a doubly-stochastic matrix $X \in \mathbb{R}^{I \times I}$ such that $XA_i = B_iX$ and $XA_i^\top = B_i^\top X$ for all $i \in M$.
2. for every $t \in T(\Gamma_M)$, $\text{soe}(t_A) = \text{soe}(t_B)$.

Theorem 3.8 is implied by the following Lemma 3.9. Inspecting the proof of this lemma, shows that $\mathbb{R}$ can be replaced by $Q$ in both Theorem 3.8 and Lemma 3.9.

**Lemma 3.9.** Let $\Gamma$ be an involution monoid. Let $I$ and $J$ be finite index sets. Let $\varphi: \Gamma \to \mathbb{R}^{I \times J}$ and $\psi: \Gamma \to \mathbb{R}^{I \times I}$ be representations of $\Gamma$. Let $\hat{\varphi}$ and $\hat{\psi}$ be the induced representations of $T(\Gamma)$. Then the following are equivalent:

1. there exists a doubly-stochastic $X \in \mathbb{R}^{I \times I}$ such that $X\varphi(g) = \psi(g)X$ for all $g \in \Gamma$,
2. there exists a pseudo-stochastic $X \in \mathbb{R}^{I \times I}$ such that $X\varphi(g) = \psi(g)X$ for all $g \in \Gamma$ and $X\hat{\varphi}(t) = \hat{\psi}(t)$ for all $t \in T(\Gamma)$,
3. for all $t \in T(\Gamma)$, $\text{soe}(t) = \text{soe}(\hat{\varphi}(t))$.

**Proof.** Item 1 implies Item 2: Let $X$ be as in Item 1. It has to be shown that $X\hat{\varphi}(t) = \hat{\psi}(t)$ for all $t \in T(\Gamma)$. The proof of the following slightly stronger claim is guided by [54, Lemma 1].

**Claim 4.** For all $t \in T(\Gamma)$, if $X(j,i) > 0$ for $i \in I$ and $j \in J$ then $\hat{\varphi}(t)(i) = \hat{\psi}(t)(j)$.

Claim 4 implies that $X\hat{\varphi}(t) = \hat{\psi}(t)$ for all $t \in T(\Gamma)$. Indeed, for $t \in T(\Gamma)$ and $j \in J$,

$$
(X\hat{\varphi}(t))(j) = \sum_{i \in I, X(i,j) > 0} X(i,j)\hat{\varphi}(i) = \sum_{i \in I, X(i,j) > 0} X(i,j)\hat{\psi}(j) = \hat{\psi}(j)(X1_i)(j) = \hat{\psi}(j). \tag{2}
$$

One may similarly see that $X^T\hat{\psi}(t) = \hat{\varphi}(t)$ for all $t \in T(\Gamma)$. This statement is applied in the inductive proof of Claim 4.

**Proof of Claim 4.** The proof is by induction on the structure of the elements of $T(\Gamma)$, cf. Definition 3.7. For the single-vertex tree, the claim is vacuous.

For the induction step, two means of constructing more complex elements $t = (T, r, e) \in T(\Gamma)$ are considered. If $t = t' \circ t''$ for two non-trivial $t', t'' \in T(\Gamma)$, the claim is readily verified. It remains to consider the case in which $r$ has a unique child $s$ in $T$. Write $t' = (T - r, s, e|_{V(\Gamma)\setminus\{t\}}) \in T(\Gamma)$ for the subtree rooted at $s$. Let $g := e(rs) \in \Gamma$.

The vectors $\hat{\varphi}(t)$ and $\hat{\psi}(t)$ satisfy the assumptions of Lemma 2.4. Indeed, by Item 1 and Equation (2),

$$
X\hat{\varphi}(t) = X\varphi(g)\hat{\varphi}(t') = \psi(g)X\varphi(t') = \psi(g)\hat{\psi}(t') = \hat{\psi}(t), \tag{3}
$$

and, alluding to the assumption that $\Gamma$ is an involution monoid,

$$
X^T\hat{\psi}(t) = X^T\varphi(g)\hat{\psi}(t') = (\psi(s^\top)X)^T\hat{\psi}(t') = (X\varphi(s^\top))^T\hat{\psi}(t') = \varphi(g)X^T\hat{\psi}(t') = \varphi(g)\hat{\varphi}(t') = \hat{\varphi}(t). \tag{4}
$$

Equations (3) and (4) in conjunction with Lemma 2.4 imply Claim 4. \hfill \square

Item 2 implies Item 1: Let $X$ be as in Item 2. Write $V \subseteq \mathbb{R}^I$ for the vector space spanned by the $\varphi(t)$ for $t \in T(\Gamma)$. Write $P \in \mathbb{R}^{I \times I}$ for the projection onto $V$. Arguing as in the proof of Lemma 2.6, it can be shown that $P\varphi(g) = \varphi(g)P$ for all $g \in \Gamma$. It follows that $XP$ satisfies the conditions of Item 2.
Claim

Proof. For $T$ to show that $\phi$ holds by assumption. Let $t \in I$ and let $C \subseteq I$ denote its equivalence class. Then $P_{e_i} = 1_C / |C|$ for $e_i \in \mathbb{R}^I$ the standard basis vector corresponding to $i$. It remains to compute $Xe_i$. Write $1_C = \sum r \in \mathbb{R}$. Then

$$(X1_C) \circ (X1_C) = \sum_{r,s} \alpha_r \alpha_s (X\hat{\phi}(t_r) \circ (X\hat{\phi}(t_s))$$

$$= \sum_{r,s} \alpha_r \alpha_s \hat{\phi}(t_r) \circ \hat{\phi}(t_s)$$

$$= \sum_{r,s} \alpha_r \alpha_s (X\hat{\phi}(t_r \circ t_s))$$

$$= \sum_{r,s} \alpha_r \alpha_s X(\hat{\phi}(t_r \circ t_s))$$

$$= X(1_C \circ 1_C)$$

$$= X1_C$$

Hence, $X1_C$ has entries in $\{0, 1\}$. Finally, observe that $X(j, i) = e^T X e_i = e^T 1_C / |C|$ is non-negative for every $j \in J$. This yields Item 1.

Item 2 implies Item 3: Let $t \in T(\Gamma)$. Then

$$\text{soe} \hat{\phi}(t) = \langle 1_I, \hat{\phi}(t) \rangle = \langle 1_I, X\hat{\phi}(t) \rangle = \langle 1_I, \hat{\psi}(t) \rangle = \text{soe} \hat{\psi}(t).$$

Item 3 implies Item 2: Write $V \leq \mathbb{R}^I$ and $W \leq \mathbb{R}^I$ for the vector spaced spanned by the $\hat{\phi}(t)$ and $\hat{\psi}(t)$ for $t \in T(\Gamma)$ respectively. Since for all $t, s \in T(\Gamma)$

$$\langle \hat{\phi}(t), \hat{\psi}(s) \rangle = \text{soe}(\hat{\phi}(t) \circ \hat{\psi}(s)) = \text{soe}(\hat{\phi}(t \circ s)) = \text{soe}(\hat{\psi}(t \circ s)) = \langle \hat{\psi}(t), \hat{\psi}(s) \rangle,$$

Lemma 2.1 implies the existence of an orthogonal map $U: V \rightarrow W$ such that $U\hat{\phi}(t) = \hat{\psi}(t)$ for all $t \in T(\Gamma)$. Extend $U$ to $X \in \mathbb{R}^I \times I$ by letting it annihilate $V^\perp$. This matrix satisfies all desired properties.

In stark contrast to Theorems 3.2 and 3.5, we give an exponential bound on the size of the trees in Theorem 3.11. Lower bounds are discussed in Remark 4.4. First we bound the depth of the trees. The depth of a tree $t = (T, r, e) \in T(\Gamma_M)$ is defined as the maximal number of edges of any path on $T$ starting in $r$.

**Lemma 3.10.** Writing $n := |I| = |J|$, the conditions of Theorem 3.8 are equivalent to the following: For every tree $t \in T(\Gamma_M)$ of depth $\leq n$, $\text{soe}(t_A) = \text{soe}(t_B)$.

**Proof.** For $d \geq 0$, write $T_A^{\leq d} \leq \mathbb{R}^I$ for the vector space spanned by the $t_A$ for all $t \in T(\Gamma_M)$ of depth $\leq d$. Write $T_A$ for the space spanned by all $t_A$ for $t \in T(\Gamma_M)$. Clearly, $T_A$ is at most $n$ dimensional. The space $T_A^{\leq 0}$ containing the all-ones vector is one-dimensional.

**Claim 5.** If $T_A^{\leq d} = T_A^{\leq d+1}$ for some $d \in \mathbb{N}$ then $T_A = T_A^{\leq d}$. In particular, $T_A^{\leq n-1} = T_A$.

**Proof of Claim.** By induction on $j \geq 1$, it is shown that $T_A^{\leq d+j} \leq T_A^{\leq d}$. The base case $j = 1$ holds by assumption. Let $t \in T(\Gamma_M)$ be a tree of depth $d + j + 1$. If $t$ can be written as $t = t^1 \circ \cdots \circ t^k$ for some trees $t^1, \ldots, t^k \in T(\Gamma_M)$ whose roots have degree one then it suffices to show that $t^i_A \leq T_A^{\leq d}$ for all $i \in [k]$ since $T_A^{\leq d}$ is closed under Schur products. Hence, it may
be supposed that the root \( r \) of \( t \) has a single child \( s \). Write \( t' \) for the subtree of \( t \) rooted at \( s \) and \( g \in \Gamma_M \) for the element associated with the edge \( rs \).

By assumption, there exist trees \( x^1, \ldots, x^m \in T(\Gamma_M) \) of depth at most \( d \) and coefficients \( a_1, \ldots, a_m \in \mathbb{R} \) such that \( t'_A = \sum_{i=1}^m a_i x^i_A \). Then \( t_A = \sum_{i=1}^m a_i g_A x^i_A \in T_A^{d+1} \). Thus, \( T_A^{d+j+1} \leq T_A^{d+1} \leq T_A^d \), as desired.

By Claim 5, every \( t_A \in T_A \) can be written as linear combination of some \( t'_A \in T_A^{\leq n-1} \). It remains to show that the coefficients in this linear combination are the same for \( A \) and \( B \).

**Claim 6.** For every \( t \in T(\Gamma_M) \), there exist coefficients \( a_1, \ldots, a_m \in \mathbb{R} \) and trees \( t^1, \ldots, t^m \in T(\Gamma_M) \) of depth at most \( n-1 \) such that

\[
t_A = \sum_i a_i t^i_A \quad \text{and} \quad t_B = \sum_i a_i t^i_B.
\]

**Proof of Claim.** By induction on the structure of \( t \). If \( t \) is the single vertex then the claim is vacuously true. If \( t \) has a unique child, write \( s \) for the subtree rooted at this child and \( g \in \Gamma_M \) for the element associated to the edge \( ts \). Observe that \( t_A = g_A s_A \) and \( t_B = g_B s_B \). The inductive hypothesis applies to \( s \) yielding coefficients \( a_1, \ldots, a_m \) and trees \( t^1, \ldots, t^m \in T(\Gamma_M) \) of depth at most \( n-1 \) such that Equation (5) holds. By Claim 5, for every \( i \in [m] \), there exist coefficients \( b_{ij} \) and trees \( r^i_j \) of depth at most \( n-1 \) such that \( g_A s^i_A = \sum b_{ij} r^i_j \). In order to conclude that the same identity holds for \( B \), observe that the tree represented by \( g s^i \) has depth at most \( n \). The same holds for all trees occurring in the following calculation:

\[
\left< g Bs^i_B - \sum b_{ij} r^i_j, g Bs^i_B - \sum b_{ij} r^i_j \right> = \langle gBs^i_B \circ gBs^i_B - 2 \sum b_{ij} \circ gBs^i_B \circ r^i_j \rangle + \sum b_{ij} b_{ik} \circ r^i_j \circ r^k_i \\
= \langle gAs^i_A \circ gAs^i_A - 2 \sum b_{ij} \circ gAs^i_A \circ r^i_j \rangle + \sum b_{ij} b_{ik} \circ r^i_j \circ r^k_i \\
= \langle gAs^i_A - \sum b_{ij} r^i_j, gAs^i_A - \sum b_{ij} r^i_j \rangle = 0.
\]

Thus, \( gBs^i_B = \sum b_{ij} r^i_j \), as desired. If \( t \) is of the form \( t^1 \circ \cdots \circ t^r \) for some trees \( t^1, \ldots, t^r \) whose roots have degree one then the first case applies to each of these subtrees. The claim follows readily.

Finally, for every tree \( t \in T(\Gamma_M) \) of arbitrary depth, let \( a_1, \ldots, a_m \in \mathbb{R} \) and \( t^1, \ldots, t^m \in T(\Gamma_M) \) be as in Claim 6. Then \( \text{soe}(t_A) = \sum a_i \text{soe}(t^i_A) = \sum a_i \text{soe}(t_B) = \text{soe}(t_B) \). \( \square \)

We conclude this section by bounding the degree of the trees which need to be considered in Theorem 3.8. In particular, it suffices to consider trees on at most \( \sum d=0 (2n-1)^d \leq (2n)^{n+1} \) vertices. In Remark 4.4, we comment on the tightness of the bounds in Theorem 3.11.

**Theorem 3.11.** Writing \( n := \| I \| = \| J \| \), the conditions of Theorem 3.8 are equivalent to the following:

For every tree \( t \in T(\Gamma_M) \) of depth \( \leq n \) and out-degree \( \leq 2n-1 \), \( \text{soe}(t_A) = \text{soe}(t_B) \).

**Proof.** Given Lemma 3.10, it suffices to show that \( \text{soe}(t_A) = \text{soe}(t_B) \) for all trees \( t \in T(\Gamma_M) \) of depth at most \( n \). To ease notation, we suppose wlog that \( I \) and \( J \) are disjoint. Similar to the set-up of the proof of Theorem 3.2, define for a tree \( t \in T(\Gamma_M) \) the block vector.
Thus, the assertion in Theorem 2.1 is a matrix of cycles, paths, and trees.

Claim 7. For every $d \geq 0$, there exist a set $T \subseteq T(\Gamma_M)$ of trees of depth $\leq d$, whose roots have out-degree $\leq 1$, and all whose out-degrees are $\leq 2n - 1$ such that

$$T_{\leq d}^{\leq 1} = \text{span}\{t^{< i}_{A \otimes B} \mid t \in T, 0 \leq i \leq 2n - 1\}.$$  

Proof of Claim. For $d = 0$, the singleton containing the one-vertex tree is as desired. For $d \geq 1$, consider the following equivalence relation on $I \cup J$: Let $i \sim_d j$ if and only if $t_{A \otimes B}(i) = t_{A \otimes B}(j)$ for all $t \in T(\Gamma_M)$ of depth $\leq d$. Observe that if $i \not\sim_d j$ then there exists $s \in T(\Gamma_M)$ of depth $\leq d$ and with root of degree 1 such that $s_{A \otimes B}(i) \neq s_{A \otimes B}(j)$. Indeed, if the root of a tree $t$ such that $t_{A \otimes B}(i) \neq t_{A \otimes B}(j)$ has higher degree then $t$ is the gluing product of multiple trees with root of degree one and one of these factors is as desired.

Let $S \subseteq T(\Gamma_M)$ be a set of trees of depth at most $d$ and with root of degree 1 such that $i \sim_d j$ if and only if $s_{A \otimes B}(i) = s_{A \otimes B}(j)$ for all $s \in S$. By Fact 2.2,

$$T_{\leq d}^{\leq 1} = \text{span}\{s^{< i}_{A \otimes B} \mid s \in S, 0 \leq i \leq 2n - 1\}.$$  

For $s \in S$, write $s'$ for the tree rooted at the unique child of the root of $s$. Moreover, write $g^s \in \Gamma_M$ for the element associated to the edge incident to the root of $s$. The tree $s'$ is of depth at most $d - 1$. Write $Q \subseteq T(\Gamma_M)$ for the of trees of depth at most $d - 1$ with roots of out-degree $\leq 1$, and all whose out-degrees are $\leq 2n - 1$, which is guaranteed to exist by induction. Then, by linearity,

$$T_{A \otimes B}^{\leq d} = \text{span}\{s^{< i}_{A \otimes B} \mid s \in S, 0 \leq i \leq 2n - 1\} = \text{span}\{(g^s s')^{< i}_{A \otimes B} \mid s \in S, 0 \leq i \leq 2n - 1\} \leq \text{span}\{(g(q^{< i}))^{< i}_{A \otimes B} \mid q \in Q, g \in \Gamma_M, 0 \leq i \leq 2n - 1, 0 \leq j \leq 2n - 1\} \leq T_{A \otimes B}^{\leq d}.$$  

Note that all trees $g(q^{< i})$ appearing in the final set are of depth $\leq d$, have roots of out-degree $\leq 1$, and only vertices of out-degree $\leq 2n - 1$.

For a vector $v \in \mathbb{R}^{I \cup J}$, write $\text{soe}_A v := \sum_{i \in I} v(i)$ and analogously $\text{soe}_B v := \sum_{j \in J} v(j)$. Let $t \in T(\Gamma_M)$ be a tree of depth at most $n$. By Claim 7, there exist $t^1, \ldots, t^r \in \Gamma_M$ of depth at most $n$ and out-degrees at most $2n - 1$ and coefficients $a_1, \ldots, a_r \in \mathbb{R}$ such that $t_{A \otimes B} = \sum_{i=1}^r a_i t^i_{A \otimes B}$. Hence,

$$\text{soe}(t_A) = \text{soe}_A(t_{A \otimes B}) = \sum a_i \text{soe}_A(t^i_{A \otimes B}) = \sum a_i \text{soe}(t^i_A) = \sum a_i \text{soe}(t^i_B) = \text{soe}(t_B).$$  

Thus, the assertion in Theorem 3.11 implies the assertion of Lemma 3.10. \qed

4 Cycles, Paths, and Trees

Two graphs $G$ and $H$ with adjacency matrices $A_G$ and $A_H$ are isomorphic if and only if there is a matrix $X$ over the non-negative integers such that $X A_G = A_H X$ and $X1 = X^T 1 = 1$, 20
(a) Series products of bilabelled graphs correspond to matrix products of their homomorphism tensors. The leftmost \((1,1)\)-bilabelled graph is the one whose homomorphism tensor is the adjacency matrix. The \((1,1)\)-bilabelled paths with labels at vertices of degree at most 1 form an involution monoid as in Definition 5.1.

\[
\text{tr} \left( \begin{array}{c}
1 \\
\end{array} \right) =
\]

(b) Identifying opposing labels and unlabelling of a bilabelled graph corresponds to taking the trace of its homomorphism tensor.

\[
\text{soe} \left( \begin{array}{c}
1 \\
\end{array} \right) =
\]

(c) Unlabelling a bilabelled graph corresponds to taking the sum-of-entries of its homomorphism tensor.

Figure 2: Combinatorial operations on bilabelled graphs.

where \(1\) is the all-ones vector. Writing the constraints as linear equations whose variables are the entries of \(X\), we obtain a system \(F_{\text{iso}}(G,H)\) that has a non-negative integer solution if and only if \(G\) and \(H\) are isomorphic. A combination of results from \([55, 17]\) shows that \(F_{\text{iso}}(G,H)\) has a non-negative rational solution if and only if \(G\) and \(H\) are homomorphism indistinguishable over the class of trees, and by \([16]\), \(F_{\text{iso}}(G,H)\) has an arbitrary rational solution if and only if \(G\) and \(H\) are homomorphism indistinguishable over the class of paths.

In this section, we reprove these results showcasing our Theorems 3.1, 3.3 and 3.8. These theorems contain the algebraic core of the arguments while the correspondence between (bi)labelled graphs and their homomorphism tensors (Section 2.6) provides the necessary combinatorial insights.

**Corollary 4.1.** For graphs \(n\)-vertex graphs \(G\) and \(H\), the following are equivalent:

1. \(G\) and \(H\) are homomorphism indistinguishable over the class of cycles,
2. \(G\) and \(H\) are homomorphism indistinguishable over the class of cycles on at most \(2n^2 - 1\) vertices,
3. there exists an orthogonal \(X \in \mathbb{R}^{V(H) \times V(G)}\) such that \(XA_G = A_H X\).

**Proof.** Apply Theorem 3.1 with \(I := V(G)\) and \(J := V(H)\), and \(A := (A_G)\) and \(B := (A_H)\). The series products of \(A\) with itself are precisely the \((1,1)\)-bilabelled paths with labels at the vertices of degree \(\leq 1\), cf. Figure 2a. Taking the traces of their homomorphism matrices amounts to identifying the labels of these paths and thus counting homomorphisms from cycles into \(G\) and \(H\), cf. Figure 2b.

By Theorem 3.2, it suffices to consider words in \(A_G\) and \(A_H\) of length at most \(2n^2 - 1\). Each letter corresponds to an edge. Thus, homomorphism counts from cycles on at most \(2n^2 - 1\) vertices suffice.

By Newton’s identities, cf. \([15, \text{Proposition 1}]\), considering cycles on at most \(n\) vertices suffices. The bound in Corollary 4.1 is suboptimal as it is derived from the more general
Theorem 3.2, which in contrary to Newton’s identities gives a criterion of simultaneous orthogonal similarity of multiple matrices, cf. [46]. For paths, we obtain an analogous result:

**Corollary 4.2.** For n-vertex graphs G and H, the following are equivalent:
1. G and H are homomorphism indistinguishable over the class of paths,
2. G and H are homomorphism indistinguishable over the class of paths on at most 2n vertices,
3. there exists a pseudo-stochastic X ∈ R^{V(H)×V(G)} such that XA_G = A_HX.

**Proof.** Recall the proof of Corollary 4.1 and invoke Theorem 3.3. Taking sums-of-entries of homomorphism matrices of (1,1)-bilabelled paths amounts to counting homomorphisms from the underlying unlabelled paths into G and H, cf. Figure 2c. By Theorem 3.5, it suffices to consider words in A_G and A_H of length at most 2n − 1. Each letter corresponds to an edge. Thus, homomorphism counts from paths on at most 2n vertices suffice. □

The classical characterisation [54] of homomorphism indistinguishability over trees involves a non-negativity condition on the matrix X. While such an assumption appears natural from the viewpoint of solving the system of equations for fractional isomorphism, it lacks an algebraic or combinatorial interpretation. Using Theorem 3.8, we reprove this known characterisation and give an alternative description that emphasises its graph-theoretic origin.

Here, the depth of a rooted tree (T, r), r ∈ V(T), is the maximum number of edges on any path from r to a leaf.

**Corollary 4.3.** For n-vertex graphs G and H, the following are equivalent:
1. G and H are homomorphism indistinguishable over the class of trees,
2. G and H are homomorphism indistinguishable over all trees T for which there exists r ∈ V(T) such that (T, r) is of depth at most n and maximum out-degree at most 2n − 1,
3. G and H are homomorphism indistinguishable over all trees on at most (2n)^n+1 vertices,
4. there exists a pseudo-stochastic matrix X ∈ Q^{V(H)×V(G)} satisfying XA_G = A_HX and one of the following equivalent conditions holds:
   a) all entries of X are non-negative,
   b) XT_G = T_H for all 1-labelled trees T ∈ T,
   c) X preserves the Schur product on RT_G, the space spanned by the T_G for T ∈ T, i.e. X(u ⊗ v) = (Xu) ⊗ (Xv) for all u, v ∈ RT_G.

**Proof.** By Theorem 3.11, the first two assertions are equivalent. A tree as in the second assertion has at most ∑_{d=1}^n(2n−1)^d ≤ (2n)^n+1 vertices. Hence, the third assertion implies the second. Clearly, the first assertion implies the third.

For the last assertion, consider the following argument: The equivalence of Items 4a and 4b is immediate from Lemma 3.9. Assuming Item 4b, Item 4c follows since X(T_G ⊗ S_G) = X((T ⊗ S)_G) = (T ⊗ S)_H = T_H ⊗ S_H for all T, S ∈ T. Conversely, by induction on the structure of T ∈ T, if T = A · S for some S ∈ T then XT_G = A_HXS_G = T_H by the assumption XA_G = A_HX. If T = R ⊗ S for some R, S ∈ T then the claim follows immediately from Item 4c. □

We finally comment on the optimality of the bounds in Corollary 4.3.

**Remark 4.4.** In Section 5.4, we argue that homomorphism counts of constant degree trees are not as expressive as homomorphism counts from all trees. In particular, by Theorem 1.3,
the bound on the maximum degree in Corollary 4.3 cannot be replaced with a constant. Furthermore, by [21], there exist graphs $G$ and $H$ on $n$ vertices which are distinguished by Colour Refinement but only in $\Theta(n)$ iterations. Thus, by [16], these graphs are homomorphism indistinguishable over all trees $T$ for which there exists $r \in V(T)$ such that the rooted tree $(T, r)$ is of depth $\Theta(n)$. Thereby, the bound in Corollary 4.3 on the depth of the trees is asymptotically tight.

5 Cyclewidth, Pathwidth, Treewidth, Treedepth, and Trees of Bounded Degree

In Corollaries 4.1 to 4.3, the machinery from Section 3 was applied to involution monoids which are generated by a single generator, namely the bilabelled edge, cf. Figure 1b. In this section, we consider involution monoids which are generated by more than one generator. In the language of Theorems 3.1, 3.3 and 3.8, this amounts to considering multiple matrices. As before, the matrices are homomorphism matrices of bilabelled graphs. Using multiple such graphs permits the treatment of more complicated graph classes such the classes of graphs of bounded cycle-, path-, treewidth, and treedepth.

The following subsections feature four different algebro-combinatorial setups, which are summarised in Figure 3. The algebraic structure of the considered class of (bi)labelled graphs determines the domain of the matrix variables in the matrix equations whose feasibility is equivalent to homomorphism indistinguishability over the family of underlying unlabelled graphs. Domains covered by our results are unitary matrices, pseudo-stochastic matrices, and doubly-stochastic matrices. In some cases, feasibility over two of these possible domains coincides (Section 5.3).
5.1 Pathwidth and Cyclewidth: Generators for Involution Monoids

The families of bicoloured graphs considered in this section all are involution monoids in the following sense. Let \( I = (I, (1, \ldots, k), (1, \ldots, k)) \) with \( V(I) = [k] \) and \( E(I) = \emptyset \) denote the identity graph, cf. Figure 5a.

**Definition 5.1.** Let \( k \geq 1 \). A set \( S \subseteq G(k, k) \) is an involution monoid if
1. \( I \in S \),
2. \( S' \in S \) for all \( S \in S \),
3. \( S \cdot S' \in S \) for all \( S, S' \in S \).

An example of an involution monoid of \((1, 1)\)-bicoloured graphs is path monoid of all \((1, 1)\)-bicoloured paths with labels at opposing ends, cf. Figure 2a. In order to derive systems of equations with finitely many equations, we consider finite generating sets of involution monoids:

**Definition 5.2.** Let \( S \) be an involution monoid. A set \( B \subseteq S \) generates \( S \) if
1. \( I \in B \),
2. \( B' \in B \) for all \( B \in B \),
3. for all \( S \in S \) there exist \( B^1, \ldots, B^\varepsilon \in B \) such that \( S = B^1 \cdots B^\varepsilon \).

For example, the path monoid is generated by the \((1, 1)\)-bicoloured graph \( A \) depicted in Figures 1b and 2a.

For a graph class \( F \) and \( N \in \mathbb{N} \), write \( F_{\leq N} := \{ F \in F \mid |V(F)| \leq N \} \). For a class \( S \subseteq G(k, k) \) of \((k, k)\)-bicoloured graphs where \( k \geq 1 \), write \( \text{soe}(S) := \{ \text{soe} S \mid S \in S \} \) and \( \text{tr}(S) := \{ \text{tr} S \mid S \in S \} \). Both \( \text{soe}(S) \) and \( \text{tr}(S) \) are classes of unlabelled graphs. The following Theorem 5.3 is immediate from Theorems 3.1 to 3.3 and 3.5.

**Theorem 5.3.** Let \( k \geq 1 \). Let \( S \subseteq G(k, k) \) be an involution monoid generated by \( B \subseteq S \). Let \( G \) and \( H \) be \( n \)-vertex graphs. Suppose that every graph in \( B \) has at most \( b \in \mathbb{N} \cup \{ \infty \} \) vertices and let \( N_1 := 2n^2b \in \mathbb{N} \cup \{ \infty \} \) and \( N_2 := 2n^2b \in \mathbb{N} \cup \{ \infty \} \). Then the following are equivalent:
1. \( G \) and \( H \) are homomorphism indistinguishable over \( \text{soe}(S) \),
2. \( G \) and \( H \) are homomorphism indistinguishable over \( \text{soe}(S)_{\leq N_1} \),
3. there exists a pseudo-stochastic \( X \in \mathbb{Q}^{|V(H)| \times |V(G)|} \) such that \( XB_G = B_H X \) for all \( B \in B \).

Furthermore, the following are equivalent:
1. \( G \) and \( H \) are homomorphism indistinguishable over \( \text{tr}(S) \),
2. \( G \) and \( H \) are homomorphism indistinguishable over \( \text{tr}(S)_{\leq N_2} \),
3. there exists an orthogonal \( U \in \mathbb{R}^{|V(H)| \times |V(G)|} \) such that \( UB_G = B_H U \) for all \( B \in B \).

**Proof.** In the set-up of Theorems 3.1 and 3.3, let \( I := V(G)^k \), \( J := V(H)^k \), and \( M := B \). Furthermore, let \( A \) (respectively, \( B \)) be the sequence of homomorphism tensors \( B_G \) (respectively, \( B_H \)) for \( B \in B \). Words \( w \in \Gamma_M \) corresponds to bicoloured graphs from \( S \) and vice-versa. The matrices \( w_A \) and \( w_B \) are homomorphism tensors of such a bicoloured graph. With these observations, Theorem 5.3 is immediate from Theorems 3.1 to 3.3 and 3.5. \( \square \)

We remark that we are only interested in the order of magnitude of the parameters \( N_1 \) and \( N_2 \). In order to state Theorem 5.3 more clearly, we chose to be slightly wasteful compared to Theorems 3.2 and 3.5.
The remainder of this section features an application of Theorem 5.3 to homomorphism indistinguishability over graphs of bounded pathwidth and cyclewidth. The prototypical example of an involution monoid is the family of graphs of pathwidth at most \( k \).

**Definition 5.4.** Let \( \mathcal{PW}^k \) denote the family of all \((k + 1, k + 1)\)-bilabelled graphs \( F = (F, u, v) \) such that \( F \) admits a path decomposition \((P, \beta)\) of width at most \( k \) with \( u, v \in V(P) \) satisfying

1. \( \beta(u) = \{u_1, \ldots, u_{k+1}\} \) and \( \beta(v) = \{v_1, \ldots, v_{k+1}\} \),
2. if \( u \neq v \) then \( \deg_P(u) = \deg_P(v) = 1 \) and if \( u = v \) then \( \deg_P(u) = \deg_P(v) = 0 \),
3. \( |\beta(s)| = k + 1 \) for all \( s \in V(P) \) and \( |\beta(s) \cap \beta(t)| = k \) for all \( st \in E(P) \).

The first two axioms of Definition 5.4 prescribe where in a path decomposition the labelled vertices have to be placed. The last axiom makes subsequent arguments easier and does not constitute a loss of generality: It is easy to see that \( \mathcal{PW}^k \) contains \( I \), is closed under reversal and series composition. Hence, it is an involution monoid as in Definition 5.1.

**Lemma 5.5.** Let \( k \geq 1 \).

1. The class \( \text{soe}(\mathcal{PW}^k) \) is the class of all graphs of pathwidth at most \( k \) on at least \( k + 1 \) vertices.
2. The class \( \text{tr}(\mathcal{PW}^k) \) is the class of all graphs of cyclewidth at most \( k \) on at least \( k + 1 \) vertices.

**Proof.** By Definition 5.4, every \( F \in \text{soe}(\mathcal{PW}^k) \) has pathwidth at most \( k \) and at least \( k + 1 \) vertices. Conversely, if \( F \) has pathwidth at most \( k \) and at least \( k + 1 \) vertices then, by Lemma 2.9, there exists a path decomposition \((P, \beta)\) of \( F \) satisfying Item 3 of Definition 5.4. The labels can be arbitrarily placed on \( F \) in accordance with Definition 5.4.

For the second claim, let \( F = (F, u, v) \in \mathcal{PW}^k \) be a bilabelled graph with path decomposition \((P, \beta)\) and \( u, v \in V(P) \) as in Definition 5.4. Let \( C \) denote the cycle obtained from \( P \) by making a fresh vertex \( w \) adjacent to \( u \) and \( v \). Extend \( \beta(w) := \beta(u) \cup \beta(v) \). In \( \text{tr}(F) \), the vertices \( u_i \) and \( v_i \) for \( i \in [k + 1] \) are respectively identified. Hence, \((C, \beta)\) gives rise to a cycle decomposition of \( \text{tr}(F) \) of width at most \( k \).

Conversely, by Lemma 2.9, if \( F \) has cyclewidth at most \( k \) and at least \( k + 1 \) vertices then there is a cycle decomposition \((C, \beta)\) of \( F \) satisfying Item 3 of Definition 5.4. Pick any vertex \( w \in V(C) \). Let \( P \) denote the path obtained from \( C \) by replacing \( w \) with two fresh vertices \( u \) and \( v \) adjacent to the two neighbours of \( w \) respectively. Write \( X \subseteq \beta(w) \) for the set of all vertices \( x \in \beta(w) \) which do not appear in all bags of \((C, \beta)\), i.e. \( x \not\in \beta(y) \) for some \( y \in V(C) \). For \( x \in X \), let \( c_1, \ldots, c_r \) and \( d_1, \ldots, d_s \) denote the vertices of \( C \) whose bags contain \( x \). Suppose that \( d_s d_{s-1} \ldots d_1 w c_1 \ldots c_r \) is a trail in \( C \) and that \( u \) and \( v \) were made adjacent to \( c_1 \) and \( v \) to \( d_1 \). Construct a graph \( F' \) from \( F \) by replacing every \( x \in X \) by two vertices \( x' \) and \( x'' \) and make \( x' \) adjacent to all neighbours of \( x \) in \( \beta(c_1) \cup \cdots \cup \beta(c_r) \) and \( x'' \) adjacent to all neighbours of \( x \) in \( \beta(d_1) \cup \cdots \cup \beta(d_s) \). Define a path decomposition \((P, \gamma)\) of \( F' \) via by letting \( \gamma(u) := (\beta(w) \setminus X) \cup \{x' \mid x \in X\} \) and \( \gamma(v) := (\beta(w) \setminus X) \cup \{x'' \mid x \in X\} \). Every other bag \( \gamma(z) \) for \( z \in V(P) \setminus \{u, v\} \) is obtained from \( \beta(z) \) by replacing \( x \in X \) by \( x' \) or \( x'' \) depending on whether \( z \) is among the \( c_1, \ldots, c_r \) or the \( d_1, \ldots, d_s \). Let \( u, v \in V(F') \) be tuples comprised of the vertices of \( \gamma(u) \) and \( \gamma(v) \) such that if \( u_i = x' \) for some \( x \in X \) and \( i \in [k + 1] \) then \( v_i = x'' \). Let \( F' := (F', u, v) \). Then \( \text{tr}(F') \cong F \), as desired. \( \square \)

To apply Theorem 5.3, it remains to give a set of generators for \( \mathcal{PW}^k \), cf. Figure 4.

**Lemma 5.6.** The set \( B^k \) consisting of the following \((k + 1, k + 1)\)-bilabelled graphs generates \( \mathcal{PW}^k \). For \( 1 \leq i \neq j \leq k + 1 \),
The identity graph \( I = (I, (1, \ldots, k + 1), (1, \ldots, k + 1)) \) with \( V(I) = [k + 1], E(I) = \emptyset \),

- the adjacency graphs \( A^{ij} = (A^{ij}, (k + 1), (k + 1)) \) with \( V(A^{ij}) = [k + 1] \) and \( E(A) = \{ij\} \),

- the forgetting graphs \( f^{i} = (F^{i}, (1, \ldots, k + 1), (1, \ldots, i - 1, i', i + 1, \ldots, k + 1)) \) with \( V(F^{i}) = [k + 1] \cup \{i'\} \) and \( E(F^{i}) = \emptyset \),

- the swap graphs \( S^{ij} = (S^{ij}, (1, \ldots, k + 1), (1, \ldots, i - 1, j, i + 1, \ldots, j - 1, i, j + 1, \ldots, k + 1)) \) with \( V(S^{ij}) = [k + 1] \) and \( E(S^{ij}) = \emptyset \).

Figure 4: Bilabelled graphs in \( B^{k} \) as defined in Lemma 5.6.

Proof. Clearly, \( B^{k} \subseteq PW^{k} \). Items 1 and 2 of Definition 5.2 are immediate. It remains to verify Item 3: To that end, let \( F \) be an arbitrary graph with a path decomposition \((P, \beta)\) with vertices \( u, v \in V(P) \) and \( u, v \in V(F)^{k + 1} \) as in Definition 5.4. The proof is by induction on \( |V(P)| \).

If \( |V(P)| = 1 \) then \( u = v \) and \( \{u_{1}, \ldots, u_{k + 1}\} = \{v_{1}, \ldots, v_{k + 1}\} \). Hence, there exists a permutation \( \sigma: [k + 1] \to [k + 1] \) such that \( u_{i} = v_{\sigma(i)} \) for all \( i \in [k + 1] \). Write \( \sigma = \tau_{1} \cdots \tau_{r} \) as product of transpositions. Then \( F = (F, u, v) \) is equal to

\[
S^{u} \cdots S^{v} \cdot \prod_{1 \leq i \neq j \leq k + 1} A_{ij}^{ij},
\]

a product of graphs in \( B^{k} \).

If \( |V(P)| \geq 2 \), let \( w \in V(P) \) denote the unique neighbour of \( u \). Let \( P' := P - u \). The subgraph \( F' \) of \( F \) induced by \( \bigcup_{p \in V(P')} \beta(p) \) satisfies Definition 5.4 with the path decomposition \((P', \beta_{|V(P')}), \) the vertices \( w, v, \) the tuple \( v \) and some tuple \( w \in V(F')^{k + 1} \) such that \( \beta(w) = \{w_{1}, \ldots, w_{k + 1}\} \) and \( w_{i} = u_{i} \) for all \( i \in [k + 1] \) \( \setminus \{\ell\} \) for some \( \ell \in [k + 1] \). Let \( F' := (F', w, v) \). Then

\[
F = \prod_{1 \leq i \neq j \leq k + 1} A_{ij}^{ij} \cdot J^{\ell} \cdot F'.
\]

The claim follows inductively. \[\square\]

In order to avoid the technicalities of working with small graphs, we record the following Lemma 5.7, which describes a padding trick.

Lemma 5.7. Let \( F' \subseteq F \) be graph classes such that \( nK_{1} \in F' \) for some \( n \geq 1 \). Suppose that for all \( F \in F \setminus F' \) it holds that \( F + \ell K_{1} \in F' \) for some \( \ell \geq 1 \). Then for all graphs \( G \) and \( H \) it holds that \( G \equiv_{F} H \) if and only if \( G \equiv_{F'} H \).
Proof. Since $F' \subseteq F$, it suffices to argue that the backward implication holds. Suppose that $G$ and $H$ are homomorphism indistinguishable over $F'$. Since $nK_1 \in F'$ for some $n \geq 1$, it holds that $|V(G)|^n = \text{hom}(nK_1, G) = \text{hom}(nK_1, H) = |V(H)|^n$. Hence, $G$ and $H$ have the same number of vertices. Suppose wlog that this number is non-zero. Let $F \in F \setminus F'$. Then $F + \ell K_1 \in F'$ for some $\ell \geq 1$. Hence, by [35, (5.28)],

$$\text{hom}(F, G) = \frac{\text{hom}(F + \ell K_1, G)}{\text{hom}(\ell K_1, G)} = \frac{\text{hom}(F + \ell K_1, H)}{\text{hom}(\ell K_1, H)} = \text{hom}(F, H),$$

which implies that $G$ and $H$ are homomorphism indistinguishable over $F$. \hfill \Box

For the case of the classes of graphs of pathwidth at most $k$ or cyclewidth at most $k$, we apply Lemma 5.7 with $F$ being the respective graph class and $F_{\geq 1} := \{ F \in F \mid |V(F)| \geq 1 \}$ assuming the role of $F'$. With this choice of $F'$, the somewhat cumbersome assumptions of Lemma 5.7 can be alleviated for graph classes which are minor-closed and closed under disjoint unions. For example, by Lemma 5.5, it holds that two graphs $G$ and $H$ are homomorphism indistinguishable over the class of graphs of pathwidth at most $k$ if and only if $G \equiv_{\text{tr}(\mathcal{P}W^k)} H$. In contrast, the class of graphs of cyclewidth at most $k$ is not closed under disjoint unions but satisfies the weaker assumptions of Lemma 5.7. Indeed, if a graph $F$ has less at most $k + 1$ vertices then it has cycle decomposition with a single bag and all graphs $F + nK_1$ for $n \in \mathbb{N}$ are also of cyclewidth at most $k$. Thus Lemmas 5.5 and 5.7 yield that two graph $G$ and $H$ are homomorphism indistinguishable over the class of graphs of cyclewidth at most $k$ if and only if $G \equiv_{\text{tr}(\mathcal{P}W^k)} H$.

This concludes the preparation for obtaining a system of matrix equations characterising homomorphism indistinguishability over graphs of bounded pathwidth and cyclewidth via Theorem 5.3. For later reference in Section 6.1, we denote the system of linear equations in Item 3 of Theorem 5.8 by $\mathcal{P}W^{k+1}(G, H)$.

Theorem 5.8. Let $k \geq 1$. For $n$-vertex graphs $G$ and $H$, the following are equivalent:

1. $G$ and $H$ are homomorphism indistinguishable over graphs of pathwidth at most $k$,
2. $G$ and $H$ are homomorphism indistinguishable over graphs of pathwidth at most $2n^{k+1}(k + 2)$ vertices,
3. there exists a pseudo-stochastic $X \in \mathbb{Q}^{V(H)^{k+1} \times V(G)^{k+1}}$ such that $XB_G = B_HX$ for all $B \in \mathcal{B}^k$.

Proof. In virtue of Lemma 5.6, we apply Theorem 5.3 to the involution monoid $\mathcal{P}W^k$ with generating set $\mathcal{B}^k$. Write $N := 2n^{k+1}(k + 2)$. Consider the following additional assertions:

4. $G$ and $H$ are homomorphism indistinguishable over graphs of pathwidth at most $k$ on at least $k + 1$ vertices,
5. $G$ and $H$ are homomorphism indistinguishable over graphs of pathwidth at most $k$ on at least $k + 1$ vertices and at most $N$ vertices.

By Theorem 5.3 and Lemma 5.5, Items 3 to 5 are equivalent. By containment of the respective graph classes, Item 1 implies Item 2, which implies Item 5. By Lemma 5.7, Items 4 and 5 are equivalent. This closes a cycle of implications. \hfill \Box

Analogously, we obtain the following theorem:

Theorem 5.9. Let $k \geq 1$. For $n$-vertex graphs $G$ and $H$, the following are equivalent:

1. $G$ and $H$ are homomorphism indistinguishable over the class of graphs of cyclewidth at most $k$,
2. G and H are homomorphism indistinguishable over the class of graphs of cyclewidth at most k on at most $2n^{2(k+1)}(k+2)$ vertices,
3. there exists an orthogonal $U \in \mathbb{R}^{V(H)^{k+1} \times V(G)^{k+1}}$ such that $UB_G = B_H U$ for all $B \in B^k$.

5.2 Treewidth: Glutinous Generation

The class of graphs of treewidth at most $k$ is generated by the same generators as $\mathcal{PW}^k$, cf. Lemma 5.6. However, instead of only considering series composition, we require the gluing product as well. To that end, recall the $k$-labelled version $I$ of the $(k,k)$-bilabelled graph $I$ from Example 2.7 and Figure 1a.

Definition 5.10. Let $k \geq 1$. Let $S \subseteq \mathcal{G}(k,k)$ be an involution monoid. The set $\mathcal{X} \subseteq \mathcal{G}(k)$ of graphs glutinously generated by $S$ is inductively defined as follows:
1. $1 \in \mathcal{X},$
2. $S \cdot X \in \mathcal{X}$ for $S \in S$ and $X \in \mathcal{X},$
3. $X \odot X' \in \mathcal{X}$ for $X, X' \in \mathcal{X}$.

For a class $\mathcal{R} \subseteq \mathcal{G}(k)$ where $k \geq 1$, write $\text{soe}(\mathcal{R}) := \{\text{soe } R \mid R \in \mathcal{R}\}$. For glutinously generated graph classes, the following general theorem follows from Theorems 3.8 and 3.11:

Theorem 5.11. Let $k \geq 1$. Let $S \subseteq \mathcal{G}(k,k)$ be an involution monoid generated by $B \subseteq S$. Let $\mathcal{X} \subseteq \mathcal{G}(k)$ be the class glutinously generated by $S$. Let $G$ and $H$ be $n$-vertex graphs. Suppose every graph in $B$ has at most $b \in \mathbb{N} \cup \{\infty\}$ vertices and let $N := (2n^k)^{\nu+1}b \in \mathbb{N} \cup \{\infty\}$. Then the following are equivalent:
1. $G$ and $H$ are homomorphism indistinguishable over $\text{soe}(\mathcal{X}),$
2. $G$ and $H$ are homomorphism indistinguishable over $\text{soe}(\mathcal{X}) \leq N,$
3. there exists a doubly-stochastic $X \in \mathcal{Q}^{V(H)^k \times V(G)^k}$ such that $XB_G = B_H X$ for all $B \in B$.

Equipped with this general theorem, we now turn to establishing that the class of graphs of bounded treewidth is subject to it.

Lemma 5.12. Let $k \geq 1$. Let $\mathcal{TW}^k \subseteq \mathcal{G}(k+1)$ denote the class which is glutinously generated by $\mathcal{PW}^k$. Then $\text{soe}(\mathcal{TW}^k)$ is the class of all graphs of treewidth at most $k$ on at least $k + 1$ vertices.

Proof. We first show that all graphs in $F = (F,u) \in \mathcal{TW}^k$ admit a tree decomposition $(T,\beta)$ of width at most $k$ such that there is $r \in V(T)$ with $\beta(r) = \{u_1,\ldots,u_{k+1}\}$. We call $r$ the root of the decomposition. The hypothesis clearly holds for $1$.

By structural induction, suppose that $F = S \cdot X$ for $X = (X,x) \in \mathcal{TW}^k$ of lesser complexity and $S = (S,u,v) \in \mathcal{PW}^k$. Let $(P,\beta)$ denote the path decomposition of $S$ with vertices $u,v \in V(P)$ as stipulated in Definition 5.4. Let $(T,\gamma)$ denote the tree decomposition of $X$ with root $r$ whose existence is guaranteed by the inductive hypothesis. Define a tree $Q$ by taking the disjoint union of $P$ and $T$ and identifying $v$ and $r$. Define $a : V(Q) \to 2^{V(F)}$ via

$$a(q) = \begin{cases} \beta(q), & \text{if } q \in V(P), \\ \gamma(q), & \text{if } q \in V(T). \end{cases}$$

Since $\beta(v) = \gamma(r)$ implicitly, the map $a$ is a tree decomposition of width at most $k$ of $F$. By construction, all labelled vertices in $F$ lie in the same bag.
If $F = X \odot X'$, a tree decomposition for $F$ can be constructed from the tree decompositions of $X$ and $X'$ by taking the disjoint union of the decomposition trees and identifying the roots.

Conversely, we consider graphs of treewidth at most $k$ with tree decompositions as in Lemma 2.9. By induction on the size of decomposition tree $T$, we show that for every graph $F$ with tree decomposition $(T, \beta)$ of width at most $k$ as in Lemma 2.9 and every $r \in V(T)$ and $u \in V(F)^{k+1}$ such that $\beta(r) = \{u_1, \ldots, u_{k+1}\}$, it holds that $F := (F, u) \in T\mathcal{W}^k$.

If $|V(T)| = 1$ then $T$ is a path. Clearly, $F' := (F, u, u) \in \mathcal{P}\mathcal{W}^k$ and $F = F' \mathcal{1} \in T\mathcal{W}^k$, as desired.

If $|V(T)| > 1$, distinguish two cases: First suppose that $r$ has only one neighbour $r'$. Define $T'$ as the tree obtained from $T$ by deleting $r$ and write $F'$ for the subgraph of $F$ induced by $\bigcup_{r' \in V(T)} \beta(r')$. Let $\beta'$ denote the restriction of $\beta$ to $V(T')$. By Lemma 2.9, there is a unique index $i \in [k+1]$ such that $u_i \in \beta(r) \setminus \beta(r')$. Write $x$ for the unique vertex in $\beta(r') \setminus \beta(r)$. Then the inductive hypothesis applies to $F', (T', \beta'), r'$ and $v := u_1 \ldots u_{i-1}u_{i+1} \ldots u_{k+1} \in V(F')^{k+1}$. Then

$$F = \prod_{i,j \in [k+1] \text{ s.t. } u_iu_j \in E(F)} A^{ij} \cdot j' : (F', v) \in T\mathcal{W}^k.$$

Finally, suppose that $r$ has multiple neighbours $r'_1, \ldots, r'_m$. For $i \in [m]$, write $T_i$ for the connected component of $r'_i$ in the forest obtained from $T$ by deleting $r'_1, \ldots, r'_{i-1}, r'_{i+1}, \ldots, r'_m$.

Write $F'_i$ for the subgraph of $F$ induced by $\bigcup_{r' \in V(T_i)} \beta(r')$ and $\beta'_i$ for the restriction of $\beta$ to $V(T'_i)$. Observe that $r$ is of degree one in all graphs $T_1, \ldots, T_m$. By the previous case, $(F'_i, u) \in T\mathcal{W}^k$. Clearly, $F = \bigcup_{i=1}^m (F'_i, u) \in T\mathcal{W}^k$.

This concludes the preparation for the proof of the main theorem of this section.

**Theorem 5.13.** Let $k \geq 1$. Let $G$ and $H$ be $n$-vertex graphs. Then the following are equivalent:

1. $G$ and $H$ are homomorphism indistinguishable over the class of graphs of treewidth at most $k$,
2. $G$ and $H$ are homomorphism indistinguishable over the class of graphs of treewidth at most $k$ on at most $(2n^{k+1})^{p^{k+1}+1}(k+2)$ vertices,
3. there exists a doubly-stochastic $X \in \mathcal{Q}^{|V(H)^{k+1} \times V(G)^{k+1}}$ such that $XB_G = BH_X$ for all $B \in \mathcal{B}^k$.

**Proof.** In virtue of Lemma 5.6, we apply Theorem 5.11 to $T\mathcal{W}^k$, which is glutinously generated by the involution monoid $\mathcal{P}\mathcal{W}^k$ with generating set $\mathcal{B}^k$. Write $N := (2n^{k+1})^{p^{k+1}+1}(k+2)$. Consider the following additional assertions:

4. $G$ and $H$ are homomorphism indistinguishable over the class of graphs of treewidth at most $k$ on at least $k+1$ vertices,
5. $G$ and $H$ are homomorphism indistinguishable over the class of graphs of treewidth at most $k$ on at least $k+1$ vertices and at most $N$ vertices.

By Theorem 5.11 and Lemma 5.12, Items 3 to 5 are equivalent. By containment of the respective graph classes, Item 1 implies Item 2, which implies Item 5. By Lemma 5.7, Items 1 and 4 are equivalent. This closes a cycle of implications.

### 5.3 Treedepth: Generation by an Involution Monoid and Closure under Gluing

In order to infer a system of equations characterising homomorphism indistinguishability over graphs of bounded treedepth, we consider another type of interaction between labelled
and bilabelled graphs. Let \( S \subseteq \mathcal{G}(k,k) \) be an involution monoid. Write \( S \mathcal{1} := \{ S \cdot 1 \mid S \in S \} \subseteq \mathcal{G}(k) \). This section is concerned with the case when \( S \mathcal{1} \) is gluing-closed.

**Definition 5.14.** Let \( k \geq 1 \). A set \( R \subseteq \mathcal{G}(k) \) is **gluing-closed** if \( R \odot R' \in R \) for all \( R, R' \in R \).

For example, the class of graphs which admit a coalgebra w.r.t. a fixed comonad is gluing-closed \([48, 14]\). Note that any glutinously generated graph class is gluing-closed. If \( S \mathcal{1} \) is gluing-closed then pseudo-stochastic solutions exist if and only if doubly-stochastic solutions exist:

**Theorem 5.15.** Let \( k \geq 1 \). Let \( S \subseteq \mathcal{G}(k,k) \) be an involution monoid generated by \( B \subseteq S \). Suppose that \( S \mathcal{1} \) is gluing-closed. Suppose that every graph in \( B \) has at most \( b \in \mathbb{N} \cup \{ \infty \} \) vertices and let \( N := 2n^k b \in \mathbb{N} \cup \{ \infty \} \). Then for graphs \( G \) and \( H \), the following are equivalent:

1. \( G \) and \( H \) are homomorphism indistinguishable over \( \text{soe}(S) \),
2. \( G \) and \( H \) are homomorphism indistinguishable over \( \text{soe}(S)_{< N} \),
3. there exists a pseudo-stochastic matrix \( X \in \mathbb{Q}^{V(H) \times V(G)} \) such that \( XB_G = B_H X \) for all \( B \in B \),
4. there exists a doubly-stochastic matrix \( X \in \mathbb{Q}^{V(H) \times V(G)} \) such that \( XB_G = B_H X \) for all \( B \in B \).

**Proof.** By Theorem 5.3, Items 1 to 3 are equivalent. Let \( \mathcal{X} \subseteq \mathcal{G}(k) \) denote the class glutinously generated by \( S \), cf. Definition 5.10. Since \( S \mathcal{1} \) is gluing-closed, it follows inductively that \( \mathcal{X} \subseteq S \mathcal{1} \). Conversely, \( S \mathcal{1} \subseteq \mathcal{X} \) since taking product of bilabelled graphs in \( S \) is one particular operation listed in Definition 5.10. Hence, \( S \mathcal{1} = \mathcal{X} \). Theorem 5.11 yields that Items 1 and 4 are equivalent.

In [23], it was shown that homomorphism indistinguishable over graphs of treedepth at most \( k \) corresponds to equivalence over the quantifier-rank-\( k \) fragment of first-order logic with counting quantifiers. We extend this characterisation by proposing a linear system of equations very similar to the one for bounded pathwidth.

**Definition 5.16.** Let \( k \geq 1 \). The set \( \mathcal{T}D^k \) is the set of all \( (k,k)\)-bilabelled graph \( F = (F, u, v) \) such that there exists a rooted forest \( \leq \) on \( F \) satisfying

1. every edge \( uv \in E(F) \) is such that \( u \leq v \) or \( v \leq u \),
2. for every leaf \( x \in V(F) \) of \( \leq \), the set \( \{ z \in V(F) \mid z \leq x \} \) has size \( k \),
3. \( u \) and \( v \) are paths from a root to a leaf i.e. \( u_1 < u_2 < \cdots < u_k \) and \( v_1 < v_2 < \cdots < v_k \).
4. the leaves \( u_k \) and \( v_k \) have the least number of common ancestors among all pairs of leaves of \( F \), i.e. writing

\[
\text{ca}(x, y) := |\{ z \in V(F) \mid z \leq x \land z \leq y \}|
\]

for \( x, y \in V(F) \), it holds that \( \text{ca}(x, y) \geq \text{ca}(u_k, v_k) \) for all pairs of leaves \( x, y \in V(F) \).

Items 1 and 2 ensure that the underlying unlabelled graph \( F \) is of treedepth at most \( k \), cf. Section 2.9. Item 3 guarantees that this property is preserved under series composition. The remaining Item 4 helps to establish that \( \mathcal{T}D^k \) is finitely generated.

**Lemma 5.17.** Let \( k \geq 1 \). \( \mathcal{T}D^k \) is an involution monoid.
Clearly, $TDB^k$ is closed under taking reverses and contains $I$. Given $F = (F, u, v)$ and $F' = (F', u', v')$ with rooted forest $\leq$ and $\leq'$, define a rooted forest $\leq''$ on $F \cdot F'$ by letting $x \leq'' y$ if $x, y \in V(F)$ and $x \leq y$ or if $x, y \in V(F')$ and $x \leq' y$. Since $v$ and $u'$ form paths from roots to leaves, this is a well-defined rooted forest. Also, in $\leq''$, $u$ and $v'$ are paths from roots to leaves.

It remains to check that Item 4 is satisfied. First observe that $ca(u_k, v_k), ca(u_k', v_k') \geq ca(u_k, v_k')$. Indeed, any common ancestor of $u_k$ and $v_k'$ must be an ancestor of $v_k$, which is identified with $u_k'$. Let $z$ denote the maximal vertex such that $z \leq'' u_k, v_k'$. Note that $z \leq'' v_k, u_k'$. Any leaf $x$ of $F$ satisfies $z \leq x$. Indeed, if $z$ and $x$ were incomparable w.r.t. then $ca(x, u_k) < ca(u_k, v_k')$ which contradicts the previous observation since $ca(x, u_k) \geq ca(u_k, v_k)$. The same argument applies to leaves of $F'$. It follows that $ca(x, y) \geq ca(u_k, v_k')$ for every pair of leaves $x, y$ in $F \cdot F'$.

The following Lemma 5.18 establishes another assumption of Theorem 5.15:

**Lemma 5.18.** Let $k \geq 1$. $TDB^k 1$ is gluing-closed.

**Proof.** Given $F = (F, u)$ and $F' = (F', u')$ with rooted forest $\leq$ and $\leq'$, define a rooted forest $\leq''$ on $F \bigcirc F'$ by letting $x \leq'' y$ if $x, y \in V(F)$ and $x \leq y$ or $x, y \in V(F')$ and $x \leq' y$. Since $u$ and $u'$ form paths from roots to leaves, this is a well-defined rooted forest. The other conditions in Definition 5.16 are easily verified.

It remains to define generators for $TDB^k$. The graphs featured in Lemma 5.19 are depicted by Figure 5.

**Lemma 5.19.** Let $k \geq 1$. Define the set $TDB^k$ as the set of the following $(k, k)$-bilabelled graphs:

- the identity graph $I = (I, (k), (k))$ with $V(I) = [k]$ and $E(I) = \emptyset$,
- the adjacency graphs $A^i = (A^i, (k), (k))$ with $V(A^i) = [k]$ and $E(A^i) = \{ij\}$ for $1 \leq i < j \leq k$,
- the join graphs $J^j = (J^j, (k), (1, \ldots, \ell, (\ell + 1)', \ldots, k'))$ with $V(J^j) = \{1, \ldots, k, (\ell + 1)', \ldots, k'\}$ and $E(J^j) = \emptyset$ for $0 \leq \ell < k$.

Then $TDB^k$ generates $TDB^k$.

**Proof.** Clearly, $TDB^k$ is closed under taking reverses and contains $I$. For the second assertions, let $F = (F, u, v) \in TDB^k$. Let $\leq$ denote a rooted forest for $F$. The proof is by induction on the number of leaves in $\leq$. 

---

Figure 5: The graphs in $TDB^k$ as defined in Lemma 5.19.
If there is only one leaf then $F$ is the product of the $A^j$ such that $1 \leq i \neq j \leq k$ and $u_i u_j \in E(F)$.

Now suppose that there are at least two leaves in $\leq$. Write $X$ for the set of all leaves $x$ of $\leq$ other than $u_k$ such that $ca(u_k, x)$ is maximal, i.e. such that $ca(u_k, x) \geq ca(u_k, y)$ for all leaves $y \neq u_k$. Let $x \in X$ be such that $ca(x, v_k)$ is minimal, i.e. $ca(x, v_k) \leq ca(y, v_k)$ for all $y \in X$. Write $D$ for the set of vertices $z \in V(F)$ such that $z \leq u_k$ and $z$ and $x$ are incomparable. Note that $D$ forms a chain in $\leq$.

Let $F'$ be the graph obtained from $F$ by deleting all vertices in $D$. The rooted forest $\leq$ restricts to a rooted forest $\leq'$ of $F'$. Let $F''$ be the subgraph of $F$ induced by the vertices $z \leq u_k$. Let $w \in V(F')^k$ be the tuple satisfying $w_1 < w_2 < \cdots < w_k = x$.

For Item 4, distinguish cases: If $ca(u_k, x) > ca(u_k, v_k)$ then there is a vertex $y$ such that $y$ is a common ancestor of $u_k$ and $x$ but $y$ is not an ancestor of $v_k$. This implies that every common ancestor of $v_k$ and $x$ is comparable with $y$ and hence $ca(x, v_k) = ca(u_k, v_k)$. Hence, $ca(a, b) \geq ca(u_k, v_k) = ca(x, v_k)$ for any pair of leaves $a, b$ in $F'$. However, if $ca(u_k, x) = ca(u_k, v_k)$ then all leaves $a$ of $F'$ are in fact in $X$ and the claim follows readily.

The bilabelled graphs $F' := (F', w, v)$ and $F'' := (F'', u, u)$ are in $T \mathcal{D}^k$ and have less leaves than $F$. The claim follows inductively, observing that $F = F'' \cdot J^\ell \cdot F'$ for $0 \leq \ell < k$ minimal such that $w_{\ell+1} \notin \{ u_1, \ldots, u_k \}$.

The above observations yield the following Theorem 5.20, which implies one of the equivalences of Theorem 1.2:

**Theorem 5.20.** Let $k \geq 1$. Let $G$ and $H$ be $n$-vertex graphs. Then the following are equivalent:

1. $G$ and $H$ are homomorphism indistinguishable over the class of graphs of treedepth at most $k$,
2. $G$ and $H$ are homomorphism indistinguishable over the class of graphs of treedepth at most $k$ on at most $4kn^k$ vertices,
3. there exists a doubly-stochastic $X \in \mathbb{Q}^{V(H)^k \times V(G)^k}$ such that $XB_G = B_H X$ for all $B \in T \mathcal{D}^k$ and
4. there exists a pseudo-doubly-stochastic $X \in \mathbb{Q}^{V(H)^k \times V(G)^k}$ such that $XB_G = B_H X$ for all $B \in T \mathcal{D}^k$.

**Proof.** In virtue of Lemmas 5.17 to 5.19, we apply Theorem 5.15 to the gluing-closed $T \mathcal{D}^k 1$ and the generating set $T \mathcal{D}^k$. Write $N := 4kn^k$. Consider the following additional assertions:

5. $G$ and $H$ are homomorphism indistinguishable over the class of graphs which admit a rooted forest satisfying Items 1 and 2 of Definition 5.16,
6. $G$ and $H$ are homomorphism indistinguishable over the class of graphs on at most $N$ vertices which admit a rooted forest satisfying Items 1 and 2 of Definition 5.16.

Observe that for every graph $F$ admitting a rooted forest satisfying Items 1 and 2 of Definition 5.16 one can pick $u, v \in V(F)^k$ such that Items 3 and 4 of Definition 5.16 are satisfied as well. Hence, by Theorem 5.15, Items 3 to 6 are equivalent. By containment of the respective graph classes, Item 1 implies Item 2, which implies Item 6.

By adding isolated vertices, any graph of treedepth at most $k$ can be turned into a graph with rooted forest satisfying Items 1 and 2 of Definition 5.16. Thus, by Lemma 5.7, Items 1 and 5 are equivalent. This closes a cycle of implications.

**5.4 Bounded Degree Trees: Inner-Product Compatibility**

In this final subsection, we turn to a class of labelled graphs which is endowed with less algebraic structure than the graph classes considered above. The class of suitably labelled
trees of bounded degree trees is inner-product compatible. This is the most general property which ensures amenability to our approach.

**Definition 5.21.** Let \( k \geq 1 \). A set \( \mathcal{R} \subseteq \mathcal{G}(k) \) is inner-product compatible if for all \( R, R' \in \mathcal{R} \) there exists \( R'' \in \mathcal{R} \) such that \( \langle R, R' \rangle = \text{soe}(R'') \).

Since \( \langle R, R' \rangle = \text{soe}(R \odot R') \) for all \( R, R' \in \mathcal{G}(k) \), all gluing-closed families are also inner-product compatible. Similarly, if \( \mathcal{R} = S1 \) for some involution monoid \( S \) then \( \mathcal{R} \) is inner-product compatible. This holds since \( \langle S_1, S_2 \rangle = \langle 1, S_1^*S_2^* \rangle = \text{soe}(S_1^*S_2^*) \) for \( S_1, S_2 \in S \).

**Theorem 5.22.** Let \( k \geq 1 \). Let \( \mathcal{R} \subseteq \mathcal{G}(k) \) be inner-product compatible containing \( 1 \). Then for graphs \( G \) and \( H \), the following are equivalent:

1. \( G \) and \( H \) are homomorphism indistinguishable over \( \text{soe}(\mathcal{R}) \),
2. there exists a pseudo-stochastic \( X \in Q^{V(H)^k \times V(G)^k} \) such that \( XR_G = R_H \) for all \( R \in \mathcal{R} \).

**Proof.** The backward direction is immediate. For the forward direction, consider the spaces \( Q R_G \) and \( Q R_H \) spanned by the \( R_G \) and \( R_H \) respectively for \( R \in \mathcal{R} \). By inner-product compatibility of \( \mathcal{R} \), for any \( R, R' \in \mathcal{R} \) there exists \( R'' \in \mathcal{R} \) such that \( \langle R_G, R_G' \rangle = \text{soe}(R''_G) = \text{soe}(R''_H) = \langle R_H, R_H' \rangle \). By Lemma 2.1, there exists an orthogonal map \( U : Q R_G \to Q R_H \) such that \( UR_G = R_H \) for all \( R \in \mathcal{R} \). In particular, \( U1_G = 1_H \) and \( U^T1_H = 1_G \). Hence, \( U \) is pseudo-stochastic.

Define \( X : Q^{V(G)^k} \to Q^{V(H)^k} \) as the map coinciding with \( U \) on \( Q R_G \) and annihilating \( (QR_G)^\perp \). Then \( XR_G = UR_G = R_H \) for all \( R \in \mathcal{R} \). Furthermore, for all \( v \in QR_G \), \( \langle v, X^T1_H \rangle = \langle Uv, 1_H \rangle = \langle v, U^T1_H \rangle = \langle v, 1_G \rangle \). For all \( v \in (QR_G)^\perp \), \( \langle v, X^T1_H \rangle = 0 = \langle v, 1_G \rangle \). Hence, \( X^T1_H = 1_G \).

As noted above, all graph classes considered in previous sections enjoy properties stronger than inner-product compatibility. The class of bounded degree trees however does not satisfy any of the aforementioned properties.

**Example 5.23.** A d-ary tree is a tree whose vertices have degree at most \( d + 1 \). For \( d \geq 1 \), the family of 1-labelled d-ary trees \( T^d \) with label at a vertex of degree at most one is inner-product compatible.

The set \( T^d \) is closed under guarded Schur products, i.e. the d-ary operation \( \odot^d \) defined as \( \odot^d(R^1, \ldots, R^d) := A \cdot (R^1 \odot \cdots \odot R^d) \) for \( R^1, \ldots, R^d \in T^d \). This operation induces a d-ary multilinear map on \( Q^{V(G)} \) for every graph \( G \), i.e. \( \odot^d_G(u_1, \ldots, u_d) := A_G(u_1 \odot \cdots \odot u_d) \) for \( u_1, \ldots, u_d \in Q^{V(G)} \).

**Theorem 5.24.** Let \( d \geq 1 \). For graphs \( G \) and \( H \), the following are equivalent:

1. \( G \) and \( H \) are homomorphism indistinguishable over the class of d-ary trees,
2. there exists a pseudo-stochastic matrix \( X \in Q^{V(H) \times V(G)} \) such that \( XT_G = T_H \) for all \( T \in T^d \),
3. there exists a pseudo-stochastic matrix \( X \in Q^{V(H) \times V(G)} \) such that \( X \) preserves \( \odot^d \) on \( Q T^d_G \), i.e. \( X(\odot^d_G(u_1, \ldots, u_d)) = \odot^d_H(Xu_1, \ldots, Xu_d) \) for all \( u_1, \ldots, u_d \in Q T^d_G \).

**Proof.** That Items 1 and 2 are equivalent follows directly from Theorem 5.22.
Assuming Item 2, let $X \in \mathbb{Q}^{V(H) \times V(G)}$ be pseudo-stochastic such that $X_T^G = T_H$ for all $T \in \mathcal{T}_d$. Then for all $T^1, \ldots, T^d \in \mathcal{T}_d$, $X(\otimes^d(T^1_G, \ldots, T^d_G)) = (\otimes^d(T^1, \ldots, T^d))_H = \otimes^d_H(X_T^G, \ldots, X_T^H)$.

Finally, Item 1 follows inductively from Item 3 observing that every $1 \neq T \in \mathcal{T}_d$ can be written as $T = \otimes^d(S^1, \ldots, S^d)$ for some $S^1, \ldots, S^d \in \mathcal{T}_d$ of lower depth.

**6 Comparison to Known Systems of Equations**

Towards understanding the power and limitations of convex optimisation approaches to the graph isomorphism problem, the level-$k$ Sherali–Adams relaxation of $F_{\text{iso}}^k(G, H)$, denoted by $F_{\text{iso}}^k(G, H)$, was studied in [4]. The system $L_{\text{iso}}^{k+1}(G, H)$ is another closely related system of interest [26], cf. Section 2.7. Every solution for $F_{\text{iso}}^k(G, H)$ yields a solution to $L_{\text{iso}}^{k+1}(G, H)$, and every solution to $L_{\text{iso}}^{k+1}(G, H)$ yields a solution to $F_{\text{iso}}^k(G, H)$ [26]. In [4, 26], it was shown that the system $L_{\text{iso}}^{k+1}(G, H)$ has a non-negative solution if and only if $G$ and $H$ are indistinguishable by the $k$-dimensional Weisfeiler–Leman algorithm. Following the results of [17, 16], the feasibility of $L_{\text{iso}}^{k+1}(G, H)$ is thus equivalent to homomorphism indistinguishability over the class of graphs of treewidth at most $k$.

The goal of this section is two-fold: First, we confirm a conjecture of [16] concerning $L_{\text{iso}}^{k+1}(G, H)$ without non-negativity constraints. Secondly, we establish that an ordered variant of $L_{\text{iso}}^{k}(G, H)$ corresponds to homomorphism indistinguishability over the class of graphs of treewidth at most $k$.

**6.1 Sherali–Adams without Non-Negativity Constraints**

Dropping non-negativity constraints in $F_{\text{iso}}^k(G, H)$ yields a system of linear equations whose feasibility characterises homomorphism indistinguishability over the class of paths [16]. It was conjectured ibidem that dropping non-negativity constraints in $L_{\text{iso}}^{k+1}(G, H)$ analogously characterises homomorphism indistinguishability over graphs of pathwidth at most $k$. One of the conjectured implications was already shown in [16]: the existence of a rational solution to $L_{\text{iso}}^{k+1}(G, H)$ implies homomorphism indistinguishability over graphs of pathwidth at most $k$.

We resolve the aforementioned conjecture by showing that the system of equations $L_{\text{iso}}^{k+1}(G, H)$ is feasible if and only if the system of equations $PW^{k+1}(G, H)$ stated in Theorem 5.8 is feasible. The proof repeatedly makes use of the observation that the equations in $L_{\text{iso}}^{k+1}(G, H)$ can be viewed as equations in $PW^{k+1}(G, H)$ where certain $(k + 1, k + 1)$-bigraphs model the continuity and compatibility equations of $L_{\text{iso}}^{k+1}(G, H)$. Building on Theorem 5.8, we obtain the following Theorem 6.1 implying Theorem 1.1.

**Theorem 6.1.** For $k \geq 1$ and graphs $G$ and $H$, the following are equivalent:

1. $G$ and $H$ are homomorphism indistinguishable over the class of graphs of pathwidth at most $k$,
2. the system of equations $PW^{k+1}(G, H)$ has a rational solution,
3. the system of equations $L_{\text{iso}}^{k+1}(G, H)$ has a rational solution.

**Proof.** Given Theorem 5.8, it suffices to show that Items 2 and 3 are equivalent. First consider the forward implication. Since $X$ already denotes the solution to the system $PW^{k+1}(G, H)$ in Theorem 5.8, the variables of $L_{\text{iso}}^{k+1}(G, H)$ will be denoted by $Y_\pi$ instead of $X_\pi$. Let $\mathcal{S}_k$ denote
the symmetric group acting on $k$ letters. For a vector $v \in V(G)^k$ and $\sigma \in \mathfrak{S}_k$, write $\sigma(v)$ for the vector $v_{\sigma(1)} \cdots v_{\sigma(k)}$.

Claim 8. Let $k \geq 2$. Let $X$ denote a solution to $\text{PW}^{k+1}(G, H)$. Then $X(\sigma(w), \sigma(v)) = X(w, v)$ for all $v \in V(G)^{k+1}$, $w \in V(H)^{k+1}$, and $\sigma \in \mathfrak{S}_{k+1}$.

Proof of Claim. Recall the swap graph $S^{ij}$ from Lemma 5.6. Let $\tau \in \mathfrak{S}_{k+1}$ denote the transposition $(ii)$. The equation $S^{ij}_w X = X S^{ij}_w$ of $\text{PW}^{k+1}(G, H)$ is equivalent to $X(\tau(w), v) = X(w, \tau(v))$ for all $v \in V(G)^{k+1}$ and $w \in V(H)^{k+1}$. Hence, writing $\sigma \in \mathfrak{S}_{k+1}$ as product of transpositions $\sigma = \tau_1 \cdots \tau_r$, it holds that $X(\sigma(w), v) = X(\tau_1 \cdots \tau_r(w), v) = X(\tau_2 \cdots \tau_r(w), \tau_1(v)) = \cdots = X(w, \tau_1(v)) = X(w, \sigma^{-1}(v))$, as desired.

The following Claim 9 shows that Equations (L1) and (L2) hold.

Claim 9. Let $\ell \geq 2$. Let $X$ denote a solution to $\text{PW}^\ell(G, H)$. Then
\[
\sum_{v' \in V(G)} X(ww, vv') = \sum_{w' \in V(H)} X(ww', vv) =: \bar{X}(w, v)
\]
for all $v \in V(G)^\ell$, $w \in V(H)^\ell$, $v \in V(G)$, and $w \in V(H)$. Furthermore, the matrix $\bar{X}$ defined above is a solution to $\text{PW}^{\ell-1}(G, H)$.

Proof of Claim. The first equality in Equation (7) is equivalent to $J^i_w X = X J^i_G$, where $J^i$ denotes the forgetting graph from Lemma 5.6. Clearly, $\bar{X}$ is pseudo-stochastic. It remains to argue that $\bar{X}$ is a solution to $\text{PW}^{\ell-1}(G, H)$.

Let $J$ denote the $(1, 1)$-bilabelled edgeless 2-vertex graphs whose labels reside on distinct vertices. For every $B \in B^{\ell-2}$, the $(\ell, \ell)$-bilabelled graph $B \otimes J$ can be written as series product of graphs in $B^{\ell-2}$. Then for arbitrary $w \in V(H)$ and $v \in V(G)$
\[
(\bar{X}B_G)(w, v) = (X(B_G \otimes J_G))(ww, vv) = \left((B_H \otimes J_H)X\right)(ww, vv) = (B_G \bar{X})(w, v).
\]
This concludes the proof.

It remains to consider Equation (L3):

Claim 10. Let $\ell \geq 2$. Let $X$ be a solution to $\text{PW}^\ell(G, H)$. Let $\pi = (w, v) \subseteq V(H) \times V(G)$ be arbitrarily ordered of length $\ell$. Suppose that $\pi$ is not a partial isomorphism. Then $X(w, v) = 0$.

Proof of Claim. If $\pi$ is not a partial isomorphism then there exists $i \neq j \in [\ell]$ such that wlog $\{v_i, v_j\} \in E(G)$ but $\{w_i, w_j\} \notin E(H)$. This implies that $A_G^{ij}(v, v) = 1$ while $A_H^{ij}(w, w) = 0$. Moreover, $X(w, v)A_G^{ij}(v, v) = (XA_G^{i:j})(w, v) = (A_H^{i:j}X)(w, v) = A_H^{i:j}(w, w)X(w, v)$ since in- and out-labels coincide. Hence, $X(w, v) = 0$.

This concludes the preparations for proving that Item 3 implies Item 2. Let $X$ denote a solution of $\text{PW}^{k+1}(G, H)$. Construct via Claim 9 solutions $X^\ell$ of $\text{PW}^\ell(G, H)$ for $1 \leq \ell \leq k + 1$ satisfying Equation (7). For $\pi = (w, v) \subseteq V(H) \times V(G)$ define $Y_{\pi} = X^{|\pi|}(w, v)$. By Claim 8, the entries of $X$ do not depend on the ordering of the indices. Thus, $Y$ is well-defined. Let finally $Y_{\emptyset} = 1$. Then Equations (L1) and (L2) hold by Equation (7). Equation (L3) holds by Claim 10, and Equation (L4) by definition. Thus, Item 3 holds.
That Item 2 implies Item 1 was shown by [16]. For the sake of completeness, we prove that Item 2 implies Item 3. To that end, let \( Y \) denote a solution of \( L_{iso}^{k+1}(G, H) \). Define a candidate solution \( X \) for \( PW^{k+1}(G, H) \) by letting \( X(w, v) := Y(w, v) \). By repeatedly applying Equations (L1) and (L2) it follows that \( X \) is pseudo-stochastic. For commutation with the graphs from Lemma 5.6, four cases have to be considered: Let \( v \in V(G)^{k+1}, w \in V(H)^{k+1} \).

Recall Equation (L3).

1. Let \( A^{ij} \) be an adjacency graph. If \( (w, v) \) is a partial isomorphism then \( A^{ij}_G(v, v) = A^{ij}_H(w, w) \) and thus \( X \) and \( A^{ij} \) commute. If \( (w, v) \) is not a partial isomorphism then \( X(w, v) = 0 \) and the tensors commute as well.
2. Let \( I^{ij} \) be an identification graph. If \( (w, v) \) is a partial isomorphism then \( v_i = v_j \) if and only if \( w_i = w_j \) and thus \( I^{ij}_G(v, v) = I^{ij}_H(w, w) \). Hence, \( X \) and \( I^{ij} \) commute. If \( (w, v) \) is not a partial isomorphism then \( X(w, v) = 0 \) and the tensors commute as well.
3. Let \( J^i \) be a forgetting graph. To ease notation, suppose \( \ell = k + 1 \). Then by Equations (L1) and (L2), writing \( v = v_1 \ldots v_{k+1} \), and \( w = w_1 \ldots w_k \),

\[
(XJ_G^{k+1})(w, v) = \sum_{x \in V(G)} X(w, v_1 \ldots v_k x) = \sum_{x \in V(G)} Y(\{(w_1, v_1), \ldots, (w_{k+1}, x)\})
\]

\[
(\text{L1}) = Y(\{(w_1, v_1), \ldots, (w_k, v_k)\}) = \sum_{y \in V(H)} Y(\{(w_1, v_1), \ldots, (w_k, v_k), (y, v_{k+1})\})
\]

\[
(\text{L2}) = \sum_{y \in V(H)} X(w_1 \ldots w_k y, v) = (J_H^{k+1} X)(w, v).
\]

4. For the swap graphs, the statement follows as in Claim 8 since the value of \( X \) does not depend on the ordering of the indices. \(\square\)

As a corollary, we show that \( PW^{k+1}(G, H) \) has a non-negative rational solution if and only if \( L_{iso}^{k+1}(G, H) \) has a non-negative rational solution. Consequently, the system of linear equations \( PW^{k+1}(G, H) \) has a non-negative rational solution if and only if \( G \) and \( H \) are homomorphism indistinguishable over graphs of treewidth at most \( k \). Hence, the systems of equations \( PW^{k+1}(G, H) \), for \( k \in \mathbb{N} \), form an alternative well-motivated hierarchy of linear programming relaxations of the graph isomorphism problem. Examining the proof of Theorem 6.1, we obtain the following corollary.

**Corollary 6.2.** Let \( k \geq 1 \). Let \( G \) and \( H \) be two graphs. Then the following are equivalent:

1. \( G \) and \( H \) are homomorphism indistinguishable over the class of graphs of treewidth at most \( k \),
2. \( PW^{k+1}(G, H) \) has a non-negative rational solution,
3. \( L_{iso}^{k+1}(G, H) \) has a non-negative rational solution.

**Proof.** The equivalence of Items 1 and 2 follows from Theorem 5.13. A combination of results of [4, 26] and [17, 16] yields that Items 1 and 3 are equivalent. For a self-contained argument, observe that the transformations devised in Claims 8 and 9 preserve non-negativity. \(\square\)

### 6.2 An Ordered Variant of Sherali–Adams and Bounded Treedepth

In this section, we reinterpret the systems of equations in Theorem 5.20 as ordered variant of \( L_{iso}^{k+1}(G, H) \). In contrast to \( L_{iso}^{k+1}(G, H) \), it is equivalent for this system to have an arbitrary rational solution and a non-negative rational solution.
Let $k \geq 1$. For graphs $G$ and $H$, consider the following system of equations $TD^k(G, H)$ with variables $X(w, v)$ for every pair of tuples $w \in V(H)^\ell$ and $v \in V(G)^\ell$ for $0 \leq \ell \leq k$. A length-$\ell$ pair $(w, v)$ is said to be a \textit{partial strong homomorphisms} if $v_i v_j \in E(G) \iff w_i w_j \in E(H)$ for all $i, j \in [\ell]$.

| $TD^k(G, H)$ |
|----------------|
| $\sum_{v' \in V(G)} X(wv, vv') = X(w, v)$ for all $w \in V(H)$ and $v \in V(G)^\ell$, $w \in V(H)^\ell$ where $0 \leq \ell < k$. (TD1) |
| $\sum_{w' \in V(H)} X(ww', vv) = X(w, v)$ for all $v \in V(G)$ and $v \in V(G)^\ell$, $w \in V(H)^\ell$ where $0 \leq \ell < k$. (TD2) |
| $X(((), ()) = 1$ |
| $X(w, v) = 0$ whenever $(w, v) \in V(H)^\ell \times V(G)^\ell$ for $1 \leq \ell \leq k$ is not a partial strong homomorphism (TD4) |

The main result of this section is the following:

\textbf{Theorem 1.2.} For every $k \geq 1$, the following are equivalent for $n$-vertex graphs $G$ and $H$:

1. $G$ and $H$ are homomorphism indistinguishable over the graphs of treedepth at most $k$,
2. the linear systems of equations $TD^k(G, H)$ has a non-negative rational solution,
3. the linear systems of equations $TD^k(G, H)$ has a rational solution.

\textbf{Proof.} Given Theorem 5.20, it suffices to show that $TD^k(G, H)$ has a (non-negative) rational solution if and only if there is a (doubly-stochastic) pseudo-stochastic matrix $X$ such that $XB_G = B_H X$ for all $B \in TD^k$.

We first consider the backward implication. Given $X \in Q^{V(H)^k \times V(G)^k}$ such that $XB_G = B_H X$ for all $B \in TD^k$, observe that if $(w, v) \in V(H)^k \times V(G)^k$ is not a partial strong homomorphism then $X(w, v) = 0$. Indeed, in this case there exist $1 \leq i \neq j \leq k$ such that $w_i w_j \in E(G) \neq v_i v_j \in E(F)$. In particular, precisely one of $A_G^{ij}(v, v)$ and $A_H^{ij}(w, w)$ is zero. Then $A_H^{ij}(w, w) X(w, v) = X(w, v) A_G^{ij}(v, v)$ implies that $X(w, v) = 0$. Hence Equation (TD4) holds for $\ell = k$. With this observation at hand, define a solution to $TD^k(G, H)$ by invoking the following claim whose proof is analogous to the proof of Claim 9.

\textbf{Claim 11.} Let $k \geq 1$. If $X \in Q^{V(H)^{k+1} \times V(G)^{k+1}}$ is doubly-stochastic and such that $XB_G = B_H X$ for all $B \in TD^k$ then

$$\sum_{v' \in V(G)} X(wv, vv') = \sum_{w' \in V(H)} X(ww', vv) =: \tilde{X}(w, v)$$

for all $v \in V(G)$, $w \in V(H)$, and $v \in V(G)^k$, $w \in V(H)^k$. Furthermore, $\tilde{X} \in Q^{V(H)^k \times V(G)^k}$ is doubly-stochastic and such that $X \tilde{B}_G = B_H \tilde{X}$ for all $B \in TD^k$.

A solution to $TD^k(G, H)$ can now be defined inductively invoking Claim 11. Equations (TD1) and (TD2) are immediate from Claim 11. Equation (TD3) follows since double stochasticity is preserved throughout the induction. Equation (TD4) follows as observed initially.

Conversely, define a matrix $X \in Q^{V(H)^k \times V(G)^k}$ by extracting the values on $V(H)^k \times V(G)^k$ from a solution to $TD^k(G, H)$. By Equations (TD1) to (TD3), $X$ is pseudo-stochastic. It remains to consider commutation with the graphs from Lemma 5.19: Let $(w, v) \in V(H)^k \times V(G)^k$. 

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• If \((w, v)\) is a partial strong homomorphism then 
  \[ A_G^{ij}(w, v) = A_H^{ij}(w, w) \]
  \(\forall 1 \leq i \neq j \leq k\). Hence, 
  \[ A_H^{ij}(w, w)X(w, v) = X(v, v)A_G^{ij}(v, v) \]
  If \((w, v)\) is not a partial strong homomorphism then the same assertions follows readily from Equation (TD4).
• For \(0 \leq \ell < k\), by repeatedly applying Equations (TD1) and (TD2),
  \[
  (XJ_G^\ell)(w, v) = \sum_{v_{\ell+1}, \ldots, v_k \in V(G)} X(w, v_1 \ldots v_{\ell+1} \ldots v_k) = X(w_1 \ldots w_\ell, v_1 \ldots v_\ell),
  \]
  which in turn is equal to \((J_H^\ell X)(w, v)\). \(\square\)

7 Homomorphism Counts from Trees Cannot Be Inferred from Homomorphism Counts from Bounded Degree Trees

In this section, we utilise the techniques introduced in Section 5.4 to show that homomorphism indistinguishability over bounded degree trees is a strictly finer relation than homomorphism indistinguishability over all trees. As a consequence [12, 17], it is not possible to simulate the 1-dimensional Weisfeiler–Leman algorithm (also known as Colour Refinement) by counting homomorphisms from trees of any fixed bounded degree.

**Theorem 1.3.** For every integer \(d \geq 1\), there exist graphs \(G\) and \(H\) such that \(G\) and \(H\) are homomorphism indistinguishable over trees of degree at most \(d\), but \(G\) and \(H\) are not homomorphism indistinguishable over the class of all trees.

After this work was first presented, Roberson [49] showed the following stronger statement: For every \(d\), the class of trees of degree at most \(d\) is homomorphism distinguishing closed, i.e. for every graph \(F\) not from this class there exists graphs \(G\) and \(H\) which are homomorphism indistinguishable over trees of degree at most \(d\) but \(\text{hom}(F, G) \neq \text{hom}(F, H)\). Roberson’s proof intricately exploits combinatorial properties of CFI graphs [12]. Despite being weaker, our Theorem 1.3 is proven by introducing a novel construction of the graphs \(G\) and \(H\) which is not akin to the ubiquitous CFI construction.

Towards Theorem 1.3, we first show that the nested subspaces \(Q^T_G^d\) for \(d \geq 1\) by which the systems of equations in Theorem 5.24 are parametrised form a strict chain.

**Theorem 7.1.** For every integer \(d \geq 1\), there exists a graph \(H\) such that \(Q^T_H^d \neq Q^T_H^{d+1}\).

7.1 Proof of Theorem 7.1

The graph in Theorem 7.1 will be constructed from a vector of distinct integers. As a first step, a multigraph adjacency matrix is constructed in Lemma 7.3. This multigraph is then turned into a simple graph in Lemma 7.4 yielding the object with the desired properties (Lemma 7.5).

All constructions in this section take place in \(\mathbb{Q}^n\) for some integer \(n\) to be fixed. Let \(1 = 1_n\) denote the all-ones vector in this space. Recall from Section 2.1 that \(\odot\) denotes the vector Schur product. The following Lemma 7.2 follows by applying arguments similar to Lemma 2.1 and Fact 2.2.

**Lemma 7.2 (Principal Sequence).** Let \(n \geq 3\). Let \(a \in \mathbb{N}^n\) be a vector with distinct entries. Let

\[
  u_0 := 1 + a, \quad u_1 := 1 - a, \quad u_i := a^\odot i, \quad (8)
\]
for $2 \leq i \leq n - 1$. Define the principal sequence of $a$ as the sequence of the vectors

$$v_0 := u_0, \quad v_{i+1} := u_{i+1} - \sum_{j=0}^{i} \frac{\langle u_{i+1}, v_j \rangle}{\langle v_j, v_j \rangle} v_j$$

(9)

for $0 \leq i \leq n - 2$. Then

1. for $1 \leq i \leq n - 1$, the vectors $v_0, \ldots, v_i$ span the same subspace as $u_0, \ldots, u_i$,
2. the vectors $v_0, \ldots, v_{n-1}$ are mutually orthogonal,
3. the vectors $v_0, \ldots, v_{n-1}$ lie in $\mathbb{Q}^n$.

**Lemma 7.3.** Let $d \geq 1$ and $n > d + 1$. Given a vector $a \in \mathbb{N}^n$ with distinct entries, there exists a symmetric matrix $M \in \mathbb{N}^{n \times n}$ satisfying the following properties:

1. if $x_1, \ldots, x_d \in S_{\leq 1}$ then $x_1 \odot \cdots \odot x_d \in S_{\leq d}$,
2. if $x_1, \ldots, x_d \in S_{\leq 1}$ then $M(x_1 \odot \cdots \odot x_d) \in S_{\leq 1}$,
3. it holds that $M((M1)_{\odot(d+1)}) \notin S_{\leq d}$.

Here, $S_{\leq 1}$ denotes the subspace of $\mathbb{Q}^n$ spanned by the first $i + 1$ vectors of the principal sequence of $a$.

**Proof.** Construct invoking Lemma 7.2 the principal sequence $v_0, \ldots, v_{n-1} \in \mathbb{Q}^n$ of the vector $a$. Define the matrix $M \in \mathbb{N}^{n \times n}$ as follows. First let

$$M_\lambda := \lambda v_0 v_0^T + v_1 v_1^T + v_{d+1} v_{d+1}^T$$

(10)

where $\lambda \in \mathbb{N}$ is chosen to be a sufficiently large positive integer such that $M_\lambda$ has only positive entries, and $1$ is not an eigenvector of $M_\lambda$. This is possible because the matrix $v_0 v_0^T$ defined via $v_0 = a + 1$ has only positive entries, and $1$ is none of its eigenvectors. Define $M \in \mathbb{N}^{n \times n}$ as the matrix obtained from $M_\lambda$ for appropriate $\lambda$ by clearing all denominators, i.e. by multiplying with a sufficiently large $\lambda' \in \mathbb{N}$. Observe that $M$ is a symmetric matrix with positive integral entries. Moreover, the rank of $M$ is exactly 3.

Having defined $M$, it remains to verify the assertions. For Item 1, if $x_1, \ldots, x_d \in S_{\leq 1}$ then each of these vectors is a linear combination of $1$ and $a$. By bilinearity of the Schur product, the product $x_1 \odot \cdots \odot x_d$ must be a linear combination of the vectors $1, \ldots, a^{\odot d}$. Hence, $x_1 \odot \cdots \odot x_d \in S_{\leq d}$.

For Item 2, if $x_1, \ldots, x_d \in S_{\leq 1}$ then $x_1 \odot \cdots \odot x_d \in S_{\leq d}$. Since $M$ annihilates all vectors in $S_{\leq d}$ except for those in $S_{\leq 1}$, it holds that $M(x_1 \odot \cdots \odot x_d) \in S_{\leq 1}$.

For Item 3, write $M1 = a1 + \beta a$, for some $a, \beta \in \mathbb{Q}$. It holds that $\beta \neq 0$ because $1$ is not an eigenvalue of $M$ by construction. The resulting expansion of $(M1)_{\odot(d+1)}$ is a linear combination of the vectors $1, a, a \odot a, \ldots, a^{(d+1)}$. Moreover, in this binomial expansion, the coefficient of $a^{(d+1)}$ is $\beta^{d+1}$, which is non-zero. The remaining terms in this expansion lie in $S_{\leq d}$ already. Hence, $(M1)_{\odot(d+1)} \notin S_{\leq d}$. Furthermore, the coefficient of $a^{(d+1)}$ in $M(M1)_{\odot(d+1)}$ is also non-zero because $v_{d+1}$ is a non-vanishing eigenvector of $M$. Hence, $M(M1)_{\odot(d+1)} \notin S_{\leq d}$. \qed

Since the matrix $M$ is symmetric and has non-negative integral entries, it can be thought of as the adjacency matrix of a multigraph, i.e. an undirected graph with multiedges. The objective is to construct a simple undirected graph $H$ such that the eigensystem of the adjacency matrix $H$ is closely related to that of $M$. 
Lemma 7.4. For every symmetric matrix \(M \in \mathbb{N}^{n \times n}\), there exists an integer \(N\) and a graph \(H\) with vertex set \([n] \times [N]\) such that \(A_H x = (Mz) \otimes 1_N\) for all \(z \in \mathbb{Q}^n\) with \(\tilde{z} := z \otimes 1_N\).

Proof. The graph \(H\) is constructed from \(M\) as follows. Fix a large positive integer \(N\) such that it is divisible by every entry of \(M\). The vertex set of \(H\) is defined to be \([n] \times [N]\). The edge set of \(H\) is determined as follows.

- For each \(u \in [n]\), the graph induced on the vertex subset \([v] \times [N]\) is set to be an arbitrary regular graph of degree \(M_{uu}\).
- For distinct \(u, v \in [n]\), the bipartite graph induced between the vertex subsets \([u] \times [N]\) and \([v] \times [N]\) is set to be an arbitrary bi-regular graph with left and right degree \(M_{uv} = M_{vu}\).

The generous choice of \(N\) ensures that the arbitrary regular and bi-regular graphs stipulated above exist, cf. e.g. [29, Lemma 3.2]. Write \(A := A_H\) for the adjacency matrix of \(H\). The entry of \(A_H(z \otimes 1_N)\) corresponding to a vertex \((u, j) \in V(H)\) is equal to

\[
\sum_{(u', j') \in V(H)} A_{(u,j),(u', j')}(z \otimes 1_N)(u', j') = \sum_{u' \in [n]} \sum_{j' \in [N]} A_{(u,j),(u', j')}(z \otimes 1_N)(u', j')
= \sum_{u' \in [n]} \sum_{j' \in [N]} A_{(u,j),(u', j')} z_{u'}
= \sum_{u' \in [n]} z_{u'} \sum_{j' \in [N]} A_{(u,j),(u', j')}
= \sum_{u' \in [n]} M_{uu'} z_{u'}
= (Mz)_{u}
\]

which does not depend on \(j\). \(\square\)

Let \(S^{d+1} := A \cdot (A1)^{\otimes d+1}\) denote the labelled star graph with label at one of its \(d + 2\) leaves. Clearly, \(S^{d+1} \in T^{d+1} \setminus T^d\).

Lemma 7.5. Let \(d \geq 1\) and \(n > d + 1\). Let \(a \in \mathbb{N}^n\) be a vector with distinct entries and principal sequence \((v_0, \ldots, v_{n-1})\). Let \(H\) denote the graph constructed from \(a\) via Lemmas 7.3 and 7.4. Then

1. for every labelled tree \(B \in T^d\), the vector \(B_H\) belongs to the span of \(\{\tilde{v}_0, \tilde{v}_1\}\).
2. the vector \(S^{d+1}_H\) does not belong to the span of \(\{\tilde{v}_0, \tilde{v}_1\}\).

Proof. Observe that for \(x, y \in \mathbb{Q}^n\), \(\tilde{x} \odot \tilde{y} = (x \otimes 1_N) \odot (y \otimes 1_N) = (x \otimes y) \otimes 1_N\). So the assertions of Lemma 7.3 on the layout of the eigenspaces of \(M\) carry over to the eigenspaces of \(A_H\).

First Item 1 is proved by structural induction on \(B\). For the base case, \(B\) is the 1-labelled one-vertex graph, and hence, \(B_H = 1_H = 1_n \otimes 1_N\). Since \(1_n\) lies in the span of \(\{v_0, v_1\}\), \(B_H\) lies in the span of \(\{\tilde{v}_0, \tilde{v}_1\}\). For the inductive step, suppose \(B = \otimes^d(C^1, \ldots, C^d) = A(C^1 \odot \cdots \odot C^d)\) for smaller \(C^1, \ldots, C^d \in T^d\). By Lemmas 7.3 and 7.4, and the inductive hypothesis, the \(C^i_H\) lie in the span of \(\{\tilde{v}_0, \tilde{v}_1\}\), and \(A_H(C^1_H \odot \cdots \odot C^d_H)\) also lies in the span of \(\{\tilde{v}_0, \tilde{v}_1\}\).

For Item 2, observe that by Lemma 7.4,

\[
S^{d+1}_H = A_H(A_H1_H)^{\odot (d+1)} = A_H(M1_n \otimes 1_N)^{\odot (d+1)} = A_H((M1_n)^{\odot (d+1)} \otimes 1_N)
= (M(M1_n)^{\odot (d+1)} \otimes 1_N).
\]

By Item 3 of Lemma 7.3, \(S^{d+1}_H\) is not contained in the span of \(\{\tilde{v}_0, \tilde{v}_1\}\). \(\square\)
This completes the preparations for the proof of Theorem 7.1.

**Proof of Theorem 7.1.** For the given degree \(d\), choose \(n > d + 1\) and an arbitrary \(a \in \mathbb{N}^n\) with distinct entries. Construct the desired graph \(H\) via Lemmas 7.3 and 7.4. Theorem 7.1 then immediately follows from Lemma 7.5. \(\square\)

### 7.2 Proof of Theorem 1.3

For a vector \(x \in \mathbb{Q}^n\) and \(p \in \mathbb{N}\) write \(\|x\|_p = \left(\sum_{i=1}^n |x_i|^p\right)^{1/p}\) for the \(p\)-norm of \(x\).

**Lemma 7.6.** Let \(d \geq 1\) and \(n > d + 1\). Let \(a, b \in \mathbb{N}^n\) be vectors with distinct entries. Suppose that \(\|a\|_i = \|b\|_i\) for all \(1 \leq i \leq 2d\), and that there exists \(\ell\) such that \(\|a\|_{\ell} \neq \|b\|_{\ell}\). Then there exist graphs \(G\) and \(H\) such that

1. \(G\) and \(H\) are homomorphism indistinguishable over the class of \(d\)-ary trees.
2. \(G\) and \(H\) are not homomorphism indistinguishable over the class of all trees.

**Proof.** Construct symmetric matrices \(M\) and \(L\) with non-negative integral entries from \(a\) and \(b\), respectively, invoking Lemma 7.3, and subsequently convert these into the adjacency matrices of simple graphs \(G\) and \(H\), respectively, via Lemma 7.4. In this process, the integers \(\lambda, \lambda',\) and \(N\) are chosen to be respectively equal for \(G\) and \(H\), which is always feasible.

For Item 1, let \(V \leq \mathbb{Q}^n\) denote the space spanned by \(1, a, \ldots, a^{\odot d}\), and analogously \(W \leq \mathbb{Q}^n\) the space spanned by \(1, b, \ldots, b^{\odot d}\). Observe that for \(0 \leq i, j \leq d\),

\[
\left\langle a^{\odot i}, b^{\odot j}\right\rangle = \|a\|_{i+j} = \|b\|_{i+j} = \left\langle b^{\odot i}, a^{\odot j}\right\rangle
\]

Hence, Lemma 2.1 guarantees the existence of an orthogonal \(U : V \rightarrow W\) such that \(Ua^{\odot i} = b^{\odot i}\) for all \(0 \leq i \leq d\). Let \(v_0, \ldots, v_d\) and \(w_0, \ldots, w_d\) denote the length-\((d + 1)\) initial segment of the principal sequence of \(a\) and of \(b\), respectively, cf. Lemma 7.2.

**Claim 12.** For all \(0 \leq i \leq d\), \(Uv_i = w_i\).

**Proof of Claim.** The claim is shown by induction on the definition of the principal sequence in Lemma 7.2. Let \(u_0, \ldots, u_d\) and \(u'_0, \ldots, u'_d\) be for \(a\) and \(b\) as in Equation (8). Clearly, \(Uu_i = u'_i\) for all \(0 \leq i \leq d\). Thus, for \(i = 0\), \(Uv_0 = U(1 + a) = 1 + b = w_0\). Furthermore, for \(i \geq 0\),

\[
Uv_{i+1} = Uu_{i+1} + \sum_{j=0}^i \frac{\left\langle u_{i+1}, v_j\right\rangle}{\left\langle v_j, v_j\right\rangle} Uv_j = u'_{i+1} + \sum_{j=0}^i \frac{\left\langle Uu_{i+1}, Uv_j\right\rangle}{\left\langle Uv_j, Uv_j\right\rangle} w_j = u'_{i+1} + \sum_{j=0}^i \frac{\left\langle u'_{i+1}, w_j\right\rangle}{\left\langle w_j, w_j\right\rangle} w_j,
\]

by orthogonality of \(U\), as desired. \(\square\)

Recall from Lemma 7.4, that \(\hat{z} = z \otimes 1_N\) denotes the lift of a vector \(z \in \mathbb{Q}^n\) to a vector in \(\mathbb{Q}^{V(G)} = \mathbb{Q}^{V(H)}\). Write \(\hat{V}\) and \(\hat{W}\) for the lifts of all vectors in \(V\) and in \(W\), respectively. The map \(U\) can be lifted to a map \(\hat{U} : \hat{V} \rightarrow \hat{W}\) via \(\hat{U}\hat{z} := (Uz) \otimes 1_N\), \(z \in V\). Checking that \(\hat{U}\) is well-defined and unitary amounts to a straightforward calculation.

Towards proving in Claim 14 that \(\hat{U}\) is a solution to the system of equations in Theorem 5.24, we show the following claim:

**Claim 13.** \(\hat{U}_G = A_H\hat{U}\) as maps \(\hat{V} \rightarrow \hat{W}\).
Proof of Claim. By Lemma 7.4 and Claim 12, for $0 \leq i \leq d$,
\[
\hat{U} A_G \hat{v}_i = \hat{U} (M v_i \otimes 1_N) = \mu_i \hat{U} (v_i \otimes 1_N) = \mu_i (\hat{U} v_i) \otimes 1_N = \mu_i w_i \otimes 1_N = L w_i \otimes 1_N = A_H \hat{U} \hat{v}_i
\]
for $\mu_i \in \{0, 1, \lambda\}$ the $i$-th eigenvalue of $M$ and $L$, cf. Equation (10).

Claim 14. For all $B \in T^{2d}$, $\hat{U} B_G = B_H$.

Proof of Claim. By structural induction on $B$. In the base case $B = 1$, the claim holds by construction observing that $1_G = 1_B \otimes 1_N = 1_H$. For the inductive step, suppose that $B = \otimes^d (C^1, \ldots, C^d)$. By Item 1 of Lemma 7.5, write $C^i_G = \alpha_i 1_G + \beta_i \hat{a}$ for some $\alpha_i, \beta_i \in \mathbb{Q}$. By induction, $\alpha_i 1_H + \beta_i \hat{b} = \hat{U} C^i_G = C^i_H$. The vector $C^i_G \otimes \cdots \otimes C^d_G$ can be written as linear combination of the vectors $1_G, \hat{a}, \ldots, \hat{a}^{\otimes d}$ since each individual vector is a linear combination of $1_G$ and $\hat{a}$. Hence, since $\hat{U} a^{\otimes i} = b^{\otimes i}$ for $0 \leq i \leq d$, $\hat{U} (C^1_G \otimes \cdots \otimes C^d_G) = C^1_H \otimes \cdots \otimes C^d_H$. By Claim 13, $\hat{U}$ preserves $\otimes^d$ and thus $\hat{U} B_G = B_H$.

By Theorem 5.24, $G$ and $H$ are homomorphism indistinguishable over the class of $d$-ary trees. It remains to verify Item 2. Let $\ell$ be the least positive integer such that $\|a\|_\ell \neq \|b\|_\ell$.

Claim 15. There exist coefficients $a, b \in \mathbb{Q}$ such that $M 1_n = a 1_n + b a$ and $L 1_n = a 1_n + b b$.

Proof of Claim. For legibility, we drop the index $n$. By definition in Lemma 7.3,
\[
\lambda' M 1 = \lambda \langle v_0, 1 \rangle v_0 + \langle v_1, 1 \rangle v_1 = \lambda \langle v_0, 1 \rangle (1 + a) + \langle v_1, 1 \rangle \left(1 - a - \frac{\langle v_1, v_0 \rangle}{\langle v_0, v_0 \rangle} (1 - a)\right).
\]
The same equality holds when $M$ is replaced by $L$, $v_0$ by $w_0$, $v_1$ by $w_1$, and $a$ by $b$. By Claim 12, the inner-products of the $v_i$ and the $w_i$ are the same, e.g. $\langle v_1, v_0 \rangle = \langle w_1, w_0 \rangle$. This yields the claim.

Let $S$ denote the star with $\ell$ leaves underlying the 1-labelled graph $(A_1)_{\otimes \ell}$. In contrary to the 1-labelled star considered in Lemma 7.5, this graph has its label at the central vertex. By Claim 15, as in Equation (11),
\[
\text{hom}(S, G) = \text{soe}(A_G 1_G)_{\otimes \ell} = N \text{soe}(M 1_n)_{\otimes \ell} = N \sum_{i=0}^{\ell} \alpha^{\ell-i} \beta^i \text{soe}(a_{\otimes i}) = N \sum_{i=0}^{\ell} \alpha^{\ell-i} \beta^i \|a\|_{\ell}^i.
\]
Replacing $a$ by $b$ yields an expression which equals $\text{hom}(S, H)$. Hence,
\[
\text{hom}(S, G) - \text{hom}(S, H) = N \beta^\ell \left(\|a\|_{\ell}^\ell - \|b\|_{\ell}^\ell\right) \neq 0
\]
since $\beta \neq 0$ as $1_n$ is neither an eigenvector of $M$ nor of $L$, and $\ell$ was chosen to be minimal.

Given Lemma 7.6, it remains to construct vectors $a, b \in \mathbb{N}^n$ such that $\|a\|_i = \|b\|_i$ for all $i \leq 2d$ but $\|a\|_\ell \neq \|b\|_\ell$ for some $\ell$. By Newton’s identities, this amounts to constructing vectors $a, b \in \mathbb{N}^n$ satisfying the former condition such that their multisets of entries are not the same. The fact that such pairs of vectors exist was established in the following number-theoretic result resolving the Prouhet–Tarry–Escott problem.
Theorem 7.7 (Prouhet–Thue–Morse Sequence [1]). Let $d \geq 1$. If the numbers in $\{0, \ldots, 2^{d+1} - 1\}$ are partitioned into two sets $S_0 = \{x_1, \ldots, x_n\}$ and $S_1 = \{y_1, \ldots, y_n\}$ of size $n = 2^d$ according to the parity of their binary representations then the following equations are satisfied:

\[
\begin{align*}
  x_1 + \cdots + x_n &= y_1 + \cdots + y_n, \\
  x_1^2 + \cdots + x_n^2 &= y_1^2 + \cdots + y_n^2, \\
  & \quad \ldots \\
  x_1^d + \cdots + x_n^d &= y_1^d + \cdots + y_n^d.
\end{align*}
\]


Proof of Theorem 1.3. Given $d \geq 1$, form sets $S_0 = \{x_1, \ldots, x_n\}$ and $S_1 = \{y_1, \ldots, y_n\}$ as in Theorem 7.7, each of size $n = 2^{2d} > d + 1$. Let $a$ and $b$ be vectors of length $n$ formed by ordering the elements of $S_0$ and $S_1$, respectively, in an arbitrary fashion.

Then, by construction, $\|a\|_\ell = \sum_{i=1}^n x_i^\ell = \sum_{i=1}^n y_i^\ell = \|b\|_\ell$ for all $1 \leq \ell \leq 2d$ but $\|a\|_\ell \neq \|b\|_\ell$ for some $\ell$ by Newton’s identities since $S_0 \neq S_1$. Consequently, Lemma 7.6 yields the two desired graphs.

\[
\square
\]

8 Conclusion

We have developed an algebraic theory of homomorphism indistinguishability that allows us to reprove known results in a unified way and derive new characterisations of homomorphism indistinguishability over bounded degree trees, graphs of bounded treedepth, graphs of bounded cyclewidth, and graphs of bounded pathwidth. The latter answers an open question from [16].

Homomorphism indistinguishabilities over various graph classes can be viewed as similarity measures for graphs, and our new results as well as many previous results show that these are natural and robust. Yet homomorphism indistinguishability only yields equivalence relations, or families of equivalence relations, and not a “quantitative” distance measure. For many applications of graph similarity, such quantitative measures are needed. Interestingly, we can derive distance measure both from homomorphism indistinguishability and from the equational characterisations we study here. For a class $\mathcal{F}$ of graphs, we can consider the \textit{homomorphism embedding} that maps graphs $G$ to the vector in $\mathbb{R}^\mathcal{F}$ whose entries are the numbers $\text{hom}(F, G)$ for graphs $F \in \mathcal{F}$. Then a norm on the space $\mathbb{R}^\mathcal{F}$ induces a graph (pseudo)metric. Such metrics give a generic family of graph kernels (see [24]). On the equational side, a notion like fractional isomorphism induces a (pseudo)metric on graphs where the distance between graphs $G$ and $H$ is $\min_X \|X A_G - A_H X\|$, where $X$ ranges over all doubly-stochastic matrices. It is a very interesting question whether the correspondence between the equivalence relations for homomorphism indistinguishability and feasibility of the systems of equations can be extended to the associated metrics. In the special case of isomorphism and homomorphism indistinguishability over all graphs, the theory of graph limits provides some answers [35]. This has recently been extended to fractional isomorphism and homomorphism indistinguishability over trees [7].

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