Lasserre Hierarchy for Graph Isomorphism and Homomorphism Indistinguishability

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───── **Abstract** ─────

We show that feasibility of the tth level of the Lasserre semidefinite programming hierarchy for graph isomorphism can be expressed as a homomorphism indistinguishability relation. In other words, we define a class $\mathcal{L}_t$ of graphs such that graphs G and H are not distinguished by the tth level of the Lasserre hierarchy if and only if they admit the same number of homomorphisms from any graph in $\mathcal{L}_t$. By analysing the treewidth of graphs in $\mathcal{L}_t$ we prove that the $3t^{\text{th}}$ level of Sherali–Adams linear programming hierarchy is as strong as the tth level of Lasserre. Moreover, we show that this is best possible in the sense that $3t$ cannot be lowered to $3t - 1$ for any t. The same result holds for the Lasserre hierarchy with non-negativity constraints, which we similarly characterise in terms of homomorphism indistinguishability over a family $\mathcal{L}_t^+$ of graphs. Additionally, we give characterisations of level-t Lasserre with non-negativity constraints in terms of logical equivalence and via a graph colouring algorithm akin to the Weisfeiler–Leman algorithm. This provides a polynomial time algorithm for determining if two given graphs are distinguished by the tth level of the Lasserre hierarchy with non-negativity constraints.

1 Introduction

The aim of this paper is to relate two rich sets of tools used to distinguish non-isomorphic graphs: the Lasserre semidefinite programming hierarchy and homomorphism indistinguishability.

Distinguishing non-isomorphic graphs is a ubiquitous problem in the theoretical and practical study of graphs. The ability of certain graph invariants to distinguish graphs has long been a rich area of study, leading to fundamental questions such as the longstanding open problem of whether almost all graphs are determined by their spectrum [35]. In practice, deploying e.g. machine learning architectures powerful enough to distinguish graphs with different features is of great importance [12]. This motivates an in-depth study of the power of various graph invariants and tools used to distinguish graphs.

Among such techniques is the Lasserre semidefinite programming hierarchy [17] which can be used to relax the integer program for graph isomorphism $\mathrm{ISO}(G, H)$, cf. Section 2.4. This yields a sequence of semidefinite programs, i.e. the level-t Lasserre relaxation of $\mathrm{ISO}(G, H)$ for $t \geq 1$, which are infeasible for more and more non-isomorphic graphs as t grows. In [33, 25, 5], it was shown that in general only the level-$\Omega(n)$ Lasserre system of equations can distinguish all non-isomorphic n-vertex graphs. In [4], the Lasserre hierarchy was compared with the Sherali–Adams[1] linear programming hierarchy [32], which is closely related to the Weisfeiler–Leman algorithm [36, 3, 13], the arguably most relevant combinatorial method for distinguishing graphs. It was shown in [4] that there exists a constant c such that, for all graphs G and H, if the level-ct Sherali–Adams relaxation of $\mathrm{ISO}(G, H)$ is feasible then so is the level-t Lasserre relaxation, which in turn implies that the level-t Sherali–Adams relaxation is feasible, cf. [18].

Another set of expressive equivalence relations comparing graphs is given by homomorphism indistinguishability, a notion originating from the study of graph substructure counts. Two graphs G and H are *homomorphism indistinguishable* over a family of graphs $\mathcal{F}$, in symbols $G \equiv_{\mathcal{F}} H$, if the number of homomorphisms from F to G is equal to the number of homomorphisms from F to H for every graph $F \in \mathcal{F}$. The study of this notion began in 1967, when Lovász [19] showed that two graphs G and H are isomorphic if and only if they are homomorphism indistinguishable over all graphs. In recent years, many prominent equivalence relations comparing graphs were characterised as homomorphism indistinguishability relations over restricted graph classes [9, 10, 11, 8, 20, 15, 2, 23, 1, 27, 26]. For example, a folklore result asserts that two graphs have cospectral adjacency matrices iff they are homomorphism indistinguishable over all cycle graphs, cf. [15]. Two graphs are quantum isomorphic iff they are homomorphism indistinguishable over all planar graphs [20]. Furthermore, feasibility of the level-t Sherali–Adams relaxation of $\mathrm{ISO}(G, H)$ has been characterised as homomorphism indistinguishability over all graphs of treewidth at most $t - 1$ [3, 13, 10]. In this way, notions from logic [10, 11, 26], category theory [8, 23, 1], algebraic graph theory [9, 15], and quantum groups [20] have been related to homomorphism indistinguishability.

1.1 Contributions

Although feasibility of the level-t Lasserre relaxation of $\mathrm{ISO}(G, H)$ was sandwiched between feasibility of the level-ct and level-t Sherali–Adams relaxation in [4], the constant c remained unknown. In fact, this c is not explicit and depends on the implementation details of an algorithm developed in that paper. Our main result asserts that c can be taken to be three and that this constant is best possible.

▶ **Theorem 1.** *For two graphs G and H and every $t \geq 1$, the following implications hold:*

$$G \simeq_{3t}^{\mathrm{SA}} H \implies G \simeq_t^{\mathrm{L}} H \implies G \simeq_t^{\mathrm{SA}} H$$

Furthermore, for every $t \geq 1$, there exist graphs G and H such that $G \simeq_{3t-1}^{\mathrm{SA}} H$ and $G \not\simeq_t^{\mathrm{L}} H$.

Here, $G \simeq_t^{\mathrm{L}} H$ and $G \simeq_t^{\mathrm{SA}} H$ denote that the level-t Lasserre relaxation and respectively the level-t Sherali–Adams relaxation of $\mathrm{ISO}(G, H)$ are feasible.

Theorem 1 is proven using the framework of homomorphism indistinguishability. In previous works [9, 22, 15, 26], the feasibility of various systems of equations associated to graphs like the Sherali–Adams relaxation of $\mathrm{ISO}(G, H)$ was characterised in terms of

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[1] Following [4], when referring to the Sherali–Adams relaxation of $\mathrm{ISO}(G, H)$ in this article, we do not refer to the original relaxation [32] but to its variant introduced by [3, 13], which corresponds more directly to other graph properties, cf. Theorem 8 and [15].

$$\begin{array}{ccccc} \mathcal{OP} & \mathcal{PW}_{2t-1} & & \mathcal{TW}_{\max\{2t-1,2\}} & \\ & \downarrow & & \downarrow & \\ \mathcal{TW}_{t-1} \longrightarrow & \mathcal{L}_t & \longrightarrow & \mathcal{L}_t^+ & \longrightarrow \mathcal{TW}_{3t-1} \end{array}$$
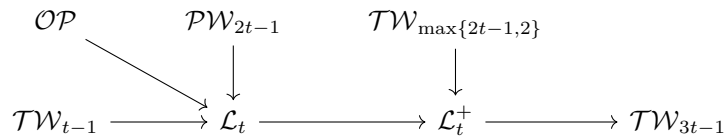
Figure 1 Relationship between $\mathcal{L}_t$, $\mathcal{L}_t^+$, the classes of graphs of bounded treewidth, bounded pathwidth, and the class of outerplanar graphs. An arrow $\mathcal{A} \to \mathcal{B}$ indicates that $\mathcal{A} \subseteq \mathcal{B}$ and thus that $G \equiv_{\mathcal{B}} H$ implies $G \equiv_{\mathcal{A}} H$ for all graphs G and H. For formal statements, see Sections 4.1 and 4.2.

homomorphism indistinguishability over certain graph classes. We continue this line of research by characterising the feasibility of the level-t Lasserre relaxation of $\mathrm{ISO}(G, H)$ by homomorphism indistinguishability of G and H over the novel class of graphs $\mathcal{L}_t$ introduced in Definition 22.

▶ **Theorem 2.** *For every integer $t \geq 1$, there is a minor-closed graph class $\mathcal{L}_t$ of graphs of treewidth at most $3t - 1$ such that for all graphs G and H it holds that $G \simeq_t^{\mathrm{L}} H$ if and only if $G \equiv_{\mathcal{L}_t} H$.*

The bound on the treewidth of graphs in $\mathcal{L}_t$ in Theorem 2 yields the upper bound in Theorem 1 given the result of [3, 13, 4, 10] that two graphs G and H satisfy $G \simeq_t^{\mathrm{SA}} H$ if and only if they are homomorphism indistinguishable over the class $\mathcal{TW}_{t-1}$ of graphs of treewidth at most $t - 1$. To our knowledge, Theorem 1 is the first result which tightly relates equivalence relations on graphs by comparing the graph classes which characterise them in terms of homomorphism indistinguishability.

Our techniques extend to a stronger version of the Lasserre hierarchy which imposes non-negativity constraints on all variables. Denoting feasibility of the level-t Lasserre relaxation of $\mathrm{ISO}(G, H)$ with non-negativity constraints by $G \simeq_t^{\mathrm{L}^+} H$, we characterise $\simeq_t^{\mathrm{L}^+}$ in terms of homomorphism indistinguishability over the graph class $\mathcal{L}_t^+$, defined in Definition 22 as a super class of $\mathcal{L}_t$. This is in line with previous work in [9, 15], where the feasibility of the level-t Sherali–Adams relaxation of $\mathrm{ISO}(G, H)$ without non-negativity constraints was characterised as homomorphism indistinguishable over the class $\mathcal{PW}_{t-1}$ of graphs of pathwidth at most $t - 1$.

▶ **Theorem 3.** *For every integer $t \geq 1$, there is a minor-closed graph class $\mathcal{L}_t^+$ of graphs of treewidth at most $3t - 1$ such that for all graphs G and H it holds that $G \simeq_t^{\mathrm{L}^+} H$ if and only if $G \equiv_{\mathcal{L}_t^+} H$.*

Given the aforementioned correspondence between the Sherali–Adams relaxation with and without non-negativity constraints and homomorphism indistinguishability over graphs of bounded treewidth and pathwidth, we conduct a detailed study of the relationship between the class of graphs of bounded treewidth, pathwidth, and the classes $\mathcal{L}_t$ and $\mathcal{L}_t^+$. Their results, depicted in Figure 1, yield independent proofs of the known relations between feasibility of the Lasserre relaxation with and without non-negativity constraints and the Sherali–Adams relaxation with and without non-negativity constraints [5, 4, 15] using the framework of homomorphism indistinguishability.

In the course of proving Theorems 2 and 3, we derive further equivalent characterisations of $\simeq_t^{\mathrm{L}}$ and $\simeq_t^{\mathrm{L}^+}$. These characterisations, which are mostly of a linear algebraic nature, ultimately yield a characterisation of $\simeq_t^{\mathrm{L}^+}$ in terms of a fragment of first-order logic with counting quantifiers and indistinguishability under a polynomial time algorithm akin to

the Weisfeiler–Leman algorithm. In this way, we obtain the following algorithmic result. It implies that *exact* feasibility of the Lasserre semidefinite program with non-negativity constraints can be tested in polynomial time. In general, only the *approximate* feasibility of semidefinite programs can be decided efficiently, e.g. using the ellipsoid method [16, 4].

▶ **Theorem 4.** *Let $t \geq 1$. Given graphs G and H, it can be decided in polynomial time whether $G \simeq_t^{\mathrm{L}^+} H$.*

Finally, for $t = 1$, we show that $\mathcal{L}_1$ and $\mathcal{L}_1^+$ are respectively equal to the class $\mathcal{OP}$ of outerplanar graphs and to the class of graphs of treewidth at most 2. The following Theorem 5 parallels a result of [20] asserting that two graphs G and H are indistinguishable under the 2-WL algorithm iff $G \simeq_1^{\mathrm{L}^+} H$.

▶ **Theorem 5.** *Two graphs G and H satisfy $G \simeq_1^{\mathrm{L}} H$ iff $G \equiv_{\mathcal{OP}} H$.*

1.2 Techniques

In the first part of the paper (Section 3), linear algebraic tools developed in [21, 20] are generalised to yield reformulations of the entire Lasserre hierarchy with and without non-negativity results. Section 4 is concerned with the graph theoretic properties of the graph classes $\mathcal{L}_t$ and $\mathcal{L}_t^+$. For understanding the homomorphism indistinguishability relations over these graph classes, the framework of bilabelled graphs and their homomorphism tensors developed in [22, 15] is used. Despite this, our approach is different from [15, 26] in the sense that here the graph classes $\mathcal{L}_t$ and $\mathcal{L}_t^+$ are inferred from given systems of equations, namely the Lasserre relaxation, rather than that a system of equations is built for a given graph class.

2 Preliminaries

2.1 Linear Algebra

Let $\mathcal{S}_+$ denote the family of real *positive semidefinite matrices*, i.e. of matrices M of the form $M_{ij} = v_i^T v_j$ for vectors $v_1, \ldots, v_n$, the *Gram vectors* of M. Write $M \succeq 0$ iff $M \in \mathcal{S}_+$. Let $\mathcal{DNN}$ denote the family of *doubly non-negative matrices*, i.e. of entry-wise non-negative positive semidefinite matrices.

A linear map $\Phi \colon \mathbb{C}^{m \times m} \to \mathbb{C}^{n \times n}$ is *trace-preserving* if $\operatorname{tr} \Phi(X) = \operatorname{tr} X$ for all $X \in \mathbb{C}^{m \times m}$, *unital* if $\Phi(\mathrm{id}_m) = \mathrm{id}_n$, $\mathcal{K}$*-preserving* for a family of matrices $\mathcal{K}$ if $\Phi(K) \in \mathcal{K}$ for all $K \in \mathcal{K}$, *positive* if it is $\mathcal{S}_+$-preserving, i.e. if $\Phi(X)$ is positive semidefinite for all positive semidefinite X, *completely positive* if $\mathrm{id}_r \otimes \Phi$ is positive for all $r \in \mathbb{N}$. The *Choi matrix* of Φ is $C_\Phi = \sum_{i,j=1}^m E_{ij} \otimes \Phi(E_{ij}) \in \mathbb{C}^{mn \times mn}$.

A *tensor* is an element $A \in \mathbb{C}^{n^t \times n^t}$ for some $n, t \in \mathbb{N}$. The symmetric group $\mathfrak{S}_{2t}$ acts on $\mathbb{C}^{n^t \times n^t}$ by permuting the coordinates, i.e. for all $\boldsymbol{u}, \boldsymbol{v} \in [n]^t$, $A^\sigma(\boldsymbol{u}, \boldsymbol{v}) := A(\boldsymbol{x}, \boldsymbol{y})$ where $\boldsymbol{x}_i := (\boldsymbol{uv})_{\sigma^{-1}(i)}$ and $\boldsymbol{y}_{j-t} := (\boldsymbol{uv})_{\sigma^{-1}(j)}$ for all $1 \leq i \leq t < j \leq 2t$.

For two vectors $v, w \in \mathbb{C}^n$, write $v \odot w$ for their *Schur product*, i.e. $(v \odot w)(i) := v(i)w(i)$ for all $i \in [n]$.

2.2 Bilabelled Graphs and Homomorphism Tensors

All graphs in this article are undirected, finite, and without multiple edges. A graph is *simple* if it does not contain any loops. A *homomorphism* $h \colon F \to G$ from a graph F to a graph G is a map $V(F) \to V(G)$ such that for all $uv \in E(F)$ it holds that $h(u)h(v) \in E(G)$.

Note that this implies that any vertex in F carrying a loop must be mapped to a vertex carrying a loop in G. Write $\hom(F, G)$ for the number of homomorphisms from F to G. For a family of graphs $\mathcal{F}$ and graphs G and H write $G \equiv_{\mathcal{F}} H$ if G and H are *homomorphism indistinguishable over* $\mathcal{F}$, i.e. $\hom(F, G) = \hom(F, H)$ for all $F \in \mathcal{F}$. Since the graphs G and H into which homomorphisms are counted, are throughout assumed to be simple, looped graphs in $\mathcal{F}$ can generally be disregarded as they do not admit any homomorphisms into simple graphs.

We recall the following definitions from [20, 15]. Let $\ell \geq 1$. An (ℓ, ℓ)-*bilabelled graph* is a tuple $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v})$ where F is a graph and $\boldsymbol{u}, \boldsymbol{v} \in V(F)^{\ell}$. The $\boldsymbol{u}$ are the *in-labelled vertices* of $\boldsymbol{F}$ while the $\boldsymbol{v}$ are the *out-labelled vertices* of $\boldsymbol{F}$. Given a graph G, the *homomorphism tensor* of $\boldsymbol{F}$ for G is $\boldsymbol{F}_G \in \mathbb{C}^{V(G)^{\ell} \times V(G)^{\ell}}$ whose $(\boldsymbol{x}, \boldsymbol{y})$-th entry is the number of homomorphisms $h \colon F \to G$ such that $h(\boldsymbol{u}_i) = \boldsymbol{x}_i$ and $h(\boldsymbol{v}_i) = \boldsymbol{y}_i$ for all $i \in [\ell]$.

For an (ℓ, ℓ)-bilabelled graph $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v})$, write soe $\boldsymbol{F} \coloneqq F$ for the underlying unlabelled graph of $\boldsymbol{F}$. Write tr $\boldsymbol{F}$ for the unlabelled graph underlying the graph obtained from $\boldsymbol{F}$ by identifying $\boldsymbol{u}_i$ with $\boldsymbol{v}_i$ for all $i \in [\ell]$. For $\sigma \in \mathfrak{S}_{2t}$, write $\boldsymbol{F}^{\sigma} \coloneqq (F, \boldsymbol{x}, \boldsymbol{y})$ where $\boldsymbol{x}_i \coloneqq (\boldsymbol{uv})_{\sigma(i)}$ and $\boldsymbol{y}_{j-t} \coloneqq (\boldsymbol{uv})_{\sigma(j)}$ for all $1 \leq i \leq t < j \leq 2t$, i.e. $\boldsymbol{F}^{\sigma}$ is obtained from $\boldsymbol{F}$ by permuting the labels according to σ. As a special case, define $\boldsymbol{F}^{*} \coloneqq (F, \boldsymbol{v}, \boldsymbol{u})$ the graph obtained by swapping in- and out-labels.

For two (ℓ, ℓ)-bilabelled graphs $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v})$ and $\boldsymbol{F}' = (F', \boldsymbol{u}', \boldsymbol{v}')$, write $\boldsymbol{F} \cdot \boldsymbol{F}'$ for the graph obtained from them by *series composition*. That is, the underlying unlabelled graph of $\boldsymbol{F} \cdot \boldsymbol{F}'$ is the graph obtained from the disjoint union of F and F' by identifying $\boldsymbol{v}_i$ and $\boldsymbol{u}'_i$ for all $i \in [\ell]$. Multiple edges arising in this process are removed. The in-labels of $\boldsymbol{F} \cdot \boldsymbol{F}'$ lie on $\boldsymbol{u}$, the out-labels on $\boldsymbol{v}'$. Moreover, write $\boldsymbol{F} \odot \boldsymbol{F}'$ for the *parallel composition* of $\boldsymbol{F}$ and $\boldsymbol{F}'$. That is, the underlying unlabelled graph of $\boldsymbol{F} \odot \boldsymbol{F}'$ is the graph obtained from the disjoint union of F and F' by identifying $\boldsymbol{u}_i$ with $\boldsymbol{u}'_i$ and $\boldsymbol{v}_i$ with $\boldsymbol{v}'_i$ for all $i \in [\ell]$. Again, multiple edges are dropped. The in-labels of $\boldsymbol{F} \odot \boldsymbol{F}'$ lie on $\boldsymbol{u}$, the out-labels on $\boldsymbol{v}$.

As observed in [20, 15], the benefit of these combinatorial operations is that they have an algebraic counterpart. Formally, for all graphs G and all (ℓ, ℓ)-bilabelled graphs $\boldsymbol{F}, \boldsymbol{F}'$, it holds that soe $\boldsymbol{F}_G = \hom(\text{soe } \boldsymbol{F}, G)$, tr $\boldsymbol{F}_G = \hom(\text{tr } \boldsymbol{F}, G)$, $(\boldsymbol{F}_G)^{\sigma} = (\boldsymbol{F}^{\sigma})_G$, $(\boldsymbol{F} \cdot \boldsymbol{F}')_G = \boldsymbol{F}_G \cdot \boldsymbol{F}'_G$, and $(\boldsymbol{F} \odot \boldsymbol{F}')_G = \boldsymbol{F}_G \odot \boldsymbol{F}'_G$.

Slightly abusing notation, we say that two graphs G and H are homomorphism indistinguishable over a family of bilabelled graphs $\boldsymbol{S}$, in symbols $G \equiv_{\mathcal{S}} H$ if G and H are homomorphism indistinguishable over the family $\{\text{soe } \boldsymbol{S} \mid \boldsymbol{S} \in \mathcal{S}\}$ of the underlying unlabelled graphs of the $\boldsymbol{S} \in \mathcal{S}$.

2.3 Pathwidth and Treewidth

▶ **Definition 6.** *Let F and T be graphs. A T-decomposition of F is a map $\beta \colon V(T) \to 2^{V(F)}$ such that*

1. $\bigcup_{t \in V(T)} \beta(t) = V(F)$,
2. *for every $e \in E(F)$, there is $t \in V(T)$ such that $e \subseteq \beta(t)$,*
3. *for every $v \in V(F)$, the set of $t \in V(T)$ such that $v \in \beta(t)$ induces a connected component of T.*

The width *of a T-decomposition β is $\max_{t \in V(T)} |\beta(t)| - 1$. For a graph class $\mathcal{T}$, the $\mathcal{T}$-width of F is the minimal width of a T-decomposition of F for $T \in \mathcal{T}$.*

The *treewidth* tw F of a graph F is the minimal width of a T-decomposition of F where T is a tree. Similarly, the *pathwidth* pw F is the minimal width of a P-decomposition of F where P is a path. For every $t \geq 0$, write $\mathcal{TW}_t$ and $\mathcal{PW}_t$ for the classes of all graphs of treewidth and respectively pathwidth at most t.

2.4 Systems of Equations for Graph Isomorphism

Two simple graphs G and H are isomorphic if and only if there exists a $\{0,1\}$-solution to the system of equations $\mathrm{ISO}(G, H)$ which comprises variables X_{gh} for $gh \in V(G) \times V(H)$ and equations

$$\sum_{h \in V(H)} X_{gh} - 1 = 0 \qquad \text{for all } g \in V(G), \tag{1}$$

$$\sum_{g \in V(G)} X_{gh} - 1 = 0 \qquad \text{for all } h \in V(H), \tag{2}$$

$$X_{gh} X_{g'h'} = 0 \qquad \begin{array}{l} \text{for all } gh, g'h' \in V(G) \times V(H) \\ \text{s.t. } \mathrm{rel}_G(g, g') \neq \mathrm{rel}_H(h, h'). \end{array} \tag{3}$$

Here, $\mathrm{rel}_G(g, g') = \mathrm{rel}_H(h', h')$ if and only if both pairs of vertices are adjacent, non-adjacent, or identical.

The Lasserre relaxation of $\mathrm{ISO}(G, H)$ is defined as follows. An element $\{g_1 h_1, \dots g_\ell h_\ell\} \in \binom{V(G) \times V(H)}{\ell}$ is a *partial isomorphism* if $g_i = g_j \Leftrightarrow h_i = h_j$ and $g_i g_j \in E(G) \Leftrightarrow h_i h_j \in E(H)$ for all $i, j \in [\ell]$. See also [28] for a comparison to the version used in [4].

▶ **Definition 7.** *Let $t \geq 1$. The level-t Lasserre relaxation for graph isomorphism has variables y_I ranging over $\mathbb{R}$ for $I \in \binom{V(G) \times V(H)}{\leq 2t}$. The constraints are*

$$M_t(y) \coloneqq (y_{I \cup J})_{I, J \in \binom{V(G) \times V(H)}{\leq t}} \succeq 0, \tag{4}$$

$$\sum_{h \in V(H)} y_{I \cup \{gh\}} = y_I \text{ for all } I \text{ s.t. } |I| \leq 2t - 2 \text{ and all } g \in V(G), \tag{5}$$

$$\sum_{g \in V(G)} y_{I \cup \{gh\}} = y_I \text{ for all } I \text{ s.t. } |I| \leq 2t - 2 \text{ and all } h \in V(H), \tag{6}$$

$$y_I = 0 \text{ if } I \text{ s.t. } |I| \leq 2t \text{ is not partial isomorphism} \tag{7}$$

$$y_\emptyset = 1. \tag{8}$$

If the system is feasible for two graphs G and H, write $G \simeq_t^{\mathrm{L}} H$. If the system together with the constraint $y_I \geq 0$ for all $I \in \binom{V(G) \times V(H)}{\leq 2t}$ is feasible, write $G \simeq_t^{\mathrm{L}^+} H$.

For a definition of the Sherali–Adams relaxation of $\mathrm{ISO}(G, H)$ in the version used here following [4], the reader is referred to [14, Appendix D.1]. Instead of feasibility of the level-t Sherali–Adams relaxation, one may think of the following equivalent notions:

▶ **Theorem 8** ([4, 10, 6]). *Let $t \geq 1$. For graphs G and H, the following are equivalent:*
1. *the level-t Sherali–Adams relaxation of $\mathrm{ISO}(G, H)$ is feasible, i.e. $G \simeq_t^{\mathrm{SA}} H$,*
2. *G and H satisfy the same sentences of t-variable first order logic with counting quantifiers,*
3. *G and H are homomorphism indistinguishable over the graphs of treewidth at most $t - 1$,*
4. *G and H are not distinguished by the $(t - 1)$-dimensional Weisfeiler–Leman algorithm,*

3 From Lasserre to Homomorphism Tensors

In this section, the tools are developed which will be used to translate a solution to the level-t Lasserre relaxation into a statement on homomorphism indistinguishability. For this purpose, three equivalent characterisations of $\simeq_t^{\mathrm{L}}$ and $\simeq_t^{\mathrm{L}^+}$ are introduced. Theorems 9 and 10 summarise our results. The notions in items 2–4 and the graph classes $\mathcal{L}_t$ and $\mathcal{L}_t^+$ are defined in Sections 3.1, 3.2, 3.4, and 4, respectively. Most of the proofs are of a linear algebraic nature. Graph theoretical repercussions are discussed in Section 4.

▶ **Theorem 9.** *Let $t \geq 1$. For graphs G and H, the following are equivalent:*

1. *the level-t Lasserre relaxation of $\mathrm{ISO}(G,H)$ is feasible,*
2. *G and H are level-t $\mathcal{S}_+$-isomorphic,*
3. *there is a level-t $\mathcal{S}_+$-isomorphism map from G to H,*
4. *G and H are partially t-equivalent,*
5. *G and H are homomorphism indistinguishable over $\mathcal{L}_t$.*

▶ **Theorem 10.** *Let $t \geq 1$. For graphs G and H, the following are equivalent:*

1. *the level-t Lasserre relaxation of $\mathrm{ISO}(G,H)$ with non-negativity constraints is feasible,*
2. *G and H are level-t $\mathcal{DNN}$-isomorphic,*
3. *there is a level-t $\mathcal{DNN}$-isomorphism map from G to H,*
4. *G and H are t-equivalent,*
5. *G and H are homomorphism indistinguishable over $\mathcal{L}_t^+$.*

Variants of the notions in items 2–4 have already been defined for the case $t = 1$ in [22]. Our contribution amounts to extending these definitions to the entire Lasserre hierarchy. A recurring theme in this context is accounting for additional symmetries. The variables y_I of the Lasserre system of equations, cf. Definition 7, are indexed by sets of vertex pairs rather than by tuples of such. Hence, when passing from such variables to tuple-indexed matrices, one must impose the additional symmetries arising this way. This is formalised at various points using an action of the symmetric group on the axes of the matrices. In the case $t = 1$, such a set up is not necessary since indices I are of size at most 2 and all occurring matrices can be taken to be invariant under transposition.

In the subsequent sections, Theorems 9 and 10 will be proven in parallel. The equivalence of items 1 and 2, 2 and 3, and 3 and 4 are established in Section 3.3, Section 3.2, and Section 3.4, respectively. The statements on homomorphism indistinguishability are proven in Section 4.

3.1 Isomorphism Relaxations via Matrix Families

In this section, as a first step towards proving Theorems 9 and 10, the notion of level-t $\mathcal{K}$-isomorphic graphs for arbitrary families of matrices $\mathcal{K}$ is introduced. In [22], level-1 $\mathcal{K}$-isomorphic graphs where studied for various families of matrices $\mathcal{K}$. In this work, the main interest lies on the family of positive semidefinite matrices $\mathcal{S}_+$ and the family of entry-wise non-negative positive semidefinite matrices $\mathcal{DNN}$. Level-t isomorphism for these families is proven to correspond to $\simeq_t^{\mathrm{L}}$ and $\simeq_t^{\mathrm{L}^+}$ respectively, cf. Theorems 16 and 17.

▶ **Definition 11.** *Let $\mathcal{K}$ be a family of matrices. Graphs G and H are said to be level-t $\mathcal{K}$-isomorphic, in symbols $G \cong_{\mathcal{K}}^t H$, if there is a matrix $M \in \mathcal{K}$ with rows and columns indexed by $(V(G) \times V(H))^t$ such that for every $g_1 h_1 \ldots g_t h_t, g_{t+1} h_{t+1} \ldots g_{2t} h_{2t} \in (V(G) \times V(H))^t$ the following equations hold:*

For every $i \in [2t]$,

$$\sum_{g_i \in V(G)} M_{g_1 h_1 \ldots g_t h_t, g_{t+1} h_{t+1} \ldots g_{2t} h_{2t}} = \sum_{h_i \in V(H)} M_{g_1 h_1 \ldots g_t h_t, g_{t+1} h_{t+1} \ldots g_{2t} h_{2t}}, \qquad (9)$$

$$\sum_{h_1', \ldots, h_{2t}' \in V(H)} M_{g_1 h_1' \ldots g_t h_t', g_{t+1} h_{t+1}' \ldots g_{2t} h_{2t}'} = 1 = \sum_{g_1', \ldots, g_{2t}' \in V(G)} M_{g_1' h_1 \ldots g_t' h_t, g_{t+1}' h_{t+1} \ldots g_{2t}' h_{2t}}. \qquad (10)$$

(a) $\boldsymbol{J}$.   **(b)** $\boldsymbol{A}^{2,2t}$.   **(c)** $\boldsymbol{I}^{2,2t}$.
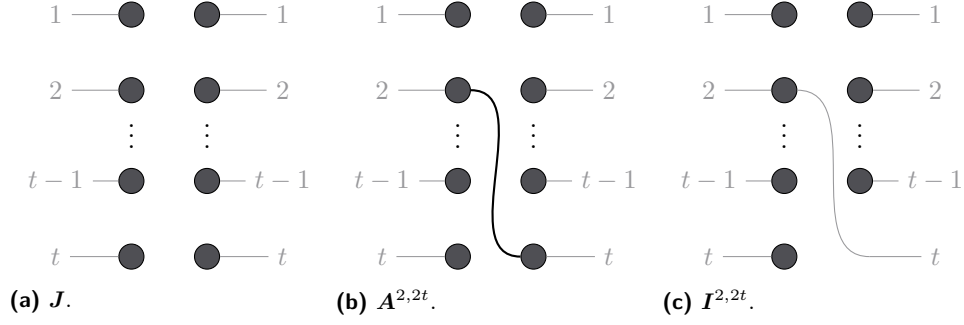
Figure 2 Examples of the atomic graphs from Definition 13. The gray lines (the *wires* [20]) indicate the in-labels (left) and out-labels (right).

If $\mathrm{rel}_G(g_1, \ldots, g_{2t}) \neq \mathrm{rel}_H(h_1, \ldots, h_{2t})$ *then*

$$M_{g_1 h_1 \ldots g_t h_t, g_{t+1} h_{t+1} \ldots g_{2t} h_{2t}} = 0. \tag{11}$$

For all $\sigma \in \mathfrak{S}_{2t}$,

$$M_{g_1 h_1 \ldots g_t h_t, g_{t+1} h_{t+1} \ldots g_{2t} h_{2t}} = M_{g_{\sigma(1)} h_{\sigma(1)} \ldots g_{\sigma(t)} h_{\sigma(t)}, g_{\sigma(t+1)} h_{\sigma(t+1)} \ldots g_{\sigma(2t)} h_{\sigma(2t)}}. \tag{12}$$

Note that for $t = 1$ and any family of matrices $\mathcal{K}$ closed under taking transposes Equation (12) is vacuous.

Systems of equations comparing graphs akin to Equations (9)–(12) were also studied by [15]. Feasibility of such equations is typically invariant under taking the complements of the graphs as remarked below. This semantic property of the relation $\cong_{\mathcal{K}}^t$ is relevant in the context of homomorphism indistinguishability as shown by [30].

▶ **Remark 12.** For a simple graph G, write $\overline{G}$ for its complement, i.e. $V(\overline{G}) := V(G)$ and $E(\overline{G}) := \binom{V(G)}{2} \setminus E(G)$. For all graphs G and H and $g_1, \ldots, g_{2t} \in V(G)$, $h_1, \ldots, h_{2t} \in V(H)$, it holds that

$$\mathrm{rel}_G(g_1, \ldots, g_{2t}) = \mathrm{rel}_H(h_1, \ldots, h_{2t}) \iff \mathrm{rel}_{\overline{G}}(g_1, \ldots, g_{2t}) = \mathrm{rel}_{\overline{H}}(h_1, \ldots, h_{2t}).$$

Thus, $G \cong_{\mathcal{K}}^t H$ if and only if $\overline{G} \cong_{\mathcal{K}}^t \overline{H}$ for all families of matrices $\mathcal{K}$ and $t \in \mathbb{N}$.

3.2 Choi Matrices and Isomorphism Maps

In this section, an alternative characterisation for level-t $\mathcal{K}$-isomorphism is given. Intuitively, the indices of the matrix $M \in \mathbb{C}^{(V(G) \times V(H))^t \times (V(G) \times V(H))^t}$ from Definition 11 are regrouped yielding a linear map $\Phi \colon \mathbb{C}^{V(G)^t \times V(G)^t} \to \mathbb{C}^{V(H)^t \times V(H)^t}$. In linear algebraic terms, M is the Choi matrix of Φ. The map Φ will later be interpreted as a function sending homomorphism tensors of (t,t)-bilabelled graphs $\boldsymbol{F}_G \in \mathbb{C}^{V(G)^t \times V(G)^t}$ with respect to G to their counterparts $\boldsymbol{F}_H$ for H.

The most basic bilabelled graphs, so called *atomic* graphs, make their first appearance in Theorem 14. These graphs are used to reformulate Equations (7) and (11). The atomic graphs are also the graphs which the sets $\mathcal{L}_t$ and $\mathcal{L}_t^+$ of Theorems 2 and 3 are generated by, cf. Definition 22. Examples are depicted in Figures 2 and 3.

▶ **Definition 13.** *Let* $t \geq 1$. *A* (t,t)-*bilabelled graph* $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v})$ *is* atomic *if all its vertices are labelled. Write* $\mathcal{A}_t$ *for the set of* (t,t)-*bilabelled atomic graphs. Note that the the the set of atomic graphs* $\mathcal{A}_t$ *is generated under parallel composition by the graphs*

- $\boldsymbol{J} \coloneqq (J, (1, \ldots, t), (t+1, \ldots, 2t))$ with $V(J) = [2t]$, $E(J) = \emptyset$,
- $\boldsymbol{A}^{ij} \coloneqq (A^{ij}, (1, \ldots, t), (t+1, \ldots, 2t))$ with $V(A^{ij}) = [2t]$, $E(A^{ij}) = \{ij\}$ for $1 \le i < j \le 2t$,
- $\boldsymbol{I}^{ij}$ for $1 \le i < j \le 2t$ which is obtained from $\boldsymbol{A}^{ij}$ by contracting the edge ij.

The following Theorem 14 relates the properties of Φ and M. In Equation (15), J denotes the all-ones matrix of appropriate dimension. Its proof is deferred to the full version [28].

▶ **Theorem 14.** *Let $t \ge 1$. Let G and H be graphs and $\mathcal{K} \in \{\mathcal{DNN}, \mathcal{S}_+\}$ be a family of matrices. Let $\Phi \colon \mathbb{C}^{V(G)^t \times V(G)^t} \to \mathbb{C}^{V(H)^t \times V(H)^t}$ be a linear map. Then the following are equivalent.*

1. *The Choi matrix C_Φ of Φ satisfies Equations (9)–(12) and $C_\Phi \in \mathcal{K}$,*

2. *Φ is a level-t $\mathcal{K}$-isomorphism map from G to H, i.e. it satisfies*

$$\Phi \text{ is completely } \mathcal{K}\text{-preserving}, \tag{13}$$

$$\Phi(\boldsymbol{A}_G \odot X) = \boldsymbol{A}_H \odot \Phi(X) \text{ for all atomic } \boldsymbol{A} \in \mathcal{A}_t \text{ and all } X \in \mathbb{C}^{V(G)^t \times V(G)^t}, \tag{14}$$

$$\Phi(J) = J = \Phi^*(J), \tag{15}$$

$$\Phi(X^\sigma) = \Phi(X)^\sigma \text{ for all } \sigma \in \mathfrak{S}_{2t} \text{ and all } X \in \mathbb{C}^{V(G)^t \times V(G)^t}. \tag{16}$$

3. *Φ^* is a level-t $\mathcal{K}$-isomorphism map from H to G.*

We remark that Theorem 14 and in particular its Equation (15) has brought us closer to interpreting the Lasserre system of equation from the perspective of homomorphism indistinguishability. As argued in Remark 15, the map Φ, which will be understood as mapping homomorphism tensors $\boldsymbol{F}_G$ to $\boldsymbol{F}_H$, is sum-preserving. Since the sum of the entries of these tensors equals the number of homomorphisms from their underlying unlabelled graphs to G and H, respectively, for establishing a connection between $\mathcal{K}$-isomorphism maps and homomorphism indistinguishability.

▶ **Remark 15.** If a linear map $\Phi \colon \mathbb{C}^{n \times n} \to \mathbb{C}^{m \times m}$ is such that $J = \Phi^*(J)$ then it is *sum-preserving*, i.e. soe $X = \text{soe}\,\Phi(X)$ for all $X \in \mathbb{C}^{n \times n}$. Indeed, soe $X = \langle X, J \rangle = \langle X, \Phi^*(J) \rangle = \langle \Phi(X), J \rangle = \text{soe}\,\Phi(X)$ where $\langle A, B \rangle \coloneqq \text{tr}(AB^*)$. In particular, if there is Φ satisfying Equations (14) and (15) for graphs G and H then $|G| = |H|$.

3.3 Connection to Lasserre

By the following Theorems 16 and 17, the notions introduced in Definition 11 and Theorem 14 are equivalent to the object of our main interest, namely feasibility of the level-t Lasserre relaxation with and without non-negativity constraints. Our results extend those of [22, Lemma 9.1] to the entire Lasserre hierarchy. The proofs are deferred to the full version [28].

▶ **Theorem 16.** *Let $t \ge 1$. Two graphs G and H are level-t $\mathcal{S}_+$-isomorphic if and only if the level-t system of the Lasserre hierarchy for graph isomorphism, i.e. Equations (4)–(8), is feasible.*

▶ **Theorem 17.** *Let $t \ge 1$. Two graphs G and H are level-t $\mathcal{DNN}$-isomorphic if and only if the level-t system of the Lasserre hierarchy for graph isomorphism Equations (4)–(8) with the additional constraint $y_I \ge 0$ for all $I \in \binom{V(G) \times V(H)}{\le 2t}$ is feasible.*

(a) J.　　(b) $A^{1,2}$.　　(c) $I^{1,2}$.
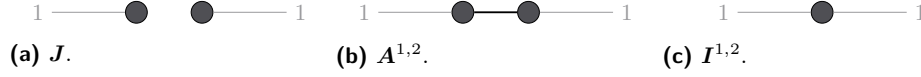
■ **Figure 3** The three atomic graphs in $\mathcal{A}_1$.

3.4 Isomorphisms between Matrix Algebras

To the two reformulations of $\simeq_t^{\mathrm{L}}$ and $\simeq_t^{\mathrm{L}^+}$ from the previous sections, a third characterisation is added in this section. It is shown that two graphs are level-t $\mathcal{S}_+$-isomorphic ($\mathcal{DNN}$-isomorphic) if and only if certain matrix algebras associated to them are isomorphic. These algebras will be identified as the algebras of homomorphism tensors for graphs from the families $\mathcal{L}_t$ and $\mathcal{L}_t^+$. The so called (partially) coherent algebras considered in this section are natural generalisations of the coherent algebra which are well-studied in the context of the 2-dimensional Weisfeiler–Leman algorithm [7].

3.4.1 Partially Coherent Algebras and $\mathcal{S}_+$-Isomorphism Maps

Let $S \subseteq \mathbb{C}^{n^t \times n^t}$. A matrix algebra $\mathcal{A} \subseteq \mathbb{C}^{n^t \times n^t}$ is *S-partially coherent* if it is unital, self-adjoint, contains the all-ones matrix, and is closed under Schur products with any matrix in S. A matrix algebra $\mathcal{A} \subseteq \mathbb{C}^{n^t \times n^t}$ is *self-symmetrical* if for every $A \in \mathcal{A}$ and $\sigma \in \mathfrak{S}_{2t}$ also $A^\sigma \in \mathcal{A}$. Note that for $t = 1$, an algebra $\mathcal{A}$ is self-symmetrical if for all $A \in \mathcal{A}$ also $A^T \in \mathcal{A}$.

▶ **Definition 18.** *Given a graph G, construct its t-partially coherent algebra $\widehat{\mathcal{A}}_G^t$ as the minimal self-symmetrical S-partially coherent algebra where S is the set of homomorphism tensors of (t, t)-bilabelled atomic graphs for G.*

Two n-vertex graphs G and H are partially t-equivalent *if there is a* partial t-equivalence, *i.e. a vector space isomorphism $\varphi\colon \widehat{\mathcal{A}}_G^t \to \widehat{\mathcal{A}}_H^t$ such that*
1. *$\varphi(M^*) = \varphi(M)^*$ for all $M \in \widehat{\mathcal{A}}_G^t$,*
2. *$\varphi(MN) = \varphi(M)\varphi(N)$ for all $M, N \in \widehat{\mathcal{A}}_G^t$,*
3. *$\varphi(I) = I$, $\varphi(\boldsymbol{A}_G) = \boldsymbol{A}_H$ for all $\boldsymbol{A} \in \mathcal{A}_t$, and $\varphi(J) = J$,*
4. *$\varphi(\boldsymbol{A}_G \odot M) = \boldsymbol{A}_H \odot \varphi(M)$ for all $\boldsymbol{A} \in \mathcal{A}_t$ and any $M \in \widehat{\mathcal{A}}_G^t$.*
5. *$\varphi(M^\sigma) = \varphi(M)^\sigma$ for all $M \in \widehat{\mathcal{A}}_G^t$ and all $\sigma \in \mathfrak{S}_{2t}$.*

The following Theorem 19 extends [22, Theorem 5.2]. Its proof is deferred to the full version [28].

▶ **Theorem 19.** *Let $t \geq 1$. Two graphs G and H are partially t-equivalent if and only if there is a level-t $\mathcal{S}_+$-isomorphism map from G to H.*

3.4.2 Coherent Algebras and $\mathcal{DNN}$-Isomorphism Maps

A matrix algebra $\mathcal{A} \subseteq \mathbb{C}^{n \times n}$ is *coherent* if it is unital, self-adjoint, contains the all-ones matrix and is closed under Schur products.

For $t = 1$, the 1-adjacency algebra as defined below is equal to the well-studied *adjacency algebra* of a graph G, cf. [7]. The latter is the smallest coherent algebra containing the adjacency matrix of the graph. The former is generated by the homomorphism tensors of $(1, 1)$-bilabelled atomic graphs. These graphs are depicted in Figure 3. Their homomorphism tensors are the all-ones matrix, the adjacency matrix of the graph, and the identity matrix.

▶ **Definition 20.** *Let $t \geq 1$. The t-adjacency algebra $\mathcal{A}_G^t$ of a graph G is the self-symmetrical coherent algebra generated by the homomorphism tensors of the atomic graphs $\mathcal{A}_t$.*
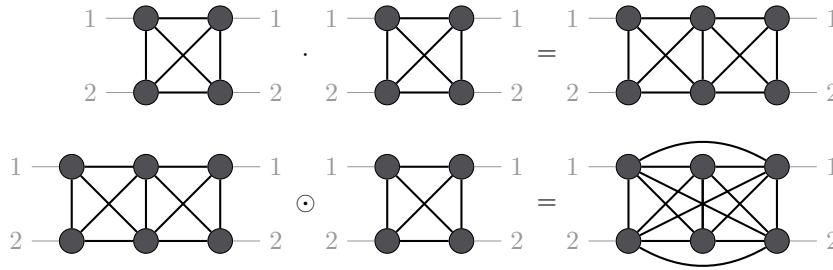
Figure 4 The bilabelled graphs in Observation 23 for $t = 2$.

Two n-vertex graphs G and H are t-equivalent if there is t-equivalence, i.e. a vector space isomorphism $\varphi \colon \mathcal{A}_G^t \to \mathcal{A}_H^t$ such that

1. $\varphi(M^*) = \varphi(M)^*$ for all $M \in \mathcal{A}_G^t$,
2. $\varphi(MN) = \varphi(M)\varphi(N)$ for all $M, N \in \mathcal{A}_G^t$,
3. $\varphi(I) = I$, $\varphi(\boldsymbol{A}_G) = \boldsymbol{A}_H$ for all $\boldsymbol{A} \in \mathcal{A}_t$, and $\varphi(J) = J$,
4. $\varphi(M \odot N) = \varphi(M) \odot \varphi(N)$ for all $M, N \in \mathcal{A}_G^t$.
5. $\varphi(M^\sigma) = \varphi(M)^\sigma$ for all $M \in \mathcal{A}_G^t$ and all $\sigma \in \mathfrak{S}_{2t}$.

The following Theorem 21 extends [22, Theorem 6.3]. Its proof is deferred to the full version [28].

▶ **Theorem 21.** *Let $t \geq 1$. Two graphs G and H are t-equivalent if and only if there is a level-t $\mathcal{DNN}$-isomorphism map from G to H.*

4 Homomorphism Indistinguishability

Using techniques from [15], we finally establish a characterisation of when the level-t Lasserre relaxation of $\mathrm{ISO}(G, H)$ is feasible in terms of homomorphism indistinguishability of G and H. In order to do so, we introduce the graph classes $\mathcal{L}_t$ and $\mathcal{L}_t^+$. In Section 4.1, we relate $\mathcal{L}_t$ and $\mathcal{L}_t^+$ to the classes of graphs of bounded treewidth and pathwidth obtaining the results depicted in Figure 1. In Section 4.2, $\mathcal{L}_1$ and $\mathcal{L}_1^+$ are identified as the classes of outerplanar graphs and graphs of treewidth two, respectively.

▶ **Definition 22.** *Let $t \geq 1$. Write $\mathcal{L}_t^+$ for the class of (t, t)-bilabelled graphs generated by the set of atomic graphs $\mathcal{A}_t$ under parallel composition, series composition, and the action of $\mathfrak{S}_{2t}$ on the labels.*

Write $\mathcal{L}_t \subseteq \mathcal{L}_t^+$ for the class of (t, t)-bilabelled graphs generated by the set of atomic graphs $\mathcal{A}_t$ under parallel composition with graphs from $\mathcal{A}_t$, series composition, and the action of $\mathfrak{S}_{2t}$ on the labels.

Note that the only difference between $\mathcal{L}_t$ and $\mathcal{L}_t^+$ is that $\mathcal{L}_t$ is closed under parallel composition with atomic graphs only. This reflects an observation by [15] relating the closure under arbitrary gluing products to non-negative solutions to systems of equations characterising homomorphism indistinguishability. Intuitively, one may use arbitrary Schur products, the algebraic counterparts of gluing, for a Vandermonde interpolation argument, cf. [14, Appendix B.4].

The following Observation 23 illustrates how the operations in Definition 22 can be used to generate more complicated graphs from the atomic graphs, cf. Figure 4.

▶ **Observation 23.** *Let $t \geq 1$. The class $\mathcal{L}_t$ contains a bilabelled graph whose underlying unlabelled graph is isomorphic to the $3t$-clique K_{3t}.*

Proof. Let $\boldsymbol{E} \coloneqq \bigodot_{1 \leq i < j \leq 2t} \boldsymbol{A}^{ij} \in \mathcal{A}_t$. The graph underlying $\boldsymbol{E} \odot (\boldsymbol{E} \cdot \boldsymbol{E})$ is isomorphic to K_{3t}. ◄

The only missing implications of Theorems 9 and 10 follow from the next two theorems:

▶ **Theorem 24.** *Let $t \geq 1$. Two graphs G and H are homomorphism indistinguishable over $\mathcal{L}_t$ if and only if they are partially t-equivalent.*

▶ **Theorem 25.** *Let $t \geq 1$. Two graphs G and H are homomorphism indistinguishable over $\mathcal{L}_t^+$ if and only if they are t-equivalent.*

For the proofs of Theorems 24 and 25, we extend the framework developed by [15]. In this work, the authors introduced tools for constructing systems of equations characterising homomorphism indistinguishably over classes of labelled graphs. A requirement of these tools is that the graph class in question is *inner-product compatible* [15, Definition 24]. This means that for every two labelled graphs $\boldsymbol{R}$ and $\boldsymbol{S}$ one can write the inner-product of their homomorphism vectors $\boldsymbol{R}_G$ and $\boldsymbol{S}_G$ as the sum-of-entries of some $\boldsymbol{T}_G$ where $\boldsymbol{T}$ is labelled graph from the class. Due to the correspondence between combinatorial operations on labelled graphs and algebraic operations on their homomorphism vectors, cf. Section 2.2, this is equivalent to the graph theoretic assumption that $\mathrm{soe}(\boldsymbol{R} \odot \boldsymbol{S}) = \mathrm{soe}(\boldsymbol{T})$, i.e. the unlabelled graph obtained by unlabelling the gluing product of $\boldsymbol{R}$ and $\boldsymbol{S}$ can be labelled such that the resulting labelled graph is in the class.

We extend this notion to bilabelled graphs. A class of (t,t)-bilabelled graphs $\mathcal{S}$ is said to be *inner-product compatible* if for all $\boldsymbol{R}, \boldsymbol{S} \in \mathcal{S}$ there is a graph $\boldsymbol{T} \in \mathcal{S}$ such that $\mathrm{tr}(\boldsymbol{R} \cdot \boldsymbol{S}^*) = \mathrm{soe}(\boldsymbol{T})$. This definition is inspired by the inner-product on $\mathbb{C}^{n \times n}$ given by $\langle A, B \rangle \coloneqq \mathrm{tr}(AB^*)$.

▶ **Lemma 26.** *Let $t \geq 1$. The classes $\mathcal{L}_t$ and $\mathcal{L}_t^+$ are inner-product compatible.*

Proof. Since $\mathcal{L}_t$ is closed under matrix products and taking transposes, it suffices to show that for every $\boldsymbol{S} \in \mathcal{L}_t$ the graph $\mathrm{tr}\,\boldsymbol{S}$ is the underlying unlabelled graph of some element of $\mathcal{L}_t$. Indeed, for every (t,t)-bilabelled graphs $\boldsymbol{F}$ it holds that $\mathrm{tr}(\boldsymbol{F}) = \mathrm{soe}(\boldsymbol{I}^{1,t+1} \odot \cdots \odot \boldsymbol{I}^{t,2t} \odot \boldsymbol{F})$ where the $\boldsymbol{I}^{ij}$ are as in Definition 13. Since $\mathcal{L}_t$ is closed under parallel composition with atomic graphs, the claim follows. For $\mathcal{L}_t^+$, an analogous argument yields the claim. ◄

The following Theorem 27, which extends the toolkit for constructing systems of equations characterising homomorphism indistinguishability over families of bilabelled graphs, is the bilabelled analogue of [15, Theorem 13]. Write $\mathbb{C}\mathcal{S}_G \subseteq \mathbb{C}^{V(G)^t \times V(G)^t}$ for the vector space spanned by homomorphism tensors $\boldsymbol{S}_G$ for $\boldsymbol{S} \in \mathcal{S}$.

▶ **Theorem 27.** *Let $t \geq 1$ and $\mathcal{S}$ be an inner-product compatible class of (t,t)-bilabelled graphs containing $\boldsymbol{J}$. For graphs G and H, the following are equivalent:*

1. *G and H are homomorphism indistinguishable over $\mathcal{S}$,*
2. *there exists a sum-preserving vector space isomorphism $\varphi \colon \mathbb{C}\mathcal{S}_G \to \mathbb{C}\mathcal{S}_H$ such that $\varphi(\boldsymbol{S}_G) = \boldsymbol{S}_H$ for all $\boldsymbol{S} \in \mathcal{S}$.*

Theorems 24 and 25 follows from this theorem as described in the full version [28].

4.1 The Classes $\mathcal{L}_t$ and $\mathcal{L}_t^+$ and Graphs of Bounded Treewidth

In this section, the classes $\mathcal{L}_t$ and $\mathcal{L}_t^+$ are compared to the classes of graphs of bounded treewidth and pathwidth. Figure 1 depicts the relationships between these classes. The first result, Lemma 28, gives an upper bound on the treewidth of graphs in $\mathcal{L}_t^+$.

▶ **Lemma 28.** *Let $t \geq 1$. The treewidth of an unlabelled graph F underlying some $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v}) \in \mathcal{L}_t^+$ is at most $3t - 1$.*

Proof. By structural induction, it is shown that every $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v}) \in \mathcal{L}_t^+$ admits a tree decomposition $\beta \colon V(T) \to 2^{V(F)}$ of width at most $3t-1$ such that the labelled vertices $\boldsymbol{u}$ and $\boldsymbol{v}$ lie together in one bag, i.e. there exists $x \in V(T)$ such that $\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_t, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_t\} \subseteq \beta(x)$.

This is clearly the case for all $\boldsymbol{F} \in \mathcal{A}_t$. Let $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v})$ and $\boldsymbol{F}' = (F', \boldsymbol{u}', \boldsymbol{v}')$ from $\mathcal{L}_t^+$ be given. Suppose there are tree decompositions $\beta \colon V(T) \to 2^{V(F)}$ and $\beta' \colon V(T') \to 2^{V(F')}$ as in the inductive hypothesis. Let $x \in V(T)$ and $x' \in V(T')$ be such that the labelled vertices of $\boldsymbol{F}$ and $\boldsymbol{F}'$ lie in $\beta(x)$ and $\beta'(x')$ respectively. Let S be the tree obtained by taking the disjoint union of T, T', and a fresh vertex y, and connecting x and x' to y.

For the graph $\boldsymbol{F} \cdot \boldsymbol{F}'$, an S-decomposition is given by the function

$$
\gamma \colon z \mapsto \begin{cases} \beta(z), & \text{if } z \in V(T), \\ \beta'(z), & \text{if } z \in V(T'), \\ \{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_t, \boldsymbol{v}_1', \ldots, \boldsymbol{v}_t', \boldsymbol{v}_1, \ldots, \boldsymbol{v}_t\}, & \text{if } z = y. \end{cases}
$$

where one may note that $\boldsymbol{v}_i = \boldsymbol{u}_i'$ for every $i \in [t]$ in $\boldsymbol{F} \cdot \boldsymbol{F}'$. It is easy to check that Definition 6 is satisfied. The decomposition is of width $3t - 1$.

For the graph $\boldsymbol{F} \odot \boldsymbol{F}'$, an S-decomposition is given by the function

$$
\gamma \colon z \mapsto \begin{cases} \beta(z), & \text{if } z \in V(T), \\ \beta'(z), & \text{if } z \in V(T'), \\ \{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_t, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_t\}, & \text{if } z = y. \end{cases}
$$

where one may note that $\boldsymbol{u}_i = \boldsymbol{u}_i'$ and $\boldsymbol{v}_i = \boldsymbol{v}_i'$ for every $i \in [t]$ in $\boldsymbol{F} \odot \boldsymbol{F}'$. Again, it is easy to check that Definition 6 is satisfied. The decomposition is of width at most $3t - 1$. ◄

Lemma 28 in conjunction with Theorems 9 and 10 implies Theorems 2 and 3. As a corollary, this yields the upper bound in Theorem 1. Indeed, by Theorem 8, $G \simeq_t^{\mathrm{SA}} H$ if and only if G and H are homomorphism indistinguishable over the class of graphs of treewidth at most $t - 1$. Hence, if $G \simeq_{3t}^{\mathrm{SA}} H$ then $G \simeq_t^{\mathrm{L}^+} H$ and in particular $G \simeq_t^{\mathrm{L}} H$.

It remains to show the lower bound asserted by Theorem 1, i.e. that $3t$ cannot be replaced by $3t - 1$ for no $t \geq 1$. To that end, first observe that Observation 23 implies that the bound in Lemma 28 is tight. However, this syntactic property of the graph class $\mathcal{L}_t$ does not suffice to derive the aforementioned semantic property of $\simeq_t^{\mathrm{SA}}$ and $\simeq_t^{\mathrm{L}}$. In fact, it could well be that for all graphs G and H if G and H are homomorphism indistinguishable over the graphs of treewidth at most $3t - 2$ also $\hom(K_{3t}, G) = \hom(K_{3t}, H)$ despite that $\mathrm{tw}\, K_{3t} > 3t - 2$. That this does not hold is implied by a conjecture of the first author [27] which asserts that every minor-closed graph class $\mathcal{F}$ which is closed under taking disjoint unions (*union-closed*) is *homomorphism distinguishing closed*, i.e. for all $F \notin \mathcal{F}$ there exist graphs G and H such that $G \equiv_{\mathcal{F}} H$ but $\hom(F, G) \neq \hom(F, H)$. Although being generally open, this conjecture was proven by Neuen [24] for the class of graphs of treewidth at most t for every t. Theorem 29 implies the last assertion of Theorem 1.

▶ **Theorem 29.** *For every $t \geq 1$, there exist graphs G and H such that $G \simeq^{\text{SA}}_{3t-1} H$ and $G \not\simeq^{\text{L}}_{t} H$.*

Proof. Towards a contraction, suppose that $G \simeq^{\text{SA}}_{3t-1} H \implies G \simeq^{\text{L}}_{t} H$ for all graphs G and H. By Theorem 8, $G \simeq^{\text{SA}}_{3t-1} H$ if and only if G and H are homomorphism indistinguishable over the class $\mathcal{TW}_{3t-2}$ of graphs of treewidth at most $3t - 2$. By Observation 23 and Theorem 9, if $G \equiv_{\mathcal{TW}_{3t-2}} H$ then $G \equiv_{\mathcal{L}_t} H$ and in particular $\hom(K_{3t}, G) = \hom(K_{3t}, H)$. As shown in [24], the class $\mathcal{TW}_{3t-2}$ is homomorphism distinguishing closed. As $\operatorname{tw} K_{3t} = 3t - 1$, it follows that there exist graphs G and H with $G \simeq^{\text{SA}}_{3t-1} H$ and $\hom(K_{3t}, G) \neq \hom(K_{3t}, H)$. In particular, $G \not\simeq^{\text{L}}_{t} H$ by Theorem 9.   ◀

It is worth noting that the classes of unlabelled graphs underlying the elements of $\mathcal{L}_t$ and $\mathcal{L}_t^+$ are themselves minor-closed and union-closed. Hence, they are subject to the aforementioned conjecture. Furthermore, by the Robertson–Seymour Theorem and [29], membership in $\mathcal{L}_t$ and $\mathcal{L}_t^+$ can be tested in polynomial time for every fixed $t \geq 1$. The proof of Lemma 30 is deferred to the full version [28].

▶ **Lemma 30.** *Let $t \geq 1$. The class of graphs underlying the elements of $\mathcal{L}_t$ and the class of graphs underlying the elements of $\mathcal{L}_t^+$ are minor-closed and union-closed.*

The remainder of this section is dedicated to some further relations between the classes of graphs of bounded treewidth or pathwidth, $\mathcal{L}_t$, and $\mathcal{L}_t^+$. Note that these facts give independent proofs for the correspondence between the feasibility of the level-t Sherali–Adams relaxation (without non-negativity constraints), which corresponds to homomorphism indistinguishability over graphs of treewidth (pathwidth) at most $t-1$, as proven by [9, 15], and the feasibility of the level-t Lasserre relaxation with and without non-negativity constraints.

First of all, it is easy to see that dropping the semidefiniteness constraint Equation (4) of the level-t Lasserre system of equations turns this system essentially into the level-$2t$ Sherali–Adams system of equations without non-negativity constraints, e.g. as defined in [14, Appendix D.1]. This is paralleled by Lemma 31.

▶ **Lemma 31.** *Let $t \geq 1$. For every graph F with $\operatorname{pw} F \leq 2t - 1$, there is a graph $\boldsymbol{F} \in \mathcal{L}_t$ whose underlying unlabelled graph is isomorphic to F.*

Furthermore, one may drop Equation (4) from the level-t Lasserre system of equations with non-negativity constraints to obtain the level-$2t$ Sherali–Adams system of equations in its original form, i.e. with non-negativity constraints. This is paralleled by Lemma 32.

▶ **Lemma 32.** *Let $t \geq 1$. For every graph F with $\operatorname{tw} F \leq 2t - 1$, there is a graph $\boldsymbol{F} \in \mathcal{L}_t^+$ whose underlying unlabelled graph is isomorphic to F.*

Since the diagonal entries of a positive semidefinite matrix are necessarily non-negative, Equation (4) implies that any solution (y_I) to the level-t Lasserre system of equations is such that $y_I \geq 0$ for all $I \in \binom{V(G) \times V(H)}{\leq t}$. Hence, such a solution is a solution to the level-t Sherali–Adams system of equations as well. This is paralleled by Lemma 33.

▶ **Lemma 33.** *Let $t \geq 1$. For every graph F with $\operatorname{tw} F \leq t - 1$, there is a graph $\boldsymbol{F} \in \mathcal{L}_t$ whose underlying unlabelled graph is isomorphic to F.*

The proofs of Lemmas 31–33 are all by inductively constructing an element of $\mathcal{L}_t^+$ using a tree decomposition of the given graph. They are deferred to the full version [28].

4.2 The Classes $\mathcal{L}_1$ and $\mathcal{L}_1^+$

The classes $\mathcal{L}_1$ and $\mathcal{L}_1^+$ can be identified as the class of outerplanar graphs and as the class of graphs of treewidth at most two, respectively. This yields Theorem 5. Proofs are deferred to the full version [28].

▶ **Proposition 34.** *The class of unlabelled graphs underlying an element of $\mathcal{L}_1^+$ coincides with the class of graphs of treewidth at most two.*

A graph F is *outerplanar* if it does not have K_4 or $K_{2,3}$ as a minor. Equivalent, it is outerplanar if it has a planar drawing such that all its vertices lie on the same face [34].

▶ **Proposition 35.** *The class of unlabelled graphs underlying an element of $\mathcal{L}_1$ coincides with the class of outerplanar graphs.*

As a corollary of Proposition 35, we observe the following:

▶ **Corollary 36.** *If $G \equiv_{\mathcal{L}_1} H$ then G is connected iff H is connected.*

5 Deciding Exact Feasibility of the Lasserre Relaxation with Non-Negativity Constraints in Polynomial Time

This section is dedicated to proving Theorem 4. To that end, it is argued that $\simeq_t^{\mathrm{L}^+}$ has equivalent characterisations in terms of logical equivalence and a colouring algorithm akin to the k-dimensional Weisfeiler–Leman algorithm [36]. This algorithm has polynomial running time. It is defined as follows:

▶ **Definition 37.** *Let $t \geq 1$, define for a graph G, $i \geq 1$, and $\boldsymbol{r}, \boldsymbol{s} \in V(G)^t$*

$$\mathsf{mwl}_G^0(\boldsymbol{rs}) := \mathrm{rel}_G(\boldsymbol{rs}),$$
$$\mathsf{mwl}_G^{i-1/2}(\boldsymbol{rs}) := \left(\mathsf{mwl}_G^{i-1}(\sigma(\boldsymbol{rs})) \mid \sigma \in \mathfrak{S}_{2t}\right),$$
$$\mathsf{mwl}_G^i(\boldsymbol{rs}) := \left(\mathsf{mwl}_G^{i-1/2}(\boldsymbol{rs}), \left\{\!\!\left\{ \left(\mathsf{mwl}_G^{i-1/2}(\boldsymbol{rt}), \mathsf{mwl}_G^{i-1/2}(\boldsymbol{ts})\right) \mid \boldsymbol{t} \in V(G)^t \right\}\!\!\right\}\right).$$

The mwl_G^i for $i \in \mathbb{N}$ define increasingly fine colourings of $V(G)^{2t}$. Let mwl_G^∞ denote the finest such colouring. Two graphs G and H are not distinguished by the t-dimensional mwl algorithm if the multisets

$$\left\{\!\!\left\{ \mathsf{mwl}_G^\infty(\boldsymbol{rs}) \mid \boldsymbol{r}, \boldsymbol{s} \in V(G)^t \right\}\!\!\right\} \quad \textit{and} \quad \left\{\!\!\left\{ \mathsf{mwl}_H^\infty(\boldsymbol{uv}) \mid \boldsymbol{u}, \boldsymbol{v} \in V(H)^t \right\}\!\!\right\}$$

are the same.

Since the finest colouring mwl_G^∞ is reached in $\leq n^{2t} - 1$ iterations for graphs on n vertices, for fixed t, it can be tested in polynomial time whether two graphs are not distinguished by the t-dimensional mwl algorithm. We are about to show that the latter happens if and only if the level-t Lasserre relaxation with non-negative constraints is feasible. As a by-product, we obtain a logical characterisation for this equivalence relation.

▶ **Definition 38.** *For $t \geq 1$, let M^t denote the fragment of first-order logic with counting quantifiers and at most $3t$ variables comprising the following expressions:*
- *$x_i = x_j$ and $Ex_i x_j$ for all $i, j \in [3t]$,*
- *if $\varphi, \psi \in \mathsf{M}^t$ then $\neg\varphi$, $\varphi \wedge \psi$, and $\varphi \vee \psi$ are in M^t,*
- *if $\varphi, \psi \in \mathsf{M}^t$ and $n \in \mathbb{N}$ then $\exists^{\geq n}\boldsymbol{y}.\ \varphi(\boldsymbol{x}, \boldsymbol{y}) \wedge \psi(\boldsymbol{y}, \boldsymbol{z})$ is in M^t. Here, the bold face letters $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$ denote t-tuples of distinct variables.*

The semantic of the quantifier $\exists^{\geq n} \boldsymbol{y}. \; \varphi(\boldsymbol{y})$ is that there exist at least n many t-tuples of vertices from the graph over which the formula is evaluated which satisfy φ. The following Theorem 39 may be thought of as a analogue of Theorem 8 for $\mathcal{L}_t^+$.

▶ **Theorem 39.** *Let $t \geq 1$. For graphs G and H, the following are equivalent:*
1. *G and H are not distinguished by the t-dimensional mwl algorithm,*
2. *G and H are homomorphism indistinguishable over $\mathcal{L}_t^+$,*
3. *G and H satisfy the same M^t-sentences.*

The proof of Theorem 39 is deferred to the full version [28]. It is conceptually similar to arguments of [6, 10, 15]. As mentioned above, Theorem 39 implies Theorem 4.

6 Conclusion

We have established a characterisation of the feasibility of the level-t Lasserre relaxation with and without non-negativity constraints of the integer program $\mathrm{ISO}(G, H)$ for graph isomorphism in terms of homomorphism indistinguishability over the graph classes $\mathcal{L}_t$ and $\mathcal{L}_t^+$. By analysing the treewidth of the graphs $\mathcal{L}_t$ and $\mathcal{L}_t^+$ and invoking results from the theory of homomorphism indistinguishability, we have determined the precise number of Sherali–Adams levels necessary such that their feasibility guarantees the feasibility of the level-t Lasserre relaxation. This concludes a line of research brought forward in [4]. For feasibility of the level-t Lasserre relaxation with non-negativity constraints, we have given, besides linear algebraic reformulations generalising the adjacency algebra of a graph, a polynomial time algorithm deciding this property.

Missing in Theorem 1 is a tight lower bound on the number of Lasserre levels necessary to ensure feasibility of a given Sherali–Adams level:

▶ **Question 40.** *Do there exist for every $t \geq 3$ graphs G and H such that $G \simeq_{t-1}^{\mathrm{L}} H$ and $G \not\simeq_t^{\mathrm{SA}} H$?*

Following the path taken in this paper, this question could potentially be resolved in two steps: Firstly, one would need to prove the graph theoretic assertion that the class $\mathcal{L}_t$ does not contain $\mathcal{TW}_t$ for all $t \geq 2$. Secondly, one would need to show that $\mathcal{L}_t$ is homomorphism distinguishing closed or at least that the homomorphism distinguishing closure [27] of $\mathcal{L}_t$ does not contain $\mathcal{TW}_t$ for all $t \geq 2$. Given the means currently available for proving such a statement [27, 24], this would involve giving game characterisations for $\mathcal{L}_t$ (mimicking the robber-cops game for $\mathcal{TW}_t$) and for $\equiv_{\mathcal{L}_t}$ (similar to the bijective $(t+1)$-pebble game for $\mathcal{TW}_t$). For the former, finding analogies to the notions of brambles or heavens seems necessary [31].

Another interesting extension of our work might be an efficient algorithm for computing an explicit partial t-equivalence between two graphs, cf. Definitions 18 and 20, or deciding that no such map exists. This would yield an efficient algorithm for deciding the exact feasibility of the Lasserre semidefinite program without non-negativity constraints, cf. [4].

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