The Complexity of Homomorphism Indistinguishability

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Abstract

For every graph class $\mathcal{F}$, let HomInd($\mathcal{F}$) be the problem of deciding whether two given graphs are homomorphism-indistinguishable over $\mathcal{F}$, i.e., for every graph F in $\mathcal{F}$, the number $\mathsf{hom}(F, G)$ of homomorphisms from F to G equals the corresponding number $\mathsf{hom}(F, H)$ for H. For several natural graph classes (such as paths, trees, bounded treewidth graphs), homomorphism-indistinguishability over the class has an efficient structural characterization, resulting in polynomial time solvability [6].

In particular, it is known that two non-isomorphic graphs are homomorphism-indistinguishable over the class $\mathcal{T}_k$ of graphs of treewidth k if and only if they are not distinguished by k-dimensional Weisfeiler-Leman algorithm, a central heuristic for isomorphism testing: this characterization implies a polynomial time algorithm for HomInd($\mathcal{T}_k$), for every fixed $k \in \mathbb{N}$. In this paper, we show that there is a polynomial-time-decidable class $\mathcal{F}$ of undirected graphs of *bounded* treewidth such that HomInd($\mathcal{F}$) is undecidable.

Our second hardness result concerns the class $\mathcal{K}$ of complete graphs. We show that HomInd($\mathcal{K}$) is co-NP-hard, and in fact, we show completeness for the class $\mathsf{C_{=}P}$ (under P-time Turing reductions). On the algorithmic side, we show that HomInd($\mathcal{P}$) can be solved in polynomial time for the class $\mathcal{P}$ of directed paths. We end with a brief study of two variants of the HomInd($\mathcal{F}$) problem: (a) the problem of lexographic-comparison of homomorphism numbers of two graphs, and (b) the problem of computing certain distance-measures (defined via homomorphism numbers) between two graphs.

1 Introduction

A classic theorem due to Lovász [12] states that two graphs G, H are isomorphic if and only if for every graph F the number $\mathsf{hom}(F, G)$ of homomorphisms from F to G is equal to the number $\mathsf{hom}(F, H)$ of homomorphisms from F to H. Jointly with Dell, the last two authors of this paper recently proved [6] that two graphs are fractionally isomorphic, or equivalently, can be distinguished by the colour refinement algorithm (see e.g. [8]), if and only if for every tree T it holds that $\mathsf{hom}(T, G) = \mathsf{hom}(T, H)$. Another well-known fact (see e.g. [20]) is that

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two graphs are co-spectral, that is, their adjacency matrices have the same sequence of eigenvalues, if and only if for every cycle C it holds that $\mathsf{hom}(C, G) = \mathsf{hom}(C, H)$. Thus counting homomorphisms from all graphs in some class gives us very interesting equivalence relations, which we call homomorphism indistinguishability: for every class $\mathcal{F}$ of graphs, two graphs G, H are *homomorphism-indistinguishable over $\mathcal{F}$* (for short: $\mathcal{F}$-HI) if and only if for every $F \in \mathcal{F}$ it holds that $\mathsf{hom}(F, G) = \mathsf{hom}(F, H)$.[1] Thus two graphs are $\mathcal{G}$-HI for the class $\mathcal{G}$ of all graphs if and only if they are isomorphic. They are $\mathcal{T}$-HI for the class $\mathcal{T}$ of trees if and only if they are fractionally isomorphic, and they are $\mathcal{C}$-HI for the class $\mathcal{C}$ of cycles if and only if they are co-spectral. We have also proved in [6] that for every k, two graphs are $\mathcal{T}_k$-HI for the class $\mathcal{T}_k$ of all graphs of tree width at most k if and only if the k-dimensional Weisfeiler-Leman algorithm does not distinguish them, and we gave a characterisation of $\mathcal{P}$-HI for the class $\mathcal{P}$ of paths in terms of a natural system of linear equations. Furthermore, the first author of this paper recently proved that two directed graphs are $\mathcal{A}$-HI for the class $\mathcal{A}$ of all directed acyclic graphs if and only if they are isomorphic [3] (also see [13]).

It follows from these results that the problem of deciding whether two graphs are homomorphism-indistinguishable over some class has a quite interesting complexity theoretic behaviour. For every class $\mathcal{F}$ of graphs, let $\mathrm{HOMIND}(\mathcal{F})$ be the problem of deciding whether two given graphs are $\mathcal{F}$-HI. Since the graph isomorphism problem is in solvable in quasipoly-nomial time [2], $\mathrm{HOMIND}(\mathcal{G})$ is in quasipolynomial time. Furthermore, it is an immediate consequence of the characterisations above that $\mathrm{HOMIND}(\mathcal{T})$, $\mathrm{HOMIND}(\mathcal{C})$, $\mathrm{HOMIND}(\mathcal{P})$, and $\mathrm{HOMIND}(\mathcal{T}_k)$ for all $k \geq 1$ are in polynomial time. This prompts the question whether $\mathrm{HOMIND}(\mathcal{F})$ is in quasipolynomial time, or even in polynomial time, for every class $\mathcal{F}$ of graphs. While this seems unlikely, it is not obvious what complexities one might expect for $\mathrm{HOMIND}(\mathcal{F})$ as $\mathcal{F}$ ranges over all classes of graphs. We study these and related questions here.

Homomorphism counts give us embeddings of graphs into an infinite dimensional vector space: for a class $\mathcal{F}$, we can associate with every graph G a *homomorphism vector* $\mathsf{Hom}_{\mathcal{F}}(G) := \big(\mathsf{hom}(F, G) \mid F \in \mathcal{F}\big) \in \mathbb{R}^{\mathcal{F}}$. Then $\mathrm{HOMIND}(\mathcal{F})$ is simply the problem of deciding whether two graphs have the same homomorphism vector. Defining a metric or, even better, an inner product on the range vector space, we obtain a (pseudo-)metric on the class of all graphs (where two non-isomorphic graphs may have distance 0). We will also study the problem of approximately computing the distance between two graphs with respect to metrics obtained this way. Such metrics are important for machine learning tasks such as clustering and classification on graphs. In fact, homomorphism vectors are closely related to the so-called graph kernels (see, e.g. [16, 17, 21]): almost all such graph kernels are defined as the inner products of homomorphism vectors for natural graph classes. Thus our results shed some new light on the complexity of computing these kernels.

At first sight, $\mathrm{HOMIND}(\mathcal{F})$ looks like a problem in co-NP: to witness that G and H are not $\mathcal{F}$-HI we just have to nondeterministically guess one $F \in \mathcal{F}$ and verify that $\mathsf{hom}(F, G) \neq \mathsf{hom}(F, H)$. But this argument is flawed for several reasons. First of all, it assumes that for given F, G we can compute $\mathsf{hom}(F, G)$ in polynomial time, which in general is not the case. Let $\#\mathrm{HOM}(\mathcal{F})$ be the problem of computing $\mathsf{hom}(F, G)$, given $F \in \mathcal{F}$ and G. Then for the class $\mathcal{G}$ of all graphs, $\#\mathrm{HOM}(\mathcal{G})$ is #P-complete. Under the complexity assumption that $\#\mathsf{W}[1] \neq \mathsf{FPT}$, it is known that $\#\mathrm{HOM}(\mathcal{F})$ is in P if and only if $\mathcal{F}$ has bounded tree

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[1] We note that homomorphism indistinguishability is incomparable to homomorphic equivalence; remember that two graphs G, H are *homomorphically equivalent* if there is a homomorphism from G to H and a homomorphism from H to G.

width [5]. This result extends to directed graphs and in fact all classes of relational structures of bounded arity. But even for $\mathcal{F}$ with tractable $\#\text{HOM}(\mathcal{F})$, the problem $\text{HOMIND}(\mathcal{F})$ is not necessarily in co-NP, because the witness F may be very large compared to G and H.

▶ **Theorem 1.** *There is a polynomial-time-decidable class $\mathcal{F}$ of undirected graphs of bounded tree width such that* $\text{HOMIND}(\mathcal{F})$ *is undecidable.*

We also prove a version of the above theorem for directed graphs (Theorem 15): the graphs in the corresponding class $\mathcal{F}$ are just directed paths padded by isolated vertices. And we cannot only prove undecidability, but also use similar arguments to obtain all kinds of complexities. So the complexity landscape for problems $\text{HOMIND}(\mathcal{F})$, which started out in quasi-polynomial time, looks fairly complicated. But admittedly the classes $\mathcal{F}$ we can use to prove Theorem 1 are quite esoteric from a graph theoretic point of view. What about "natural" graph classes? For the class $\mathcal{K}$ of all complete graphs, the corresponding problem $\text{HOMIND}(\mathcal{K})$ turns out to be hard.

▶ **Theorem 2.** $\text{HOMIND}(\mathcal{K})$ *is* co-NP*-hard.*

For an upper bound, note that $\text{HOMIND}(\mathcal{K}) \in \mathsf{P}^{\#\mathsf{P}}$, because to decide whether for two n-vertex graphs G, H it holds that $\mathsf{hom}(K, G) = \mathsf{hom}(K, H)$ for all complete graphs K, we only need to check the equality for all K of size at most n. Actually, we pinpoint the exact complexity of $\text{HOMIND}(\mathcal{K})$ by proving it to be complete for the complexity class $\mathsf{C}_=\mathsf{P}$ (see Theorem 18). This implies that $\text{HOMIND}(\mathcal{K})$ is not in the polynomial hierarchy PH unless PH collapses (see Corollary 22).

We also look at tractable cases of the homomorphism indistinguishability problem. In particular, we prove that $\text{HOMIND}(\mathcal{P}_\rightarrow)$ is in P for the class $\mathcal{P}_\rightarrow$ of directed paths (see Theorem 23).

In the last section we look at variants of $\text{HOMIND}(\mathcal{F})$. A first such variant is the problem $\text{HOMLEX}(\mathcal{F})$ of lexicographically comparing the homomorphism vectors over $\mathcal{F}$ of two input graphs. Of course the lexicographical order depends on some order of the graphs in $\mathcal{F}$; the simple classes $\mathcal{F}$ we consider (directed paths and cycles as well as complete graphs) have only one graph per size, and we can use the natural order by size. We prove that $\text{HOMLEX}(\mathcal{P}_\rightarrow)$ and $\text{HOMLEX}(\mathcal{C}_\rightarrow)$ are in polynomial time for the classes $\mathcal{P}_\rightarrow$ and $\mathcal{C}_\rightarrow$ of directed paths and cycles and that $\text{HOMLEX}(\mathcal{K})$ is $\#\mathsf{P}$-complete.

Finally, we study the problem of computing the distance between two graphs with respect to various metrics defined on the homomorphism vectors $\mathsf{Hom}_\mathcal{F}(G)$. We prove that if $\mathcal{F}$ is a polynomial time enumerable class of graphs for which $\#\text{HOM}(\mathcal{F})$ is in polynomial time then the distance between two graphs can be approximated up to an arbitrarily small additive error ε in polynomial time. This is not a deep result, but we believe it is quite relevant, because computing distances between graphs (even approximately) with respect to various distance measures tends to be a very hard algorithmic problem (e.g. [1, 9, 11, 14, 15]). Here we have a family of natural metrics for which it is tractable.

2   Preliminaries

Directed Graphs.   A directed graph (or digraph) G consists of a finite set of vertices $V(G)$ (or V_G) and a set of edges $E(G) \subseteq V \times V$. A subgraph H of a directed graph G is a graph satisfying $V_H \subseteq V_G$ and $E_H \subseteq E_G \cap (V_H \times V_H)$. We assume familiarity with the basic terminology from graph theory, e.g., path, cycle etc., which can be found in e.g., [7]. Given two digraphs G and H, a homomorphism from G to H is an edge-preserving mapping from $V(G)$ to $V(H)$, i.e., a mapping $\varphi : V_G \rightarrow V_H$ such that its natural extension to $V_G \times V_G$ satisfies $\varphi(E_G) \subseteq E_H$.

A set X of vertices of a directed graph G is a *clique* if for all distinct $x, y \in X$, either $(x, y) \in E(G)$ or $(y, x) \in E(G)$. For every $k \geq 1$, let $c_k(G)$ be the number of cliques of size k in G. For every directed graph G and every $k \geq 1$, let $d_k(G)$ be the number of directed paths of length $k - 1$ in G. We call a directed graph P a *partial order* if it is acyclic and the edge relation is transitive. Observe that if P is a partial order then the edge relation induces a linear order on every clique. Furthermore, a subgraph Q of P is a directed path if and only if $V(Q)$ is a clique in P. Thus for every $k \geq 1$ we have $c_k(P) = d_k(P)$.

Denote $\mathsf{hom}(G, H)$ to be the number of homomorphisms from G to H. For a class $\mathcal{F}$ of graphs and a graph G, the *homomorphism vector of G over $\mathcal{F}$* is

$$\mathsf{Hom}_{\mathcal{F}}(G) := \big(\mathsf{hom}(F, G) \mid F \in \mathcal{F}\big).$$

Undirected Graphs.   The notions of subgraph, homomorphisms and homomorphism vector have analogous standard definitions in the undirected case. Denote the edge $\{u, v\}$ of an undirected graph as uv. Let K_k denote the undirected k-clique, i.e. the graph defined by $V(G) = [k]$ and $E(G) = \binom{[k]}{2}$.

▶ **Definition 3.** *Let G, H be two undirected graphs. The product graph $G \otimes H$ is defined by*

$$V(G \otimes H) := V(G) \times V(H),$$
$$E(G \otimes H) := \big\{\{(u, v), (u', v')\} \mid uu' \in E(G) \text{ and } vv' \in E(H)\big\}.$$

Let G, H be two graphs, and $k \geq 1$. The following folklore lemma states that the homomorphism numbers are multiplicative for the above-mentioned product operation.

▶ **Lemma 4.** *For every graph F, $\mathsf{hom}(F, G \otimes H) = \mathsf{hom}(F, G) \cdot \mathsf{hom}(F, H)$.*

It is well-known that for every $k \in \mathbb{N}$ and every graph G, $c_k(G) = \frac{\mathsf{hom}(K_k, G)}{k!}$.

▶ **Corollary 5.** *$c_k(G \otimes H) = k! \cdot c_k(G) \cdot c_k(H)$.*

The following construction will be useful later.

▶ **Proposition 6.** *Let n, ℓ, k be fixed positive integers such that $k \leq n$ and $\ell \leq \binom{n}{k}$. In time $\mathrm{poly}(n)$, we can construct a graph P satisfying $c_k(P) = \ell$.*

Proof. Let

$$n_1 := \max\left\{n' \;\middle|\; n' \geq k \text{ and } \binom{n'}{k} \leq \ell\right\}, \quad i_1 := \max\left\{i \;\middle|\; i \cdot \binom{n_1}{k} \leq \ell\right\}.$$

Clearly, $k \leq n_1 \leq n$ and $1 \leq i_1$, and both can be computed in time $\mathrm{poly}(n)$. Moreover, the remainder

$$\ell' := \ell - i_1 \cdot \binom{n_1}{k} < \ell$$

satisfies $0 \leq \ell' < \binom{n_1}{k}$. An exhaustive application of this rule ensures the existence of numbers $1 \leq s \leq n$, $1 \leq i_1, \ldots, i_s$, and $n_s < n_{s-1} < \cdots < n_1 \leq n$ such that

$$\ell = i_1 \cdot \binom{n_1}{k} + \cdots + i_s \cdot \binom{n_s}{k}.$$

Moreover, all $i_1, \ldots, i_s$ and $n_1, \ldots, n_s$ can be computed in time $\mathrm{poly}(n)$. Finally, the desired graph P consists of i_1 disjoint copies of K_{n_1}, i_2 disjoint copies of K_{n_2}, and so on. Clearly, $c_k(P) = \ell$ by our construction.   ◀

Cayley-Hamilton. The famous Cayley-Hamilton theorem states that the substitution of a matrix in its characteristic polynomial results in the zero matrix. Formally, let $A \in \mathbb{F}^{n \times n}$ be a square matrix over a field $\mathbb{F}$.

▶ **Theorem 7** (Cayley-Hamilton). *Let $p(\lambda) = \det(\lambda I_n - A)$ denote the characteristic polynomial of A. Then, $p(A) = 0$.*

Let $\mathrm{sum}(A)$ denote the sum of all entries of A. Recall that the trace of a matrix A, denoted by $\mathrm{tr}(A)$, is the sum of diagonal entries of A. The following lemma is standard.

▶ **Lemma 8.** *Let $A = A(G)$ be the adjacency matrix of a digraph G and $k \geq 1$. The number of walks of length k in A is equal to $\mathrm{sum}(A^k)$. Equivalently, $\mathrm{sum}(A^k) = \mathsf{hom}(P_k, G)$.*

Similarly, the number of closed walks of length k in G is equal to $\mathrm{tr}(A^k)$. Equivalently, $\mathrm{tr}(A^k) = \mathsf{hom}(C_k, G)$.

The following is a consequence of the Cayley-Hamilton theorem and is utilised in Section 6 for our tractability result regarding $\textsc{HomInd}(\mathcal{P}_\rightarrow)$ for the class $\mathcal{P}_\rightarrow$ of directed paths.

▶ **Corollary 9.** *Let $A \in \mathbb{F}^{n \times n}$. There exist $a_1, \ldots, a_n \in \mathbb{R}$ such that for every $\ell \geq 0$*

$$A^{n+\ell} = \sum_{i \in [n]} a_i A^{i+\ell-1}.$$

Thus

$$\mathrm{sum}(A^{n+\ell}) = \sum_{i \in [n]} a_i \cdot \mathrm{sum}(A^{i+\ell-1}) \quad and \quad \mathrm{tr}(A^{n+\ell}) = \sum_{i \in [n]} a_i \cdot \mathrm{tr}(A^{i+\ell-1}).$$

3 Combinatorial Constructions

Theorem 10 presents our main construction, which is at the heart of both our undecidability results in Section 4 and our hardness results in Section 5. Essentially, for an arbitrary $k \geq 1$, we construct two partial orders that have the same number of directed paths on i vertices for every $i \geq 1$ except for $i = k$. Hence, these partial orders are distinguished by the directed path of length $k - 1$ but not by any other directed path.

▶ **Theorem 10.** *For every $k \geq 1$, there are partial orders P_k, Q_k of order $|P_k|, |Q_k| \leq \max\{1, 2(k-1)\}$ such that*

$$d_i(P_k) = d_i(Q_k) \qquad \qquad for\ 1 \leq i \leq k-1, \qquad (1)$$
$$d_k(P_k) = 1, \quad d_k(Q_k) = 0, \qquad \qquad \qquad (2)$$
$$d_i(P_k) = d_i(Q_k) = 0 \qquad \qquad for\ all\ i > k. \qquad (3)$$

Proof. For a directed graph G, a set $X \subseteq V(G)$, and a fresh vertex $x \notin V(G)$, let $G \rhd_X x$ be the graph obtained from G by adding vertex x and edges from all vertices in X to x. Formally, $V(G \rhd_X x) := V(G) \cup \{x\}$ and $E(G \rhd_X x) := E(G) \cup \{(x', x) \mid x' \in X\}$.
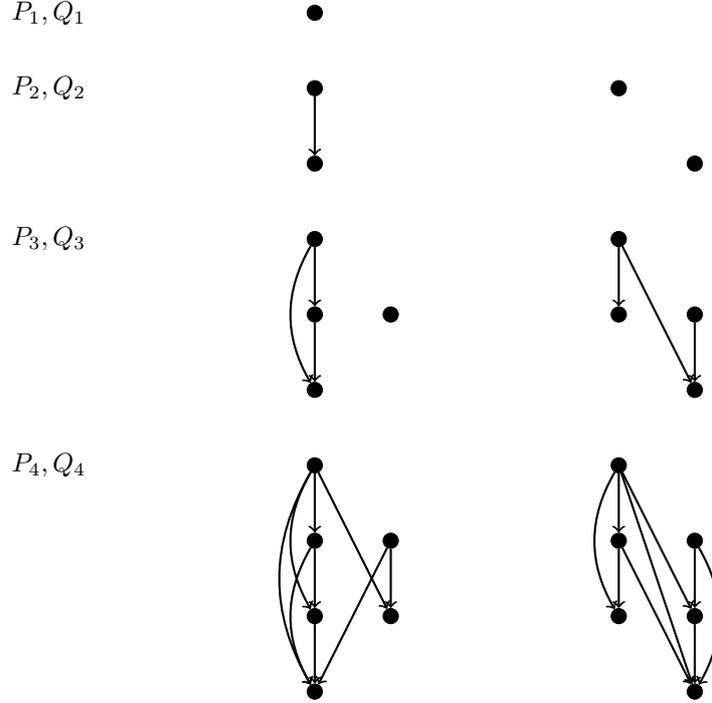
Let us describe the construction of the directed graphs P_k, Q_k. Let v_i for $i \geq 1$ and w_i for $i \geq 2$ be fresh vertices. Let

$$\begin{aligned}
V_1 &:= \{v_1\}, & P_1 &:= (V_1, \emptyset), \\
W_1 &:= \emptyset, & Q_1 &:= (W_1, \emptyset), \\
V_2 &:= \{v_1, v_2\}, & P_2 &:= (\{V_2, \{(v_1, v_2)\}\}), \\
W_2 &:= \{v_1, w_2\} & Q_2 &:= (W_2, \emptyset),
\end{aligned}$$

and for $k \geq 2$, noting that $W_{k-1} \subseteq V_k$ and $V_{k-1} \subseteq W_k$, let

$$V_{k+1} := V_k \cup \{v_{k+1}, w_k\}, \qquad\qquad P_{k+1} := (P_k \rhd_{V_k} v_{k+1}) \rhd_{W_{k-1}} w_k,$$
$$W_{k+1} := W_k \cup \{v_k, w_{k+1}\}, \qquad\qquad Q_{k+1} := (Q_k \rhd_{W_k} w_{k+1}) \rhd_{V_{k-1}} v_k.$$

Figure 1 illustrates the construction for $1 \leq k \leq 4$.

Figure 1 The graphs P_k, Q_k for $k = 1, \ldots, 4$.

Note that both P_k and Q_k are directed acyclic graphs. Obviously, we have $|V_k|, |W_k| \leq \max\{1, 2(k-1)\}$ for all k. By $G[X]$, we denote the induced subgraph of a set X in a graph G. Observe that for all $\ell \geq k \geq 1$ we have $P_\ell[X] = P_k[X]$ for all $X \subseteq V_k$ and $Q_\ell[Y] = Q_k[Y]$ for all $Y \subseteq W_k$.

▷ **Claim 11.** For all $\ell > k \geq 1$ it holds that $P_\ell[W_k] = Q_k$ and $Q_\ell[V_k] = P_k$.

Proof. It suffices to prove the claim for $\ell = k + 1$. The proof is by induction on k. For $k = 1, 2$, the assertion is immediate from Figure 1. For the inductive step, let $k \geq 2$. By the induction hypothesis, we have $P_k[W_{k-1}] = Q_{k-1}$. To construct Q_k from Q_{k-1}, we add the vertex w_k and edges from all vertices in W_{k-1} to w_k. Moreover, we add v_{k-1} and edges from all vertices in V_{k-2} to v_{k-1}. Both of these vertices and all these edges are present in P_{k+1}:

- v_{k-1} and edges from all vertices in V_{k-2} to v_{k-1} have already been added in the transition from P_{k-2} to P_{k-1};
- w_k and edges from all vertices in W_{k-1} to w_k are added in the transition from P_k to P_{k+1}.

Thus $P_{k+1}[W_k] = Q_k$. The argument that $Q_{k+1}[V_k] = P_k$ is similar. ◁

Since $V_{k+1} = V_k \cup W_k \cup \{v_{k+1}\}$ and $W_{k+1} = V_k \cup W_k \cup \{w_{k+1}\}$, a consequence of this claim is that

$$P_{k+1} \cap Q_{k+1} = P_{k+1} \setminus \{v_{k+1}\} = Q_{k+1} \setminus \{w_{k+1}\} = P_k \cup Q_k. \tag{4}$$

▷ **Claim 12.** The edge relations of P_k and Q_k are transitive.

Proof. This follows by induction from (4), because v_k and w_k have out-degree 0 in P_k, Q_k, respectively. ◁

Thus P_k and Q_k are partial orders.

▷ **Claim 13.** For all graphs G and all subsets $X \subseteq G$ we have

$$c_1\big(G \rhd_X x\big) = c_1(G) + 1, \tag{5}$$
$$c_i\big(G \rhd_X x\big) = c_i(G) + c_{i-1}\big(G[X]\big) \qquad\qquad \text{for } i \geq 2. \tag{6}$$

Proof. Straightforward. ◁

Thus for $k \geq 2$ and $i \geq 2$ we have

$$c_i(P_{k+1}) = c_i(P_k) + c_{i-1}(P_k) + c_{i-1}(Q_{k-1}) \tag{7}$$

and similarly

$$c_i(Q_{k+1}) = c_i(Q_k) + c_{i-1}(Q_k) + c_{i-1}(P_{k-1}). \tag{8}$$

Now we prove (1)-(3) by induction on k. We have already noted that it holds for $k = 1, 2$. For the inductive step, let $k \geq 2$ and $i \geq 1$.

Case 1: $i = 1$. We have $c_1(P_{k+1}) = |V_{k+1}| = 2k = |W_{k+1}| = c_1(Q_{k+1})$.

Case 2: $2 \leq i \leq k - 1$. We have $c_i(P_k) = c_i(Q_k)$, $c_{i-1}(P_k) = c_{i-1}(Q_k)$ and $c_{i-1}(P_{k-1}) = c_{i-1}(Q_{k-1})$ by the induction hypothesis, and by (7) and (8) this implies $c_i(P_{k+1}) = c_i(P_{k+1})$.

Case 3: $i = k$. We have $c_i(P_k) = c_i(Q_k) + 1$ and $c_{i-1}(P_k) = c_{i-1}(Q_k)$ and $c_{i-1}(P_{k-1}) = c_{i-1}(Q_{k-1}) + 1$ by the induction hypothesis. Thus by (7) and (8),

$$c_i(P_{k+1}) = c_i(P_k) + c_{i-1}(P_k) + c_{i-1}(Q_{k-1})$$
$$= c_i(Q_k) + 1 + c_{i-1}(Q_k) + c_{i-1}(P_{k-1}) - 1 = c_i(Q_{k+1}),$$

which completes the proof of (1).

Case 4: $i = k + 1$. We have $c_i(P_k) = c_i(Q_k) = 0$ and $c_{i-1}(P_k) = 1, c_{i-1}(Q_k) = 0$ and $c_{i-1}(P_{k-1}) = c_{i-1}(Q_{k-1}) = 0$ by the induction hypothesis. Thus by (7) and (8),

$$c_i(P_{k+1}) = c_i(P_k) + c_{i-1}(P_k) + c_{i-1}(Q_{k-1}) = 1,$$
$$c_i(Q_{k+1}) = c_i(Q_k) + c_{i-1}(Q_k) + c_{i-1}(P_{k-1}) = 0.$$

This proves (2).

Case 5: $i \geq k + 2$. We have $c_i(P_k) = c_i(Q_k) = c_{i-1}(P_k) = c_{i-1}(Q_k) = c_{i-1}(P_{k-1}) = c_{i-1}(Q_{k-1}) = 0$ by the induction hypothesis. Thus by (7) and (8), $c_i(P_{k+1}) = c_i(Q_{k+1}) = 0$. This proves (3).

Now assertions (1)–(3) follow, because for partial orders G we have $c_k(G) = d_k(G)$ for all $k \geq 1$. ◀

As the construction of Theorem 10 yields partial orders, for which directed path counts and clique counts are the same, we also obtain an undirected version for clique counts with Corollary 14.

▶ **Corollary 14.** *For every $k \geq 1$ there are undirected graphs G_k, H_k of order $|G_k|, |H_k| \leq \max\{1, 2(k-1)\}$ such that*

$$c_i(G_k) = c_i(H_k) \qquad\qquad\qquad for\ 1 \leq i \leq k - 1, \tag{9}$$

$$c_k(G_k) = 1, \quad c_k(H_k) = 0, \tag{10}$$

$$c_i(G_k) = c_i(H_k) = 0 \qquad\qquad\qquad for\ all\ i > k. \tag{11}$$

Proof. Let G_k, H_k be the undirected graphs underlying the partial orders P_k, Q_k of Theorem 10. ◀

We also show how to generalise Theorem 10 and Corollary 14 such that number of directed paths of length $k - 1$ and the number of cliques of size k in these graphs, respectively, can freely be chosen. The exact statements and their proofs can be found in the full version of the paper.

4   Undecidability Results

We proceed to derive undecidability results for $\text{HomInd}(\mathcal{F})$ using the combinatorial constructions of Section 3. Before we prove our main theorem (Theorem 1), the following version for the case of directed graphs will be necessary.

▶ **Theorem 15.** *There is a polynomial time decidable class $\mathcal{F}$ of directed graphs of tree width 1 such that $\text{HomInd}(\mathcal{F})$ is undecidable.*

Proof. Let us fix some Gödel numbering of deterministic Turing machines such that M_j denotes the machine with Gödel number j. For every pair $(j, t) \in \mathbb{N}^2$, let $F_{j,t}$ be the graph that is the disjoint union of a directed path $P_{j+1}^{\rightarrow}$ of length $(j + 1)$ and an independent set of size t. Let $\mathcal{F}$ be the class of all graphs $F_{j,t}$ such that M_j halts in t steps when started on the empty input word. Clearly, $\mathcal{F}$ is decidable in polynomial time.

Observe that for every graph G and all $j, t \in \mathbb{N}$ we have

$$\text{hom}(F_{j,t}, G) = \text{hom}(P_{j+1}, G) \cdot |G|^t. \tag{12}$$

Let G_k, H_k be the graphs constructed in Theorem 10. It is easy to note that $\text{hom}(F_{0,t}, G_1) = 1 \neq 0 = \text{hom}(F_{0,t}, H_1)$ and $\text{hom}(F_{j,t}, G_1) = \text{hom}(F_{j,t}, H_1) = 0$ for $j \geq 1$. For $k \geq 2$, recall that $|G_k| = |H_k| = 2(k - 1)$ and that $\text{hom}(P_j^{\rightarrow}, G_k) = \text{hom}(P_j^{\rightarrow}, H_k)$ if and only if $j \neq k$. Thus it follows from (12) that for all j, t we have

$$\text{hom}(F_{j,t}, G_k) \neq \text{hom}(F_{j,t}, H_k) \iff j = k - 1. \tag{13}$$

This implies

$$\text{Hom}_{\mathcal{F}}(G_k) \neq \text{Hom}_{\mathcal{F}}(H_k) \iff F_{(k-1),t} \in \mathcal{F} \text{ for some } t \in \mathbb{N}$$
$$\iff M_{k-1} \text{ halts on the empty input word.}$$

This proves that $\text{HomInd}(\mathcal{F})$ is undecidable. Since every graph in $\mathcal{F}$ is a directed path with some padded isolated vertices, the treewidth of $\mathcal{F}$ is 1. Hence, proved. ◀

The above proof can be easily modified to invoke Corollary 14 instead of Theorem 10, which yields the following corollary.

▶ **Corollary 16.** *There is a polynomial time decidable class $\mathcal{F}$ of undirected graphs such that $\text{HomInd}(\mathcal{F})$ is undecidable.*

In particular, every graph in this class of undirected graphs is a clique (padded with isolated vertices), and therefore, this class has unbounded treewidth. Our main theorem, Theorem 1, is a sharper version of the above corollary.

4.1   Proof of Theorem 1

The proof of Theorem 1 is obtained by replacing the directed graphs $F_{j,t}, G_k, H_k$ (constructed in the proof of Theorem 15) by their suitably-defined undirected versions $\widetilde{F}_{j,t}, \widetilde{G}_k, \widetilde{H}_k$. The two key requirements of this transformation are (a) the homomorphism numbers are preserved, i.e., $\mathsf{hom}(F_{j,t}, G_k) = \mathsf{hom}(\widetilde{F}_{j,t}, \widetilde{G}_k)$ and $\mathsf{hom}(F_{j,t}, H_k) = \mathsf{hom}(\widetilde{F}_{j,t}, \widetilde{H}_k)$, and (b) the treewidth of the transformed graphs is bounded. To satisfy these properties, we devise suitable gadgets to encode the direction of an edge: our gadgets employ homomorphically incomparable Kneser graphs in order to control the homomorphism numbers of the resulting undirected graphs. The end result of our gadget construction is the following technical lemma (note that our construction there does not exploit any special properties of the present graphs and works for arbitrary directed graphs). The proof is deferred to the full version of the paper.

Let $\mathcal{F}$ be the class of all directed graphs $F_{j,t}$ arising in the proof of Theorem 15, such that $\textsc{HomInd}(\mathcal{F})$ is undecidable.

▶ **Lemma 17.** *Given graphs $F_{j,t}, G_k, H_k$ (constructed in the proof of Theorem 15), we can construct corresponding undirected graphs $\widetilde{F}_{j,t}, \widetilde{G}_k, \widetilde{H}_k$ in polynomial time, satisfying the following properties.*

1. *For all $j, t \in \mathbb{N}$ there exists a positive integer $C_{j,t}$ such that for every $k \in \mathbb{N}$,*

$$\mathsf{hom}(\widetilde{F}_{j,t}, \widetilde{G}_k) = C_{j,t} \cdot \mathsf{hom}(F_{j,t}, G_k),$$
$$\mathsf{hom}(\widetilde{F}_{j,t}, \widetilde{H}_k) = C_{j,t} \cdot \mathsf{hom}(F_{j,t}, H_k).$$

2. *There exists a fixed positive integer ℓ such that for every $j, t \in \mathbb{N}$, the graph $\widetilde{F}_{j,t}$ has treewidth at most ℓ.*

3. *Let $\widetilde{\mathcal{F}}$ be the class of all undirected graphs $\widetilde{F}_{j,t}$ such that $F_{j,t} \in \mathcal{F}$. Then $\widetilde{\mathcal{F}}$ is polynomial time decidable.*

From the above lemma, we can deduce Theorem 1 as follows.

Proof of Theorem 1. The proof follows the proof of Theorem 15 closely. By Lemma 17 and Equation 13,

$$\mathsf{hom}(\widetilde{F}_{j,t}, \widetilde{G}_k) \neq \mathsf{hom}(\widetilde{F}_{j,t}, \widetilde{H}_k) \iff j = k - 1. \tag{14}$$

This implies

$$\begin{aligned}
\mathsf{Hom}_{\widetilde{\mathcal{F}}}(\widetilde{G}_k) \neq \mathsf{Hom}_{\widetilde{\mathcal{F}}}(\widetilde{H}_k) &\iff \widetilde{F}_{(k-1),t} \in \widetilde{\mathcal{F}} \text{ for some } t \in \mathbb{N} \\
&\iff F_{(k-1),t} \in \mathcal{F} \text{ for some } t \in \mathbb{N} \\
&\iff M_{k-1} \text{ halts on the empty input word.}
\end{aligned}$$

This proves that $\textsc{HomInd}(\widetilde{\mathcal{F}})$ is undecidable. By Lemma 17, $\widetilde{\mathcal{F}}$ has bounded treewidth and is polynomial-time-decidable. Hence, proved.   ◀

5   Hardness for Cliques

The construction of Corollary 14 allows for a simple proof of the co-NP-hardness of $\textsc{HomInd}(\mathcal{K})$.

Proof of Theorem 2. We reduce the co-NP-hard problem

$$\overline{\textsc{Clique}} = \{(F, k) \mid F \text{ graph without a } k\text{-clique}\}$$

to $\textsc{HomInd}(\mathcal{K})$. To this end, we use Corollary 14 to construct two graphs G_k and H_k in time polynomial in $k \leq n$. Then, the graphs

$$F_1 := F \otimes G_k \quad \text{and} \quad F_2 := F \otimes H_k.$$

can be constructed in time $\text{poly}(n)$. Corollary 5, together with (9)-(11), implies that

$$c_i(F_1) = c_i(F_2) \qquad\qquad\qquad \text{for } 1 \leq i \leq k - 1, \qquad (15)$$

$$c_k(F_1) = k! \cdot c_k(F), \quad c_k(F_2) = 0, \qquad\qquad\qquad\qquad\qquad (16)$$

$$c_i(F_1) = c_i(F_2) = 0 \qquad\qquad\qquad \text{for all } i > k. \qquad\qquad (17)$$

Hence, the mapping $F \mapsto (F_1, F_2)$ is the desired polynomial-time many-one reduction as $c_k(F) = 0$ if and only if $c_i(F_1) = c_i(F_2)$ for every $i \geq 1$. ◀

A more refined argument gives us a more precise classification of the complexity of $\textsc{HomInd}(\mathcal{K})$.

▶ **Theorem 18.** $\textsc{HomInd}(\mathcal{K})$ *is complete for* $\mathsf{C_=P}$ *under polynomial time Turing reductions.*

The complexity class $\mathsf{C_=P}$ was introduced in [18, 22]. Here we use the following equivalent definition from [10].

▶ **Definition 19.** *Let L be a decision problem. Then $L \in \mathsf{C_=P}$ if and only if there is a function f in $\#\mathrm{P}$ and a function g computable in polynomial time such that for every instance x of L*

$$x \in L \quad \Longleftrightarrow \quad f(x) = g(x).$$

Before giving the proof of Theorem 18, we derive some of its consequences, which shows that $\textsc{HomInd}(\mathcal{K})$ is apparently much harder than co-NP as stated in Theorem 2, and in fact, unlikely to be in the polynomial hierarchy (PH).

It is clear that every problem in $\mathsf{C_=P}$ can be decided in polynomial time with an oracle to a problem in $\#\mathrm{P}$. The following slightly weak converse is also easy to see (cf. [4], Section 1.2).

▶ **Proposition 20.** $\mathrm{P}^{\#\mathrm{P}} \subseteq \mathrm{NP}^{\mathsf{C_=P}}$.

Thus Theorem 18 implies that:

▶ **Corollary 21.** $\mathrm{P}^{\#\mathrm{P}} \subseteq \mathrm{NP}^{\textsc{HomInd}(\mathcal{K})}$.

Combined with renowned Toda's Theorem [19], we conclude that $\textsc{HomInd}(\mathcal{K})$ is above the polynomial hierarchy.

▶ **Corollary 22.** $\textsc{HomInd}(\mathcal{K})$ *is not in* PH, *unless* PH *collapses.*

Now we are ready to prove Theorem 18: the proof is deferred to the full version of the paper.

6   Tractable Cases

▶ **Theorem 23.** HOMIND$(\mathcal{F})$ *can be solved in polynomial time for the class $\mathcal{F}$ of directed paths.*

The proof of the theorem is deferred to the full version of the paper.

7   Related Problems

For a class of graphs $\mathcal{F}$, let $\mathcal{F}_k$ denote the class of all graphs $F \in \mathcal{F}$ of order k. For classes $\mathcal{F}$ where there is at most one graph $F \in \mathcal{F}$ of order k for every $k \geq 1$, it is only natural to consider the entries $\mathsf{hom}(F, G)$ of a homomorphism vector $\mathsf{Hom}_\mathcal{F}(G)$ as sorted by the order of F. Then it becomes possible to compare these vectors using the lexicographical ordering $\leq_\ell$, and for such a class $\mathcal{F}$, we let HOMLEX$(\mathcal{F})$ denote the following decision problem: given graphs G and H, decide whether $\mathsf{Hom}_\mathcal{F}(G) \leq_\ell \mathsf{Hom}_\mathcal{F}(H)$.

For the classes of directed paths and directed cycles, the proof of Theorem 23 immediately yields that the corresponding decision problems can be decided in polynomial time as, given graphs G and H with $|V(G)| = |V(H)| = n$, it suffices to consider the first $2n$ paths and n cycles, respectively.

▶ **Theorem 24.** HOMLEX$(\mathcal{F})$ *can be solved in polynomial time for the class of directed paths and the class of directed cycles.*

For the class of all complete graphs, the hardness of the HOMLEX$(\mathcal{K})$ is expected.

▶ **Theorem 25.** HOMLEX$(\mathcal{K})$ *is complete for* #P *under polynomial time Turing reductions.*

The proof is deferred to the full version of the paper.

A more interesting direction is to consider the similarity of homomorphism vectors as this induces a measure of similarity on the graphs themselves (see e.g. [13], Lemma 10.22 and Lemma 10.32). It is not clear how exactly the distance of homomorphism vectors should be defined, but some natural candidates are the following:

(a) $d^1_\mathcal{F}(G, H) := \displaystyle\sum_{\substack{k \geq 1 \\ \mathcal{F}_k \neq \emptyset}} \frac{1}{k^k |\mathcal{F}_k|} \sum_{F \in \mathcal{F}_k} |\mathsf{hom}(F, G) - \mathsf{hom}(F, H)|$

(b) $d^\infty_\mathcal{F}(G, H) := \displaystyle\sum_{\substack{k \geq 1 \\ \mathcal{F}_k \neq \emptyset}} \frac{1}{k^k} \max_{F \in \mathcal{F}_k} |\mathsf{hom}(F, G) - \mathsf{hom}(F, H)|$

(c) $d^2_\mathcal{F}(G, H) := \sqrt{\displaystyle\sum_{\substack{k \geq 1 \\ \mathcal{F}_k \neq \emptyset}} \frac{1}{k^k |\mathcal{F}_k|} \sum_{F \in \mathcal{F}_k} (\mathsf{hom}(F, G) - \mathsf{hom}(F, H))^2}$

The scaling by k^k in the definitions is quite arbitrary and ensures that the sums converge: Let G and H be graphs with $|V(G)| \geq |V(H)|$. As the number of homomorphisms from a k-vertex graph to an n-vertex graph is at most n^k, we for example have

$$\sqrt[k]{\frac{1}{k^k |\mathcal{F}_k|} \sum_{F \in \mathcal{F}_k} |\mathsf{hom}(F, G) - \mathsf{hom}(F, H)|} \leq \sqrt[k]{\frac{|V(G)|^k}{k^k}} = \frac{|V(G)|}{k} \xrightarrow{k \to \infty} 0,$$

which implies convergence of the sum in the definition of $d^1_\mathcal{F}$ by the root test. Of course, one may also scale by a different factor, e.g., $k!$, and possibly even make it depend on the orders of G and H. It is not hard to see that $d^1_\mathcal{F}$, $d^\infty_\mathcal{F}$, and $d^2_\mathcal{F}$ are pseudometrics on graphs. For $d^2_\mathcal{F}$,

this follows directly from the fact that it is the pseudometric induced by an inner product on homomorphism vectors proposed by Dell, Grohe, and Rattan [6].

For "simple-enough" classes of graphs, these pseudometrics can be computed up to an arbitrarily small additive error ε in polynomial time in the straightforward way: compute "enough" terms by computing the first graphs in $\mathcal{F}$ and then counting homomorphisms from them one by one. To this end, we call a class of graphs $\mathcal{F}$ polynomial-time enumerable if there is a polynomial-time algorithm that, on input 1^k, outputs all graphs in $\mathcal{F}_k$. Theorem 26 only considers $d^1_{\mathcal{F}}$ for simplicity, but the calculations can directly be adapted to $d^\infty_{\mathcal{F}}$ and $d^2_{\mathcal{F}}$. The proof is deferred to the full version of the paper.

▶ **Theorem 26.** *Let $\mathcal{F}$ be a polynomial-time enumerable class of graphs for which $\#\mathrm{HOM}(\mathcal{F})$ is in polynomial time. Then, for every $\varepsilon > 0$, there is a polynomial-time algorithm $D^\varepsilon_{\mathcal{F}}$ that takes two graphs G and H as input and outputs a real number $D^\varepsilon_{\mathcal{F}}(G, H)$ such that $|d^1_{\mathcal{F}}(G, H) - D^\varepsilon_{\mathcal{F}}(G, H)| \leq \varepsilon$ holds for all G and H.*

Among the classes to which Theorem 26 applies are the class $\mathcal{C}$ of all cycles, the class $\mathcal{P}$ of all paths, and for every fixed $d \geq 1$, the class of all complete d-ary trees.

8 Conclusion

We established the rich complexity-theoretic behaviour of the problem $\mathrm{HOMIND}(\mathcal{F})$ for a variety of graph classes. It was already known that this problem can be solved in polynomial time for the class of paths, trees and bounded treewidth graphs. Our results are complementary: there exist polynomial-time-decidable graph classes for which this problem is undecidable, even though these graph classes satisfy strong structural restrictions (such as bounded treewidth). For the class of complete graphs and directed paths, we also provide tight upper and lower bounds for the complexity of $\mathrm{HOMIND}(\mathcal{F})$. Our techniques rely on combinatorial constructions of graphs with almost-identical homomorphism vectors: these constructions might be of independent interest.

Perhaps the most interesting direction of further work is the study of graph metrics induced by homomorphism vectors. These metrics induce natural measures of similarity between graphs: such measures serve as an important black-box component for the design of practical graph learning algorithms. Therefore, a better understanding of these metrics will enable a theoretical analysis of practical graph learning tools.

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