THE COMPLEXITY OF COUNTING SURJECTIVE HOMOMORPHISMS AND COMPACTIONS *

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Abstract.
A homomorphism from a graph G to a graph H is a function from the vertices of G to the vertices of H that preserves edges. A homomorphism is *surjective* if it uses all of the vertices of H and it is a *compaction* if it uses all of the vertices of H and all of the non-loop edges of H. Hell and Nešetřil gave a complete characterisation of the complexity of deciding whether there is a homomorphism from an input graph G to a fixed graph H. A complete characterisation is not known for surjective homomorphisms or for compactions, though there are many interesting results. Dyer and Greenhill gave a complete characterisation of the complexity of counting homomorphisms from an input graph G to a fixed graph H. In this paper, we give a complete characterisation of the complexity of counting surjective homomorphisms from an input graph G to a fixed graph H and we also give a complete characterisation of the complexity of counting compactions from an input graph G to a fixed graph H. In an addendum we use our characterisations to point out a dichotomy for the complexity of the respective approximate counting problems (in the connected case).

1. Introduction.

A homomorphism from a graph G to a graph H is a function from $V(G)$ to $V(H)$ that preserves edges. That is, the function maps every edge of G to an edge of H. Many structures in graphs, such as proper colourings, independent sets, and generalisations of these, can be represented as homomorphisms, so the study of graph homomorphisms has a long history in combinatorics [3, 4, 20, 21, 24, 26].

Much of the work on this problem is algorithmic in nature. A very important early work is Hell and Nešetřil's paper [22], which gives a complete characterisation of the complexity of the following decision problem, parameterised by a fixed graph H: "Given an input graph G, determine whether there is a homomorphism from G to H." Hell and Nešetřil showed that this problem can be solved in polynomial time if H has a loop or is loop-free and bipartite. They showed that it is NP-complete otherwise. An important generalisation of the homomorphism decision problem is the list-homomorphism decision problem. Here, in addition to the graph G, the input specifies, for each vertex v of G, a list S_v of permissible vertices of H. The problem is to determine whether there is a homomorphism from G to H that maps each vertex v of G to a vertex in S_v. Feder, Hell and Huang [12] gave a complete characterisation of the complexity of this problem. This problem can be solved in polynomial time if H is a so-called bi-arc graph, and it is NP-complete otherwise.

More recent work has restricted attention to homomorphisms with certain properties. A function from $V(G)$ to $V(H)$ is *surjective* if every element of $V(H)$ is the image of at least one element of $V(G)$. So a homomorphism from G to H is surjective if every vertex of H is "used" by the homomorphism. There is still no complete

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characterisation of the complexity of determining whether there is a surjective homomorphism from an input graph G to a graph H, despite an impressive collection of results [1, 17, 18, 19, 27]. A homomorphism from $V(G)$ to $V(H)$ is a *compaction* if it uses every vertex of H and also every non-loop edge of H (so it is surjective both on $V(H)$ and on the non-loop edges in $E(H)$). Compactions have been studied under the name "homomorphic image" [20, 24] and even under the name "surjective homomorphism" [6, 26]. Once again, despite much work [1, 30, 31, 32, 33, 34], there is still no characterisation of the complexity of determining whether there is a compaction from an input graph G to a graph H.

Dyer and Greenhill [10] initiated the algorithmic study of *counting* homomorphisms. They gave a complete characterisation of the graph homomorphism counting problem, parameterised by a fixed graph H: "Given an input graph G, determine how many homomorphisms there are from G to H." Dyer and Greenhill showed that this problem can be solved in polynomial time if every component of H is a clique with all loops present or a biclique (complete bipartite graph) with no loops present. Otherwise, the counting problem is #P-complete. Díaz, Serna and Thilikos [8] and Hell and Nešetřil [23] have shown that the same dichotomy characterisation holds for the problem of counting list homomorphisms.

The main contribution of this paper is to give complete dichotomy characterisations for the problems of counting compactions and surjective homomorphisms. Our main theorem, Theorem 1.2, shows that the characterisation for compactions is different from the characterisation for counting homomorphisms. If every component of H is (i) a star with no loops present, (ii) a single vertex with a loop, or (iii) a single edge with two loops then counting compactions to H is solvable in polynomial time. Otherwise, it is #P-complete. We also obtain the same dichotomy for the problem of counting list compactions. Thus, even though the decision problem is still open for compactions, our theorem gives a complete classification of the complexity of the corresponding counting problem.

There is evidence that computational problems involving surjective homomorphisms are more difficult than those involving (unrestricted) homomorphisms. For example, suppose that H consists of a 3-vertex clique with no loops together with a single looped vertex. As [1] noted, the problem of deciding whether there is a homomorphism from a loop-free input graph G to H is trivial (the answer is yes, since all vertices of G may be mapped to the loop) but the problem of determining whether there is a surjective homomorphism from a loop-free input graph G to H is NP-complete. (To see this, recall the NP-hard problem of determining whether a connected loop-free graph G' that is not bipartite is 3-colourable. Given such a graph G', we may determine whether it is 3-colourable by letting G consist of the disjoint union of G' and a loop-free clique of size 4, and then checking whether there is a surjective homomorphism from G to H.) There is also evidence that *counting* problems involving surjective homomorphisms are more difficult than those involving unrestricted homomorphisms. In Section 4.3 we consider a *uniform* homomorphism-counting problem where all connected components of G are cliques without loops and all connected components of H are cliques with loops, but both G and H are part of the input. It turns out (Theorem 4.4) that in this uniform case, counting homomorphisms is in FP but counting surjective homomorphisms is #P-complete. Despite this evidence, we show (Theorem 1.3) that the problem of counting surjective homomorphisms to a fixed graph H has the same complexity characterisation as the problem of counting all homomorphisms to H: The problem is solvable in polynomial time if every component of H is a clique with loops or a biclique without loops. Otherwise, it is #P-complete. Once again, our dichotomy characterisation extends to the problem of counting surjective list homomorphisms. Even though the decision problem is still open for surjective homomorphisms, our theorem gives a complete complexity classification of the corresponding counting problem.

In Section 1.2 we will introduce one more related counting problem — the problem of counting *retractions*. Informally, if G is a graph containing an induced copy of H then a retraction from G to H is a homomorphism from G to H that maps the induced copy to itself. Retractions are well-studied in combinatorics, often from an algorithmic perspective [1, 11, 12, 13, 31, 33]. A complexity classification is not known for the decision problem (determining whether there is a retraction from an input to H). Nevertheless, it is easy to give a complexity characterisation for the corresponding counting problem (Corollary 1.7). This characterisation, together with our main results, implies that a long-standing conjecture of Winkler about the complexity of the decision problems for compactions and retractions is false in the counting setting. See Section 1.2 for details.

Finally, in an addendum to this work, we address the relaxed versions of the counting problems where the goal is to *approximately* count surjective homomorphisms, compactions and retractions. We use our theorems to give a complexity dichotomy in the connected case for all three of these problems.

1.1. Notation and Theorem Statements. In this paper graphs are undirected and may contain loops. A homomorphism from a graph G to a graph H is a function $h\colon V(G) \to V(H)$ such that, for all $\{u, v\} \in E(G)$, the image $\{h(u), h(v)\}$ is in $E(H)$. We use $N\big(G \to H\big)$ to denote the number of homomorphisms from G to H. A homomorphism h is said to "use" a vertex $v \in V(H)$ if there is a vertex $u \in V(G)$ such that $h(u) = v$. It is *surjective* if it uses every vertex of H. We use $N^{\mathrm{sur}}\big(G \to H\big)$ to denote the number of surjective homomorphisms from G to H. A homomorphism h is said to use an edge $\{v_1, v_2\} \in E(H)$ if there is an edge $\{u_1, u_2\} \in E(G)$ such that $h(u_1) = v_1$ and $h(u_2) = v_2$. It is a *compaction* if it uses every vertex of H and every non-loop edge of H. We use $N^{\mathrm{comp}}\big(G \to H\big)$ to denote the number of compactions from G to H. H is said to be *reflexive* if every vertex has a loop. It is said to be *irreflexive* if no vertex has a loop. We study the following computational problems[1], which are parameterised by a graph H.

Name. #Hom(H).
Input. Irreflexive graph G.
Output. $N\big(G \to H\big)$.

Name. #Comp(H).
Input. Irreflexive graph G.
Output. $N^{\mathrm{comp}}\big(G \to H\big)$.

Name. #SHom(H).
Input. Irreflexive graph G.
Output. $N^{\mathrm{sur}}\big(G \to H\big)$.

A *list homomorphism* generalises a homomorphism in the same way that a list colouring of a graph generalises a (proper) colouring. Suppose that G is an irreflexive

[1]The reason that the input graph G is restricted to be irreflexive in these problems, but that H is not restricted, is that this is the convention in the literature. Since our results will be complexity classifications, parameterised by H, we strengthen the results by avoiding restrictions on H. Different conventions are possible regarding G, but hardness results are typically the most difficult part of the complexity classifications in this area, so restricting G leads to technically-stronger results.

graph and that H is a graph. Consider a collection of sets $\mathbf{S} = \{S_v \subseteq V(H) : v \in V(G)\}$ A *list homomorphism* from $(G, \mathbf{S})$ to H is a homomorphism h from G to H such that, for every vertex v of G, $h(v) \in S_v$. The set S_v is referred to as a "list", specifying the allowable targets of vertex v. We use $N\big((G, \mathbf{S}) \to H\big)$ to denote the number of list homomorphisms from $(G, \mathbf{S})$ to H, $N^{\mathrm{sur}}\big((G, \mathbf{S}) \to H\big)$ to denote the number of surjective list homomorphisms from $(G, \mathbf{S})$ to H and $N^{\mathrm{comp}}\big((G, \mathbf{S}) \to H\big)$ to denote the number of list homomorphisms from $(G, \mathbf{S})$ to H that are compactions. We study the following additional computational problems, again parameterised by a graph H.

Name. #LHom(H).
Input. Irreflexive graph G and a collection of lists $\mathbf{S} = \{S_v \subseteq V(H) : v \in V(G)\}$.
Output. $N\big((G, \mathbf{S}) \to H\big)$.

Name. #LComp(H).
Input. Irreflexive graph G and a collection of lists $\mathbf{S} = \{S_v \subseteq V(H) : v \in V(G)\}$.
Output. $N^{\mathrm{comp}}\big((G, \mathbf{S}) \to H\big)$.

Name. #LSHom(H).
Input. Irreflexive graph G and a collection of lists $\mathbf{S} = \{S_v \subseteq V(H) : v \in V(G)\}$.
Output. $N^{\mathrm{sur}}\big((G, \mathbf{S}) \to H\big)$.

In order to state our theorems, we define some classes of graphs. A graph H is a *clique* if, for every pair (u, v) of distinct vertices, $E(H)$ contains the edge $\{u, v\}$. (Like other graphs, cliques may contain loops but not all loops need to be present.) H is a *biclique* if it is bipartite (disregarding any loops) and there is a partition of $V(H)$ into two disjoint sets U and V such that, for every $u \in U$ and $v \in V$, $E(H)$ contains the edge $\{u, v\}$. A biclique is a *star* if $|U| = 1$ or $|V| = 1$ (or both). Note that a star may have only one vertex since, for example, we could have $|U| = 1$ and $|V| = 0$. We sometimes use the notation $K_{a,b}$ to denote an irreflexive biclique whose vertices can be partitioned into U and V with $|U| = a$ and $|V| = b$. The size of a graph is the number of vertices that it has. We can now state the theorem of Dyer and Greenhill [10], as extended to list homomorphisms by Díaz, Serna and Thilikos [8] and Hell and Nešetřil [23].

THEOREM 1.1 (Dyer, Greenhill). *Let H be a graph. If every connected component of H is a reflexive clique or an irreflexive biclique, then the problems #Hom(H) and #LHom(H) are in* FP. *Otherwise, #Hom(H) and #LHom(H) are* #P*-complete.*

We can also state the main results of this paper.

THEOREM 1.2. *Let H be a graph. If every connected component of H is an irreflexive star or a reflexive clique of size at most* 2 *then #Comp(H) and #LComp(H) are in* FP. *Otherwise, #Comp(H) and #LComp(H) are* #P*-complete.*

THEOREM 1.3. *Let H be a graph. If every connected component of H is a reflexive clique or an irreflexive biclique, then #SHom(H) and #LSHom(H) are in* FP. *Otherwise, #SHom(H) and #LSHom(H) are* #P*-complete.*

The tractability results in Theorem 1.2 follow from the fact that the number of compactions from a graph G to a graph H can be expressed as a linear combination of the number of homomorphisms from G to certain subgraphs of H, see Section 3.1. A proof sketch of the intractability result in Theorem 1.2 is given at the beginning of Section 3.2. Theorem 1.3 is simpler, see Section 4.

1.2. Reductions and Retractions. In the context of two computational problems P_1 and P_2, we write $\mathrm{P}_1 \leq \mathrm{P}_2$ if there exists a polynomial-time Turing reduction from P_1 to P_2. If there exist such reductions in both directions, we write $\mathrm{P}_1 \equiv \mathrm{P}_2$. Theorems 1.1, 1.2 and 1.3 imply the following observation.

Observation 1.4. *Let H be a graph. Then*

$$\#\mathit{Hom}(H) \equiv \#\mathit{LHom}(H) \equiv \#\mathit{SHom}(H) \equiv \#\mathit{LSHom}(H) \\ \leq \#\mathit{Comp}(H) \equiv \#\mathit{LComp}(H).$$

In order to see how Observation 1.4 contrasts with the situation concerning decision problems, it is useful to define decision versions of the computational problems that we study. Thus, $\mathrm{Hom}(H)$ is the problem of determining whether $N\big(G \to H\big) = 0$, given an input G of $\#\mathrm{Hom}(H)$. The decision problems $\mathrm{Comp}(H)$, $\mathrm{SHom}(H)$ and $\mathrm{LHom}(H)$ are defined similarly.

It is also useful to define the notion of a *retraction*. Suppose that H is a graph with $V(H) = \{v_1, \ldots, v_c\}$ and that G is an irreflexive graph. We say that a tuple $(u_1, \ldots, u_c)$ of c distinct vertices of G induces a copy of H if, for every $1 \leq a < b \leq c$, $\{u_a, u_b\} \in E(G) \iff \{v_a, v_b\} \in E(H)$. A *retraction* from $(G; u_1, \ldots, u_c)$ to H is a homomorphism h from G to H such that, for all $i \in [c]$, $h(u_i) = v_i$. We use $N^{\mathrm{ret}}\big((G; u_1, \ldots, u_c) \to H\big)$ to denote the number of retractions from $(G; u_1, \ldots, u_c)$ to H. We briefly consider the retraction counting and decision problems, which are parameterised by a graph H with $V(H) = \{v_1, \ldots, v_c\}$.[2]

Name. $\#\mathrm{Ret}(H)$.
Input. Irreflexive graph G and a tuple $(u_1, \ldots, u_c)$ of distinct vertices of G that induces a copy of H.
Output. $N^{\mathrm{ret}}\big((G; u_1, \ldots, u_c) \to H\big)$.

Name. $\mathrm{Ret}(H)$.
Input. Irreflexive graph G and a tuple $(u_1, \ldots, u_c)$ of distinct vertices of G that induces a copy of H.
Output. Does $N^{\mathrm{ret}}\big((G; u_1, \ldots, u_c) \to H\big) = 0$?

The following observation appears as Proposition 1 of [1]. The proposition is stated for more general structures than graphs, but it applies equally to our setting.

Proposition 1.5 (Bodirsky et al.). *Let H be a graph. Then*

$$\mathit{Hom}(H) \leq \mathit{SHom}(H) \leq \mathit{Comp}(H) \leq \mathit{Ret}(H) \leq \mathit{LHom}(H).$$

We have already mentioned the fact (pointed out by Bodirsky et al.) that if H is an irreflexive 3-vertex clique together with a single looped vertex, then $\mathrm{Hom}(H)$ is in P, but $\mathrm{SHom}(H)$ is NP-complete. There are no known graphs H separating $\mathrm{SHom}(H)$, $\mathrm{Comp}(H)$ and $\mathrm{Ret}(H)$. Moreover, Bodirsky et al. mention a conjecture [1, Conjecture 2], attributed to Peter Winkler, that, for all graphs H, $\mathrm{Comp}(H)$ and $\mathrm{Ret}(H)$ are polynomially Turing equivalent.

The following observation, together with our theorems, implies Corollary 1.8 (below), which shows that the generalisation of Winkler's conjecture to the counting setting is false unless FP = #P, since $\#\mathrm{Comp}(H)$ and $\#\mathrm{Ret}(H)$ are not polynomially Turing equivalent for all H.

[2] Once again, some works would allow G to have loops, and would insist that loops are preserved in the induced copy of H. We prefer to stick with the convention that G is irreflexive, but this does not make a difference to the complexity classifications that we describe.

Observation 1.6. *Let H be a graph. Then*

$$\#Ret(H) \le \#LHom(H) \text{ and } \#Hom(H) \le \#Ret(H).$$

Proof. Let $V(H) = \{v_1, \dots, v_c\}$. We first reduce #Ret($H$) to #LHom($H$). Consider an input to #Ret(H) consisting of G and $(u_1, \dots, u_c)$. For each $a \in [c]$, let S_{u_a} be the set containing the single vertex v_a. For each $v \in V(G) \setminus \{u_1, \dots, u_c\}$, let $S_v = V(H)$. Let $\mathbf{S} = \{S_v : v \in V(G)\}$. Then $N^{\text{ret}}\big((G; u_1, \dots, u_c) \to H\big) = N\big((G, \mathbf{S}) \to H\big)$.

We next reduce #Hom(H) to #Ret(H). Let E^0 be the set of all non-loop edges of H. Consider an input G to #Hom(H). Suppose without loss of generality that $V(G)$ is disjoint from $V(H) = \{v_1, \dots, v_c\}$. Let G' be the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E^0$. Then $(v_1, \dots, v_c)$ induces a copy of H in G' and $N\big(G \to H\big) = N^{\text{ret}}\big((G'; v_1, \dots, v_c) \to H\big)$. ∎

Observation 1.6 immediately implies the following dichotomy characterisation for the problem of counting retractions.

Corollary 1.7. *Let H be a graph. If every connected component of H is a reflexive clique or an irreflexive biclique, then #Ret(H) is in* FP. *Otherwise, #Ret(H) is* #P*-complete.*

Proof. The corollary follows immediately from Observation 1.6 and Theorem 1.1. ∎

Corollary 1.8. *Let H be a graph. Then*

$$\#Hom(H) \equiv \#LHom(H) \equiv \#SHom(H) \equiv \#LSHom(H) \equiv \#Ret(H) \le$$
$$\#Comp(H) \equiv \#LComp(H).$$

Furthermore, there is a graph H for which #Comp(H) and #LComp(H) are #P*-complete, but #Hom(H), #LHom(H), #SHom(H), #LSHom(H) and #Ret(H) are in* FP.

Proof. Theorems 1.1, 1.2, 1.3 and Corollary 1.7 give complexity classifications for all of the problems. The reductions in the corollary follow from three easy observations.

- All problems in FP are trivially inter-reducible.
- All #P-complete problems are inter-reducible.
- All problems in FP are reducible to all #P-complete problems.

The separating graph H can be taken to be any reflexive clique of size at least 3 or any irreflexive biclique that is not a star. ∎

1.3. Related Work. This section was added after the announcement of our results (https://arxiv.org/abs/1706.08786v1), in order to draw attention to some interesting subsequent work [7, 5].

Both our tractability results and our hardness results rely on the fact (see Theorem 3.8) that the number of compactions from G to H can be expressed as a linear combination of the number of homomorphisms from G to certain subgraphs J of H. A similar statement applies to surjective homomorphisms.

As we note in the paper, these kinds of linear combinations have been noticed in related contexts before, for example in [2, Lemma 4.2] and in [26]. We use the linear combination of Theorem 3.8, together with interpolation, to prove hardness. Although it is standard to restrict the input graph G to be irreflexive (and this restriction makes the results stronger) the fact that G is required to be irreflexive causes severe difficulties.

In fact, Dell's note about our paper [7] shows that, if you weaken the theorem statements by allowing the input G to have loops, then a simpler interpolation based on a very recent paper by Curticapean, Dell and Marx [6] can be used to make the proofs very elegant! The exact same idea, written more generally, was also discovered by Chen [5].

2. Preliminaries. It will often be technically convenient to restrict the problems that we study by requiring the input graph G to be connected. In each case, we do this by adding a superscript "C" to the name of the problem. For example, the problem $\#\mathrm{Hom}^{\mathrm{C}}(H)$ is defined as follows.

Name. $\#\mathrm{Hom}^{\mathrm{C}}(H)$.
Input. A *connected* irreflexive graph G.
Output. $N\big(G \to H\big)$.

It is well known and easy to see (See, e.g., [26, (5.28)]) that if G is an irreflexive graph with components $G_1, \ldots, G_t$ then $N\big(G \to H\big) = \prod_{i\in[t]} N\big(G_i \to H\big)$. Similarly, given $\mathbf{S} = \{S_v \subseteq V(H) : v \in V(G)\}$ let $\mathbf{S}_i = \{S_v : v \in V(G_i)\}$. Then $N\big((G, \mathbf{S}) \to H\big) = \prod_{i\in[t]} N\big((G_i, \mathbf{S}_i) \to H\big)$. Thus, Dyer and Greenhill's theorem (Theorem 1.1) can be re-stated in the following convenient form.

THEOREM 2.1 (Dyer, Greenhill). *Let H be a graph. If every connected component of H is a reflexive clique or an irreflexive biclique, then $\#Hom^C(H)$, $\#Hom(H)$, $\#LHom^C(H)$ and $\#LHom(H)$ are all in* FP. *Otherwise, $\#Hom^C(H)$, $\#Hom(H)$, $\#LHom^C(H)$ and $\#LHom(H)$ are all* #P*-complete.*

Finally, we introduce some frequently used notation. For every positive integer n, we define $[n] = \{1, \ldots, n\}$.

A subgraph H' of H is said to be *loop-hereditary* with respect to H if for every $v \in V(H')$ that is contained in a loop in $E(H)$, v is also contained in a loop in $E(H')$.

We indicate that two graphs G_1 and G_2 are isomorphic by writing $G_1 \cong G_2$.

Given sets S_1 and S_2, we write $S_1 \oplus S_2$ for the disjoint union of S_1 and S_2. Given graphs G_1 and G_2, we write $G_1 \oplus G_2$ for the graph $(V(G_1) \oplus V(G_2), E(G_1) \oplus E(G_2))$. If V is a set of vertices then we write $G_1 \oplus V$ as shorthand for the graph $G_1 \oplus (V, \emptyset)$. Similarly, if M is a matching (a set of disjoint edges) with vertex set V, then we write $G_1 \oplus M$ as shorthand for the graph $G_1 \oplus (V, M)$.

3. Counting Compactions. The section is divided into a short subsection on tractable cases and the main subsection on hardness results which also contains the proof of the final dichotomy result, Theorem 1.2.

3.1. Tractability Results. The tractability result in Lemma 3.1 follows from the fact (see Theorem 3.8) that the number of compactions from G to H can be expressed as a linear combination of the number of homomorphisms from G to certain subgraphs J of H. While we need the full details of our particular linear expansion to derive our hardness results, the following simpler version suffices for tractability.

LEMMA 3.1. *Let H be a graph such that every connected component is an irreflexive star or a reflexive clique of size at most* 2*. Then $\#Comp(H)$ and $\#LComp(H)$ are in* FP.

Proof. First we deal with the case that H is the empty graph. Suppose that H is the empty graph and let $(G, \mathbf{S})$ be an instance of $\#\mathrm{LComp}(H)$. If G is empty then $N^{\mathrm{comp}}\big((G, \mathbf{S}) \to H\big) = 1$. Otherwise, $N^{\mathrm{comp}}\big((G, \mathbf{S}) \to H\big) = 0$. Thus, if H is empty, then $\#\mathrm{LComp}(H)$ is in FP. Obviously, this also implies that $\#\mathrm{Comp}(H)$ is in FP.

Let $\mathcal{H}$ be the set of all non-empty graphs in which every connected component is an irreflexive star or a reflexive clique of size at most 2. We will show that for every $H \in \mathcal{H}$, #LComp(H) is in FP. To do this, we need the following notation. Given a graph H, let $m(H)$ denote the sum of $|V(H)|$ and the number of non-loop edges of H. We will use induction on $m(H)$.

The base case is $m(H) = 1$. In this case, H has only one vertex w. If G is non-empty and has $w \in S_v$ for every vertex $v \in V(G)$ then $N^{\mathrm{comp}}\big((G, \mathbf{S}) \to H\big) = 1$. Otherwise, $N^{\mathrm{comp}}\big((G, \mathbf{S}) \to H\big)$ is 0. So #LComp(H) is in FP.

For the inductive step, consider some $H \in \mathcal{H}$ with $m(H) > 1$. Let $(G, \mathbf{S})$ be an instance of #LComp(H). If G is empty then $N^{\mathrm{comp}}\big((G, \mathbf{S}) \to H\big) = 0$, so suppose that G is non-empty. For every subgraph H' of H let $\mathbf{S}_{H'}$ denote the set of lists $\mathbf{S}_{H'} = \{S_v \cap V(H') : v \in V(G)\}$. It is easy to see that $N\big((G, \mathbf{S}) \to H\big) = \sum_{H'} N^{\mathrm{comp}}\big((G, \mathbf{S}_{H'}) \to H'\big)$, where the sum is over all loop-hereditary subgraphs H' of H. This observation is well known and is implicit, e.g, in the proof of a lemma of Borgs, Chayes, Kahn and Lovász [2, Lemma 4.2] (in a context without lists or loops).

A subgraph H' of H is said to be a *proper* subgraph of H if either $V(H')$ is a strict subset of $V(H)$ or $E(H')$ is a strict subset of $E(H)$ (or both). For every graph H, let $Sub^{<}(H)$ denote the set of non-empty proper subgraphs of H that are loop-hereditary with respect to H. Note that if $H \in \mathcal{H}$ and $H' \in Sub^{<}(H)$ then $H' \in \mathcal{H}$ and $m(H') < m(H)$. We can refine the summation as follows.

$$N\big((G, \mathbf{S}) \to H\big) = N^{\mathrm{comp}}\big((G, \mathbf{S}) \to H\big) + \sum_{H' \in Sub^{<}(H)} N^{\mathrm{comp}}\big((G, \mathbf{S}_{H'}) \to H'\big). \qquad \square$$

Since $H \in \mathcal{H}$, every component of H is a reflexive clique or an irreflexive biclique, so Theorem 1.1 shows that the quantity $N\big((G, \mathbf{S}) \to H\big)$ on the left-hand side can be computed in polynomial time. By induction, we see that every term of the form $N^{\mathrm{comp}}\big((G, \mathbf{S}_{H'}) \to H'\big)$ can also be computed in polynomial time. Subtracting this from the left-hand side, we obtain $N^{\mathrm{comp}}\big((G, \mathbf{S}) \to H\big)$, as desired.

Thus, we have proved that #LComp(H) is in FP. The problem #Comp(H) is a restriction of #LComp(H), so it is also in FP.

3.2. Hardness Results. This is the key section of this work. In this section, we consider a graph H that has a connected component that is not an irreflexive star or a reflexive clique of size at most 2. The objective is to show that #Comp(H) and #LComp(H) are #P-hard (this is the hardness content of Theorem 1.2).

We start with a brief proof sketch. The easy case is when H contains a component that is not a reflexive clique or an irreflexive biclique. In this case, Dyer and Greenhill's Theorem 1.1 shows that #Hom(H) is #P-hard. We obtain the desired hardness by giving (in Theorem 3.4) a polynomial-time Turing reduction from #Hom(H) to #Comp(H). The result is finished off with a trivial reduction from #Comp(H) to #LComp(H). The proof of Theorem 3.4 is not difficult — given an input G to #Hom(H), we add isolated vertices and edges to G and recover the desired quantity $N\big(G \to H\big)$ using an oracle for #Comp(H) and polynomial interpolation. There are small technical issues related to size-1 components in H, and these are dealt with in Lemma 3.2.

The more interesting case is when every component of H is a reflexive clique or an irreflexive biclique, but some component is either a reflexive clique of size at least 3 or an irreflexive biclique that is not a star. The first milestone is Lemma 3.14, which shows #P-hardness in the special case where H is connected. We prove Lemma 3.14

in a slightly stronger setting where the input graph G is connected. This allows us, in the remainder of the section, to generalise the connected case to the case in which H is not connected.

The main difficulty, then, is Lemma 3.14. The goal is to show that #Comp(H) is #P-hard when H is a reflexive clique of size at least 3 or an irreflexive biclique that is not a star. Our main method for solving this problem is a technique (Theorem 3.8) that lets us compute the number of compactions from a connected graph G to a connected graph H using a weighted sum of homomorphism counts, say $N\big(G \to J_1\big), \dots, N\big(G \to J_k\big)$. An important feature is that some of the weights might be negative.

Our basic approach will be to find a constituent J_i such that $\#\mathrm{Hom}^{\mathrm{C}}(J_i)$ is #P-hard and to reduce $\#\mathrm{Hom}^{\mathrm{C}}(J_i)$ to the problem of computing the weighted sum. Of course, if computing $N\big(G \to J_1\big)$ is #P-hard and computing $N\big(G \to J_2\big)$ is #P-hard, it does not follow that computing a weighted sum of these is #P-hard.

In order to solve this problem, in Lemmas 3.10 and 3.11 we use an argument similar to that of Lovász [25, Theorem 3.6] to prove the existence of input instances that help us to distinguish between the problems $\#\mathrm{Hom}^{\mathrm{C}}(J_1), \dots, \#\mathrm{Hom}^{\mathrm{C}}(J_k)$. Theorem 3.12 then provides the desired reduction from a chosen $\#\mathrm{Hom}^{\mathrm{C}}(J_i)$ to the problem of computing the weighted sum. Theorem 3.12 is proved by a more complicated interpolation construction, in which we use the instances from Lemma 3.11 to modify the input.

Having sketched the proof at a high level, we are now ready to begin. We start by working towards the proof of Theorem 3.4. The first step is to show that deleting size-1 components from H does not add any complexity to #Comp(H).

Lemma 3.2. *Let H be a graph that has exactly q size-1 components. Let H' be the graph constructed from H by removing all size-1 components. Then #Comp(H') $\leq$ #Comp(H).*

Proof. Let $W = \{w_1, \dots, w_q\}$ be the vertices of H that are contained in size-1 components. We can assume $q \geq 1$, otherwise $H' = H$. Let G' be an input to #Comp(H') and note that G' might contain isolated vertices. For any non-negative integer t, let V_t be a set of t isolated vertices, distinct from the vertices of G', and let $G_t = G' \oplus V_t$. For all $i \in \{0, \dots, t\}$, we define $S^i(G')$ to be the number of homomorphisms σ from G' to H with the following properties:

1. σ uses all non-loop edges of H'.
2. $|\sigma(V(G')) \cap \{w_1, \dots, w_q\}| = i$,

where $\sigma(V(G'))$ is the image of $V(G')$ under the map σ. We define $N^i(V_t)$ as the number of homomorphisms τ from V_t to H such that $\{w_1, \dots, w_i\} \subseteq \tau(V(V_t))$. Intuitively, $N^i(V_t)$ is the number of homomorphisms from V_t to H that use at least a set of i arbitrary but fixed vertices of H, as the particular choice of vertices $\{w_1, \dots, w_i\}$ is not important when counting homomorphisms from a set of isolated vertices. For any compaction $\gamma\colon V(G_t) \to V(H)$, the restriction $\gamma|_{V(G)}$ has to use all non-loop edges in H'. As H' does not have size-1 components, this implies that all vertices other than $w_1, \dots, w_q$ are used by $\gamma|_{V(G)}$. Say, additionally, that γ uses $q - i$ vertices from W, for some $i \in \{0, \dots, q\}$. Then, $\gamma|_{V_t}$ has to use the remaining i vertices. Thus, for each fixed $t \geq 0$, we obtain a linear equation:

$$\underbrace{N^{\mathrm{comp}}\big(G_t \to H\big)}_{b_t} = \sum_{i=0}^{q} \underbrace{S^{q-i}(G')}_{x_i}\underbrace{N^i(V_t)}_{a_{t,i}}. \quad (399)$$

By choosing $q+1$ different values for the parameter t we obtain a system of linear equations. Here, we choose $t = 0, \dots, q$. Then the system is of the form $\mathbf{b} = \mathbf{A}\mathbf{x}$ for

$$\mathbf{b} = \begin{pmatrix} b_0 \\ \vdots \\ b_q \end{pmatrix} \qquad \mathbf{A} = \begin{pmatrix} a_{0,0} & \dots & a_{0,q} \\ \vdots & \ddots & \vdots \\ a_{q,0} & \dots & a_{q,q} \end{pmatrix} \qquad \text{and} \qquad \mathbf{x} = \begin{pmatrix} x_0 \\ \vdots \\ x_q \end{pmatrix}.$$

Note, that the vector $\mathbf{b}$ can be computed using $q+1$ #Comp(H) oracle calls. Further,

$$x_q = S^0(G') = N^{\text{comp}}\big(G' \to H'\big).$$

Thus, determining $\mathbf{x}$ is sufficient for computing the sought-for $N^{\text{comp}}\big(G' \to H'\big)$. It remains to show that the matrix $\mathbf{A}$ is of full rank and is therefore invertible.

If $t < i$, we observe that $a_{t,i} = 0$ as we cannot use at least i vertices of H when we have fewer than i vertices in the domain. For the diagonal elements with $t \in \{0, \dots, q\}$ we have that $a_{t,t} = N^t(V_t) = t!$ (note that $0! = 1$). Hence,

$$\mathbf{A} = \begin{pmatrix} 0! & 0 & \cdots & 0 \\ * & 1! & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ * & \cdots & * & q! \end{pmatrix}$$

is a triangular matrix with non-zero diagonal entries, which completes the proof. ∎

LEMMA 3.3. *Let H be a graph without any size-1 components. Then #Hom(H) $\leq$ #Comp(H).*

Proof. The proof is by interpolation and is somewhat similar to the proof of Lemma 3.2. Let G be an input to #Hom(H). We design a graph $G_t = G \oplus I_t$ as an input to the problem #Comp(H) by adding a set I_t of t disjoint new edges to the graph G.

We introduce some notation. Let $E^0(H)$ be the set of non-loop edges of H and let $r = \big|E^0(H)\big|$. Let $S^k(G)$ be the number of homomorphisms σ from G to H that use exactly k of the non-loop edges of H (additionally, σ might use any number of loops). Let $\{e_1, \dots, e_k\}$ be a set of k arbitrary but fixed non-loop edges from H. We define $N^k(I_t)$ as the number of homomorphisms τ from I_t to H such that $\{e_1, \dots, e_k\}$ are amongst the edges used by τ. Note that the particular choice of edges $\{e_1, \dots, e_k\}$ is not important when counting homomorphisms from an independent set of edges to H—$N^k(I_t)$ only depends on the numbers k and t.

We observe that, for each compaction $\gamma\colon V(G_t) \to V(H)$, the restriction $\gamma|_{V(G)}$ uses some set $F \subseteq E^0(H)$ of non-loop edges and does not use any other non-loop edges of H. Suppose that F has cardinality $|F| = r - k$ for some $k \in \{0, \dots, r\}$. Then $\gamma|_{V(I_t)}$ uses at least the remaining k fixed non-loop edges of H. As H does not have any size-1 components, this ensures at the same time that γ is surjective.

Therefore, we obtain the following linear equation for a fixed $t \geq 0$:

$$\underbrace{N^{\text{comp}}\big(G_t \to H\big)}_{b_t} = \sum_{k=0}^{r} \underbrace{S^{r-k}(G)}_{x_k} \underbrace{N^k(I_t)}_{a_{t,k}}.$$

As in the proof of Lemma 3.2, we choose $t = 0, \dots, r$ to obtain a system of linear equations with

$$\mathbf{b} = \begin{pmatrix} b_0 \\ \vdots \\ b_r \end{pmatrix} \qquad \mathbf{A} = \begin{pmatrix} a_{0,0} & \cdots & a_{0,r} \\ \vdots & \ddots & \vdots \\ a_{r,0} & \cdots & a_{r,r} \end{pmatrix} \qquad \text{and} \qquad \mathbf{x} = \begin{pmatrix} x_0 \\ \vdots \\ x_r \end{pmatrix}.$$

We can compute $\mathbf{b}$ using a #Comp(H) oracle. Further,

$$\sum_{k=0}^{r} x_k = \sum_{k=0}^{r} S^{r-k}(G) = \sum_{k=0}^{r} S^k(G) = N\big(G \to H\big).$$

Thus, determining the vector $\mathbf{x}$ is sufficient for computing the sought-for number of homomorphisms $N\big(G \to H\big)$.

Finally, we show that $\mathbf{A}$ is invertible. If $t < k$, we observe that $a_{t,k} = N^k(I_t) = 0$, as clearly it is impossible to use more than t edges of H when there are only t edges in I_t. Further, for the diagonal elements it holds that for $t \in [r]$ we have $a_{t,t} = N^t(I_t) = 2^t t!$ as there are $t!$ possibilities for assigning the edges in I_t to the fixed set of t edges of H and there are 2^t vertex mappings for each such assignment of edges, also $N^0(I_0) = 1$. Hence,

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ * & 2^1 1! & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ * & \cdots & * & 2^r r! \end{pmatrix}$$

is a triangular matrix with non-zero diagonal entries and is therefore invertible. □

THEOREM 3.4. *Let H be a graph. Then #Hom(H) ≤ #Comp(H).*

Proof. Let H' be the graph constructed from H by removing all size-1 components. By Lemma 3.2 we obtain #Comp(H') ≤ #Comp(H). Then Lemma 3.3 can be applied to the graph H' and thus we obtain #Hom(H') ≤ #Comp(H') ≤ #Comp(H). Finally, it follows from Theorem 1.1 that #Hom(H') ≡ #Hom(H), which gives #Hom(H) ≡ #Hom(H') ≤ #Comp(H') ≤ #Comp(H). □

Theorem 3.4 shows that hardness results from Theorem 1.1 will carry over from #Hom(H) to #Comp(H). We also know some cases where #Comp(H) is tractable from Lemma 3.1. The complexity of #Comp(H) is still unresolved if every component of H is a reflexive clique or an irreflexive biclique, but some reflexive clique has size greater than 2, or some irreflexive biclique is not a star. This is the case described at length at the beginning of the section. Recall that the first step is to specify a technique (Theorem 3.8) that lets us compute the number of compactions from a connected graph G to a connected graph H using a weighted sum of homomorphism counts, say $N\big(G \to J_1\big), \dots, N\big(G \to J_k\big)$. Towards this end, we introduce some definitions which we will use repeatedly in the remainder of this section.

DEFINITION 3.5. *A* weighted graph set *is a tuple $(\mathcal{H}, \lambda)$, where $\mathcal{H}$ is a set of* non-empty, pairwise non-isomorphic, connected *graphs and λ is a function $\lambda \colon \mathcal{H} \to \mathbb{Z}$.*

DEFINITION 3.6. *Let H be a connected graph. By Sub(H) we denote the set of non-empty, loop-hereditary, connected subgraphs of H. Let $\mathcal{S}_H$ be a set which contains exactly one representative of each isomorphism class of the graphs in Sub(H). Finally, for $H' \in \mathcal{S}_H$, we define $\mu_H(H')$ to be the number of graphs in Sub(H) that are isomorphic to H'.*

Note that for a connected graph H, we have $\mu_H(H) = 1$.

DEFINITION 3.7. *For each non-empty connected graph H, we define a weight function λ_H which assigns an integer weight to each non-empty connected graph J.*

- *If J is not isomorphic to any graph in $\mathcal{S}_H$, then $\lambda_H(J) = 0$.*
- *If $J \cong H$, then $\lambda_H(J) = 1$.*
- *Finally, if J is isomorphic to some graph in $\mathcal{S}_H$ but $J \ncong H$, we define $\lambda_H(J)$ inductively as follows.*

$$\lambda_H(J) = - \sum_{\substack{H' \in \mathcal{S}_H \\ s.t.\ H' \ncong H}} \mu_H(H') \lambda_{H'}(J).$$

Note that λ_H is well-defined as all graphs $H' \in \mathcal{S}_H$ with $H' \ncong H$ are smaller than H either in the sense of having fewer vertices or in the sense of having the same number of vertices but fewer edges.

The following theorem is the key to our approach for computing the number of compactions from a connected graph G to a connected graph H using a weighted sum of homomorphism counts. In the Appendix, we give an illustrative example where we verify the theorem for the case $H = K_{2,3}$ and we give the intuition behind the definitions. Here we go on to give the formal statement and proof.

THEOREM 3.8. *Let H be a non-empty connected graph. Then for every non-empty, irreflexive and connected graph G we have*

$$N^{comp}\big(G \to H\big) = \sum_{J \in \mathcal{S}_H} \lambda_H(J) N\big(G \to J\big).$$

Proof. Let $H_1, H_2, \dots$ be the set of non-empty connected graphs sorted by some fixed ordering that ensures that if H_i is isomorphic to a subgraph of H_j, then $i \leq j$. We verify the statement of the theorem by induction over the graph index with respect to this ordering. Let G be non-empty, irreflexive and connected.

For the base case, H_1 is K_1, which is the graph with one vertex and no edges. In this case, $\mathcal{S}_{H_1} = \{K_1\}$ and $\lambda_{K_1}(K_1) = 1$. Also

$$N^{\text{comp}}\big(G \to K_1\big) = N\big(G \to K_1\big).$$

So the theorem holds in this case.

Now assume that the statement holds for all graphs up to index i and consider the graph H_{i+1}. For ease of notation we set $H = H_{i+1}$. We use the fact that every homomorphism from a connected graph G to H_{i+1} is a compaction onto some non-empty, loop-hereditary and connected subgraph of H_{i+1} and vice versa. Thus, it holds that

$$\begin{aligned} N\big(G \to H\big) &= \sum_{H' \in \mathcal{S}_H} \mu_H(H') \cdot N^{\text{comp}}\big(G \to H'\big) \\ &= N^{\text{comp}}\big(G \to H\big) + \sum_{\substack{H' \in \mathcal{S}_H \\ \text{s.t. } H' \ncong H}} \mu_H(H') \cdot N^{\text{comp}}\big(G \to H'\big). \end{aligned}$$

Thus, we can rearrange and use the induction hypothesis to obtain

$$\begin{aligned} N^{\mathrm{comp}}\big(G \to H\big) &= N\big(G \to H\big) - \sum_{\substack{H' \in \mathcal{S}_H \\ \text{s.t. } H' \not\cong H}} \mu_H(H') \cdot N^{\mathrm{comp}}\big(G \to H'\big) \\ &= N\big(G \to H\big) - \sum_{\substack{H' \in \mathcal{S}_H \\ \text{s.t. } H' \not\cong H}} \mu_H(H') \cdot \sum_{J \in \mathcal{S}_{H'}} \lambda_{H'}(J) N\big(G \to J\big). \end{aligned}$$

Then we change the order of summation and use that $\lambda_{H'}(J) = 0$ if J is not isomorphic to any graph in $\mathcal{S}_{H'}$ to collect all coefficients that belong to a particular term $N\big(G \to J\big)$. We obtain

$$\begin{aligned} N^{\mathrm{comp}}\big(G \to H\big) &= N\big(G \to H\big) - \sum_{\substack{J \in \mathcal{S}_H \\ \text{s.t. } J \not\cong H}} \Big(\sum_{\substack{H' \in \mathcal{S}_H \\ \text{s.t. } H' \not\cong H}} \mu_H(H') \lambda_{H'}(J) \Big) N\big(G \to J\big) \\ &= \sum_{J \in \mathcal{S}_H} \lambda_H(J) N\big(G \to J\big). \end{aligned}$$

∎

We remark that Theorem 3.8 can be generalised to graphs H and G with multiple connected components by looking at all subgraphs of H, rather than just at the connected ones. However, within this work, the version for connected graphs suffices.

Let $(\mathcal{H}, \lambda)$ be a weighted graph set. The following parameterised problem is not natural in its own right, but it helps us to analyse the complexity of $\#\mathrm{Comp}^{\mathrm{C}}(H)$:

Name. $\#\mathrm{GraphSetHom}^{\mathrm{C}}((\mathcal{H}, \lambda))$.
Input. An irreflexive, connected graph G.
Output. $Z_{\mathcal{H},\lambda}(G) = \begin{cases} 0 & \text{if } G \text{ is empty} \\ \sum_{J \in \mathcal{H}} \lambda(J) N\big(G \to J\big) & \text{otherwise.} \end{cases}$

Corollary 3.9. *Let H be a non-empty connected graph. Then*

$$\#\mathit{Comp}^{C}(H) \equiv \#\mathit{GraphSetHom}^{C}((\mathcal{S}_H, \lambda_H)).$$

Proof. The corollary follows directly from Theorem 3.8. ∎

Corollary 3.9 gives us the desired connection between weighted graph sets and compactions. We will use this later in the proof of Lemma 3.14 to establish the #P-hardness of $\#\mathrm{Comp}^{\mathrm{C}}(H)$ when H is either a reflexive clique of size at least 3 or an irreflexive biclique that is not a star.

Our next goal is to prove Theorem 3.12, which states that, for certain weighted graph sets $(\mathcal{H}, \lambda)$, determining $Z_{\mathcal{H},\lambda}(G)$ is at least as hard as computing $N\big(G \to J\big)$ for some graph J from the set $\mathcal{H}$ with $\lambda(J) \neq 0$. To this end, we first introduce two lemmas that help us to distinguish between different graphs J in the interpolation that we will later use to prove Theorem 3.12.

For the following lemmas, we introduce some new notation. For a graph G with distinguished vertex $v \in V(G)$ and a graph H with distinguished vertex $w \in V(H)$, the quantity $N\big((G,v) \to (H,w)\big)$ denotes the number of homomorphisms h from G to H with $h(v) = w$. Analogously, $N^{\mathrm{inj}}\big((G,v) \to (H,w)\big)$ denotes the number of injective homomorphisms h from G to H with $h(v) = w$. If there exists an isomorphism from G to H that maps v onto w, we write $(G,v) \cong (H,w)$, otherwise we write

$(G,v) \not\cong (H,w)$. In the following lemma, we show that for two such target entities (H_1,w_1) and (H_2,w_2) that are non-isomorphic, there exists an input which separates them. To this end, we use an argument very similar to that presented in [16, Lemma 3.6] and in the textbook by Hell and Nešetřil [24, Theorem 2.11], which goes back to the works of Lovász [25, Theorem 3.6].

LEMMA 3.10. *Let H_1 and H_2 be connected graphs with distinguished vertices $w_1 \in V(H_1)$ and $w_2 \in V(H_2)$ such that $(H_1,w_1) \not\cong (H_2,w_2)$. Suppose that one of the following cases holds:*

Case 1. H_1 and H_2 are reflexive graphs.

Case 2. H_1 and H_2 are irreflexive bipartite graphs, each of which contains at least one edge.

Then

i) There exists a connected irreflexive graph G with distinguished vertex $v \in V(G)$ for which $N\big((G,v) \to (H_1,w_1)\big) \neq N\big((G,v) \to (H_2,w_2)\big)$.

ii) In Case 2 we can assume that G contains at least one edge and is bipartite.

Proof. In order to shorten the proof, we define some notation that depends on which case holds. In Case 1, we say that a tuple (G,v) consisting of a graph G with distinguished vertex v is *relevant* if G is connected and reflexive. In Case 2, we say that it is relevant if G is connected, irreflexive and bipartite and contains at least one edge. We start with a claim that applies in either case.

Claim: There exists a relevant (G,v) such that

$$N\big((G,v) \to (H_1,w_1)\big) \neq N\big((G,v) \to (H_2,w_2)\big).$$

Proof of the claim: To prove the claim, assume for a contradiction that for all relevant (G,v) we have

$$N\big((G,v) \to (H_1,w_1)\big) = N\big((G,v) \to (H_2,w_2)\big). \tag{3.1}$$

The contradiction will follow from the following subclaim:

Subclaim: For every relevant (G,v),

$$N^{\text{inj}}\big((G,v) \to (H_1,w_1)\big) = N^{\text{inj}}\big((G,v) \to (H_2,w_2)\big).$$

Proof of the subclaim: The proof of the subclaim is by induction on the number of vertices of G. For the base case of the induction we treat the two cases separately.

In Case 1, the base case of the induction is $|V(G)| = 1$. The relevant (G,v) is the graph consisting of the single (looped) vertex v. For every reflexive graph H and vertex $w \in V(H)$ we have that $N\big((G,v) \to (H,w)\big) = N^{\text{inj}}\big((G,v) \to (H,w)\big)$. Therefore, (3.1) implies that the subclaim is true for this (G,v).

In Case 2, the base case of the induction is $|V(G)| = 2$. (There are no relevant (G,v) with $|V(G)| < 2$ since G has to contain an edge.) Consider a relevant (H,w). Since H is irreflexive and the two vertices of G are connected by an edge (so cannot be mapped by a homomorphism to the same vertex of H) we have $N\big((G,v) \to (H,w)\big) = N^{\text{inj}}\big((G,v) \to (H,w)\big)$. Once again, (3.1) implies that the subclaim is true for this (G,v).

For the inductive step, suppose that the subclaim holds for all relevant (G,v) in which G has up to $k-1$ vertices. Consider a relevant (G,v) with $|V(G)| = k$. Let Θ

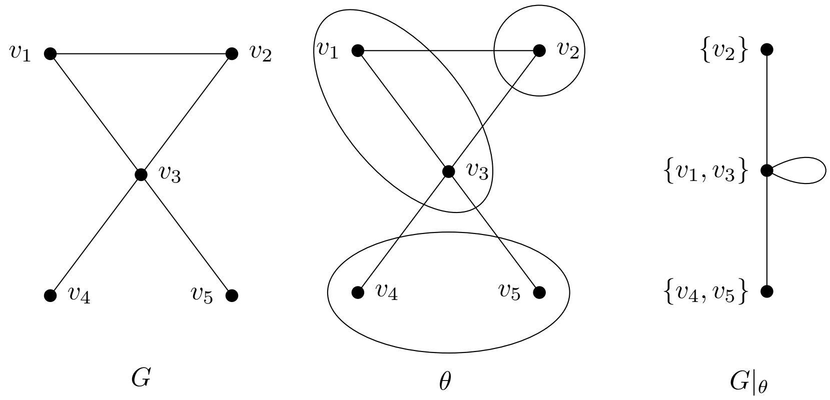


FIG. 1. *Graph G and the corresponding quotient graph $G|_\theta$ for $\theta = \{\{v_2\}, \{v_1, v_3\}, \{v_4, v_5\}\}$.*

be the set of partitions of $V(G)$ — that is, each $\theta \in \Theta$ is a set $\{U_1, \dots, U_j\}$ for some integer j such that the elements of θ are non-empty and pairwise disjoint subsets of $V(G)$ with $\bigcup_{i=1}^{j} U_i = V(G)$. For $\theta \in \Theta$ with $\theta = \{U_1, \dots, U_j\}$, by $G|_\theta$ we denote the corresponding *quotient graph*, i.e. let $G|_\theta$ be the graph with vertices $\{U_1, \dots, U_j\}$ that has an edge $\{U_i, U_{i'}\}$ if and only if there exist $v \in U_i$ and $u \in U_{i'}$ with $\{v, u\} \in E(G)$. Therefore, $G|_\theta$ might have loops but no multi-edges, see Figure 1. Let v_θ denote the vertex of $G|_\theta$ which corresponds to the equivalence class of θ that contains the distinguished vertex v. Finally, let τ denote the partition of $V(G)$ into singletons. Then for every relevant (H, w) it holds that

$$
\begin{aligned}
N\big((G,v) \to (H,w)\big) &= \sum_{\theta \in \Theta} N^{\mathrm{inj}}\big((G|_\theta, v_\theta) \to (H,w)\big) \\
&= N^{\mathrm{inj}}\big((G|_\tau, v_\tau) \to (H,w)\big) + \sum_{\theta \in \Theta \setminus \{\tau\}} N^{\mathrm{inj}}\big((G|_\theta, v_\theta) \to (H,w)\big) \\
&= N^{\mathrm{inj}}\big((G,v) \to (H,w)\big) + \sum_{\theta \in \Theta \setminus \{\tau\}} N^{\mathrm{inj}}\big((G|_\theta, v_\theta) \to (H,w)\big), \qquad (3.2)
\end{aligned}
$$

where the third equality follows as $G|_\tau = G$.

Now we show that only relevant tuples $(G|_\theta, v_\theta)$ actually contribute to the sum in (3.2). First, note that since G is connected, so is $G|_\theta$.

In Case 1, every quotient graph $G|_\theta$ is reflexive. Therefore, for every $\theta \in \Theta \setminus \{\tau\}$, the tuple $(G|_\theta, v_\theta)$ is relevant.

In Case 2, H is an irreflexive bipartite graph with at least one edge. Therefore, we have $N^{\mathrm{inj}}\big((G|_\theta, v_\theta) \to (H,w)\big) > 0$ only if $G|_\theta$ is an irreflexive bipartite graph and also, θ is a proper vertex-colouring of G, i.e. every part of θ is an independent set. For such a partition θ, $G|_\theta$ has at least one edge if G does. We have now shown that only relevant tuples $(G|_\theta, v_\theta)$ contribute to the sum in (3.2).

Therefore, let Γ be the set of all partitions θ of $V(G)$ such that $(G|_\theta, v_\theta)$ is relevant. Then, we can rephrase (3.2) as follows.

$$
N\big((G,v) \to (H,w)\big) = N^{\mathrm{inj}}\big((G,v) \to (H,w)\big) + \sum_{\theta \in \Gamma \setminus \{\tau\}} N^{\mathrm{inj}}\big((G|_\theta, v_\theta) \to (H,w)\big). \qquad (3.3)
$$

To prove the subclaim, we can set (H, w) in (3.3) to be (H_1, w_1). Similarly, we can set it to be (H_2, w_2). Then, we can use the induction hypothesis, the subclaim, on all tuples $(G|_\theta, v_\theta)$ in the sum as all these tuples are relevant and the partitions $\theta \in \Gamma\backslash\{\tau\}$ have strictly fewer than k parts. Applying (3.1), we obtain

$$N^{\text{inj}}\big((G,v) \to (H_1,w_1)\big) = N^{\text{inj}}\big((G,v) \to (H_2,w_2)\big),$$

which completes the induction and the proof of the subclaim. **(End of the proof of the subclaim.)**

We show next how to use the subclaim to derive a contradiction. In particular, in the subclaim we can set (G, v) to be either (H_1, w_1) or (H_2, w_2). This implies $(H_1, w_1) \cong (H_2, w_2)$, which gives the desired contradiction. Thus, we have shown contrary to (3.1) that there exists a relevant (G, v) with

$$N\big((G,v) \to (H_1,w_1)\big) \neq N\big((G,v) \to (H_2,w_2)\big)$$

and therefore we have proved the claim. **(End of the proof of the claim.)**

In Case 2, the claim is identical to the statement of the lemma. However, in Case 1 a relevant tuple (G, v) contains a reflexive graph G, whereas for the statement of the lemma, G has to be irreflexive. This is easily fixed as we can set G^0 to be the graph constructed from G by removing all loops. Using the fact that H_1 and H_2 are reflexive, we obtain for $i = 1$ and $i = 2$ that

$$N\big((G^0,v) \to (H_i,w_i)\big) = N\big((G,v) \to (H_i,w_i)\big).$$

Hence, the choice (G^0, v) has all the desired properties. ∎

In the following lemma, we generalise the pairwise property from Lemma 3.10. The result and the proof are adapted versions of [15, Lemma 6]. For ease of notation let $\binom{[k]}{2}$ denote the set of all pairs $\{i, j\}$ with $i, j \in [k]$ and $i \neq j$.

LEMMA 3.11. *Let $H_1, \ldots, H_k$ be connected graphs with distinguished vertices $w_1, \ldots, w_k$ where $w_i \in V(H_i)$ for all $i \in [k]$ and, for every pair $\{i, j\} \in \binom{[k]}{2}$, we have $(H_i, w_i) \ncong (H_j, w_j)$. Suppose that one of the following cases holds:*

Case 1. $\forall i \in [k]$, H_i is a reflexive graph.

Case 2. $\forall i \in [k]$, H_i is an irreflexive bipartite graph that contains at least one edge.

Then

i) There exists a connected irreflexive graph G with a distinguished vertex $v \in V(G)$ such that, for every $\{i, j\} \in \binom{[k]}{2}$, it holds that $N\big((G,v) \to (H_i,w_i)\big) \neq N\big((G,v) \to (H_j,w_j)\big)$.

ii) In Case 2 we can assume that G contains at least one edge and is bipartite.

Proof. Again, we use the notion of relevant tuples but slightly modify the definition from the one given in the proof of Lemma 3.10. A tuple (G, v) is called relevant if G is a connected *irreflexive* graph and, in Case 2, if additionally G contains at least one edge and is bipartite. We show that there exists a relevant (G, v) such that for every $\{i, j\} \in \binom{[k]}{2}$ we have

$$N\big((G,v) \to (H_i,w_i)\big) \neq N\big((G,v) \to (H_j,w_j)\big).$$

We use induction on k, which is the number of graphs $H_1, \ldots, H_k$. The base case for $k = 2$ is covered by Lemma 3.10. Now let us assume that the statement holds for $k-1$ and the inductive step is for k. By the inductive hypothesis there exists a relevant (G, v) such that without loss of generality (possibly by renaming the graphs $H_1, \dots, H_k$)

$$N\big((G,v) \to (H_2, w_2)\big) > \dots > N\big((G,v) \to (H_k, w_k)\big).$$

Let $i^* \in [k] \setminus \{1\}$ be an index with

$$N\big((G,v) \to (H_1, w_1)\big) = N\big((G,v) \to (H_{i^*}, w_{i^*})\big).$$

If no such index exists, we can simply choose the graph G which then fulfils the statement of the lemma. Using the base case, there exists a relevant (G', v') such that

$$N\big((G',v') \to (H_1, w_1)\big) > N\big((G',v') \to (H_{i^*}, w_{i^*})\big),$$

possibly renaming (H_1, w_1) and (H_{i^*}, w_{i^*}). Let $i \in [k]$.

First, we show that for all $i \in [k]$ we have $N\big((G',v') \to (H_i, w_i)\big) \geq 1$. This is clearly true for Case 1, where w_i has a loop. In this case, we can always map all vertices of G' to the single vertex w_i.

In Case 2, as H_i is connected and contains at least one edge, there is some $w \in V(H_i)$ such that $\{w, w_i\} \in E(H_i)$. Since (G', v') is relevant, G' is connected and bipartite and has at least one edge. Let $\{A, B\}$ be a partition of $V(G')$ such that $v' \in A$ and A and B are independent sets of G. There is a homomorphism h from G' to H_i with $h(v') = w_i$ which maps all vertices in A to w_i and all vertices in B to w.

Therefore, in both cases we have shown that for all $i \in [k]$ we have

$$N\big((G',v') \to (H_i, w_i)\big) \geq 1.$$

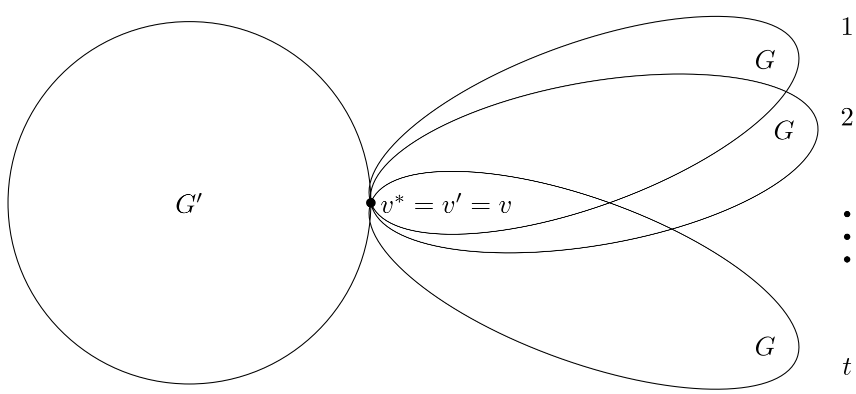


FIG. 2. (G^*, v^*).

For a yet to be determined number t we construct a graph G^* from (G, v) and (G', v') by taking the graph G' and t copies of G and identifying the vertex v' with the t copies of v and call the resulting vertex v^*, cf. Figure 2. Note that from the fact that (G, v) and (G', v') are relevant, it is straightforward to show that (G^*, v^*) is relevant as well. Then, for any graph H and $w \in V(H)$ it holds that

$$N\big((G^*,v^*) \to (H, w)\big) = N\big((G',v') \to (H, w)\big) \cdot N\big((G,v) \to (H, w)\big)^t.$$

The goal is to choose t sufficiently large to achieve

$$\begin{aligned} N\big((G^*,v^*)\to(H_2,w_2)\big) > \ldots > N\big((G^*,v^*)\to(H_{i^*-1},w_{i^*-1})\big) \\ > N\big((G^*,v^*)\to(H_1,w_1)\big) \\ > N\big((G^*,v^*)\to(H_{i^*},w_{i^*})\big) \\ > \ldots \\ > N\big((G^*,v^*)\to(H_k,w_k)\big). \end{aligned}$$

Accordingly, we define a permutation σ of the indices $\{1,\ldots,k\}$ that inserts index 1 between position i^*-1 and i^*. The domain of σ corresponds to the new indices to which we assign the former indices. To avoid confusion, we give the function table in Table 1

Table 1
Function table of σ.

i	1	$\cdots$	i^*-2	i^*-1	i^*	$\cdots$	k
$\sigma(i)$	2	$\cdots$	i^*-1	1	i^*	$\cdots$	k

Formally,

$$\sigma(i) = \begin{cases} i+1 & \text{if } i \le i^*-2 \\ 1 & \text{if } i = i^*-1 \\ i & \text{otherwise.} \end{cases}$$

Let $M = N\big((G,v)\to(H_2,w_2)\big)$. As $N\big((G',v')\to(H_j,w_j)\big) \ge 1$ for all $j\in[k]$, it is well-defined to set

$$C = \max_{j\in[k]\setminus\{i^*-1\}} \frac{N\big((G',v')\to(H_{\sigma(j+1)},w_{\sigma(j+1)})\big)}{N\big((G',v')\to(H_{\sigma(j)},w_{\sigma(j)})\big)}$$

and $t=\lceil CM\rceil$. Let G^* be as defined above. For ease of notation, for $j\in[k-1]$, we set

$$\xi(j) = \frac{N\big((G^*,v^*)\to(H_{\sigma(j)},w_{\sigma(j)})\big)}{N\big((G^*,v^*)\to(H_{\sigma(j+1)},w_{\sigma(j+1)})\big)}.$$

We want to show $\xi(j)>1$ for all $j\in[k-1]$ to complete the proof.

For $j=i^*-1$ we obtain

$$\begin{aligned} \xi(j) &= \frac{N\big((G^*,v^*)\to(H_{\sigma(i^*-1)},w_{\sigma(i^*-1)})\big)}{N\big((G^*,v^*)\to(H_{\sigma(i^*)},w_{\sigma(i^*)})\big)} \\ &= \frac{N\big((G^*,v^*)\to(H_1,w_1)\big)}{N\big((G^*,v^*)\to(H_{i^*},w_{i^*})\big)} \\ &= \frac{N\big((G',v')\to(H_1,w_1)\big)}{N\big((G',v')\to(H_{i^*},w_{i^*})\big)} > 1. \end{aligned}$$

For $j \in [k-1] \setminus \{i^*-1\}$ we have

$$\xi(j) = \frac{N\big((G^*, v^*) \to (H_{\sigma(j)}, w_{\sigma(j)})\big)}{N\big((G^*, v^*) \to (H_{\sigma(j+1)}, w_{\sigma(j+1)})\big)}$$
$$= \frac{N\big((G', v') \to (H_{\sigma(j)}, w_{\sigma(j)})\big) \cdot N\big((G, v) \to (H_{\sigma(j)}, w_{\sigma(j)})\big)^t}{N\big((G', v') \to (H_{\sigma(j+1)}, w_{\sigma(j+1)})\big) \cdot N\big((G, v) \to (H_{\sigma(j+1)}, w_{\sigma(j+1)})\big)^t}$$
$$\geq \frac{1}{C}\left(\frac{N\big((G, v) \to (H_{\sigma(j)}, w_{\sigma(j)})\big)}{N\big((G, v) \to (H_{\sigma(j+1)}, w_{\sigma(j+1)})\big)}\right)^t.$$

Since $N\big((G, v) \to (H_{\sigma(j)}, w_{\sigma(j)})\big) \geq 1 + N\big((G, v) \to (H_{\sigma(j+1)}, w_{\sigma(j+1)})\big)$ for

$$j \in [k-1] \setminus \{i^*-1\}$$

we have

$$\xi(j) \geq \frac{1}{C}\left(1 + \frac{1}{N\big((G, v) \to (H_{\sigma(j+1)}, w_{\sigma(j+1)})\big)}\right)^t.$$

Using $(1+x)^t \geq 1 + tx > tx$ for $t \geq 1$, $x \geq 0$ we obtain

$$\xi(j) > \frac{t}{C \cdot N\big((G, v) \to (H_{\sigma(j+1)}, w_{\sigma(j+1)})\big)}.$$

Finally, we use that for all $j \in [k-1] \setminus \{i^*-1\}$ we have

$$N\big((G, v) \to (H_2, w_2)\big) > N\big((G, v) \to (H_{\sigma(j+1)}, w_{\sigma(j+1)})\big)$$

and conclude

$$\xi(j) > \frac{t}{C \cdot N\big((G, v) \to (H_2, w_2)\big)} \geq \frac{t}{CM} \geq 1.$$

Thus, we have shown $\xi(j) > 1$ as required, which completes the proof. ∎

In the following theorem, we use the separating instances that we obtain from Lemma 3.11 for interpolation-based reductions to $\#\mathrm{GraphSetHom}^{\mathrm{C}}((\mathcal{H}, \lambda))$.

THEOREM 3.12. *Let $(\mathcal{H}, \lambda)$ be a weighted graph set for which one of two cases holds:*

Case 1. All graphs in $\mathcal{H}$ are reflexive.

Case 2. All graphs in $\mathcal{H}$ are irreflexive and bipartite.

Then, for all $H \in \mathcal{H}$ with $\lambda(H) \neq 0$, $\#Hom^{C}(H) \leq \#GraphSetHom^{C}((\mathcal{H}, \lambda))$.

Proof. If, in Case 2, $\mathcal{H}$ contains a graph without edges, i.e. a single-vertex graph K_1, let $(\mathcal{H}', \lambda')$ be a weighted graph set constructed from $(\mathcal{H}, \lambda)$ by removing the K_1 and its corresponding weight $\lambda(K_1)$. As $\#\mathrm{Hom}(K_1)$ is in FP we have

$$\#\mathrm{GraphSetHom}^{\mathrm{C}}((\mathcal{H}', \lambda')) \leq \#\mathrm{GraphSetHom}^{\mathrm{C}}((\mathcal{H}, \lambda))$$

and

$$\#\mathrm{Hom}^{\mathrm{C}}(K_1) \leq \#\mathrm{GraphSetHom}^{\mathrm{C}}((\mathcal{H}, \lambda)).$$

Therefore, for the remainder of this proof, we assume that every graph in $\mathcal{H}$ contains at least one edge. Let $\mathcal{H}^{\neq 0} = \{H_1, \ldots, H_k\}$ be the set of graphs in $\mathcal{H}$ that are assigned non-zero weights by λ. Note that all graphs in $\mathcal{H}^{\neq 0}$ are pairwise non-isomorphic, connected and non-empty by definition of a weighted graph set. Thus, for every pair $\{i,j\} \in \binom{[k]}{2}$ and every $w_i \in V(H_i)$, $w_j \in V(H_j)$ we have $(H_i, w_i) \ncong (H_j, w_j)$.

Now, for each graph H_i we collect the vertices which are in the same orbit of the automorphism group of H_i. Formally, for each $i \in [k]$ and $w \in V(H_i)$, let $[w]$ be the orbit of w, i.e. the set of vertices w' such that $(H_i, w') \cong (H_i, w)$. Let W be a set which contains exactly one representative from each such orbit. Further, for each $i \in [k]$ set $W_i = W \cap V(H_i)$. Then, for each $w, w' \in W_i$ with $w' \neq w$, we have $(H_i, w) \ncong (H_i, w')$.

Let $k' = \sum_{i=1}^{k} |W_i|$ and let $(H'_1, w'_1), \ldots, (H'_{k'}, w'_{k'})$ be an enumeration of the tuples $\{(H_i, w_i) : i \in [k],\ w_i \in W_i\}$. Then we can apply Lemma 3.11 to the input $(H'_1, w'_1), \ldots, (H'_{k'}, w'_{k'})$ to obtain a connected irreflexive graph J with distinguished $u \in V(J)$ such that for every $i, j \in [k]$ and for all $w_i \in W_i$, $w_j \in W_j$ we have $N\big((J,u) \to (H_i, w_i)\big) \neq N\big((J,u) \to (H_j, w_j)\big)$.

Let $i \in [k]$ and suppose that $H_i \in \mathcal{H}$ and $\lambda(H_i) \neq 0$. Let G be a non-empty graph which is an input to the problem $\#\mathrm{Hom}^{\mathrm{C}}(H_i)$. Let v be an arbitrary vertex of G. We use the same construction as in Figure 2 to design a graph G_t as input to the problem $\#\mathrm{GraphSetHom}^{\mathrm{C}}((\mathcal{H}, \lambda))$ by taking t copies of J as well as the graph G and identifying the t copies of vertex u with the vertex $v \in V(G)$. As both G and J are connected, G_t is as well. Then, using an oracle for $\#\mathrm{GraphSetHom}^{\mathrm{C}}((\mathcal{H}, \lambda))$, we can compute $Z_{\mathcal{H},\lambda}(G_t)$ with

$$\begin{aligned} Z_{\mathcal{H},\lambda}(G_t) &= \sum_{H \in \mathcal{H}} \lambda(H) N\big(G_t \to H\big) \\ &= \sum_{i \in [k]} \lambda(H_i) N\big(G_t \to H_i\big) \\ &= \sum_{i \in [k]} \lambda(H_i) \sum_{w \in V(H_i)} N\big((G,v) \to (H_i, w)\big) \cdot N\big((J,u) \to (H_i, w)\big)^t \qquad (3.4) \end{aligned}$$

Now we collect the terms which belong to vertices in the same orbit. To this end, for $w \in W$ and $i \in [k]$ such that $w \in V(H_i)$, we define $\lambda_w = |[w]| \cdot \lambda(H_i)$, $N_w(G) = N\big((G,v) \to (H_i, w)\big)$ and $N_w(J) = N\big((J,u) \to (H_i, w)\big)$. Let $W = \{w_0, \ldots, w_r\}$. Then, continuing from Equation (3.4):

$$\begin{aligned} Z_{\mathcal{H},\lambda}(G_t) &= \sum_{i \in [k]} \lambda(H_i) \sum_{w \in V(H_i)} N\big((G,v) \to (H_i, w)\big) \cdot N\big((J,u) \to (H_i, w)\big)^t \\ &= \sum_{w \in W} \lambda_w N_w(G) N_w(J)^t. \end{aligned}$$

By choosing $r+1$ different values for the parameter t — here it is sufficient to choose $t = 0, \ldots, r$ — we obtain a system of linear equations $\mathbf{b} = \mathbf{A}\mathbf{x}$ as follows:

$$\mathbf{b} = \begin{pmatrix} Z_{\mathcal{H},\lambda}(G_0) \\ \vdots \\ Z_{\mathcal{H},\lambda}(G_r) \end{pmatrix} \quad \mathbf{A} = \begin{pmatrix} \lambda_{w_0} N_{w_0}(J)^0 & \ldots & \lambda_{w_r} N_{w_r}(J)^0 \\ \vdots & \ddots & \vdots \\ \lambda_{w_0} N_{w_0}(J)^r & \ldots & \lambda_{w_r} N_{w_r}(J)^r \end{pmatrix} \quad \mathbf{x} = \begin{pmatrix} N_{w_0}(G) \\ \vdots \\ N_{w_r}(G) \end{pmatrix}$$

The vector $\mathbf{b}$ can be computed using $r+1$ $\#\mathrm{GraphSetHom}^{\mathrm{C}}((\mathcal{H}, \lambda))$ oracle calls. Then

$$N\big(G \to H_i\big) = \sum_{w \in W_i} |[w]| N_w(G).$$

Thus, determining x is sufficient for computing the sought-for $N\big(G \to H_i\big)$. It remains to show that the matrix $\mathbf{A} \in \mathbb{Z}^{(r+1)\times(r+1)}$ is of full rank and therefore invertible. This can be easily seen by dividing each column by its first entry. The division is well-defined as for $t \in \{0 \dots, r\}$ we have $\lambda_{w_t} \neq 0$ by definition of $\mathcal{H}^{\neq 0}$. The columns of the resulting matrix are pairwise different by the choice of (J, u) and as a consequence the resulting matrix is a Vandermonde matrix and therefore invertible. ∎

Next, we give a short technical lemma which follows from Definition 3.7 and is used in Lemma 3.14 to show that Theorem 3.12 gives hardness results for $\#\mathrm{Comp}^{\mathrm{C}}(H)$.

LEMMA 3.13. *Let H be a connected graph with at least one non-loop edge. Let H^- be the graph obtained from H by deleting exactly one non-loop edge (but keeping all vertices). If H^- is connected, then $\lambda_H(H^-) \neq 0$.*

Proof. As H^- is non-empty and connected, it is a valid input to λ_H and from the definition of λ_H (Definition 3.7) we obtain

$$\lambda_H(H^-) = -\sum_{\substack{H' \in \mathcal{S}_H \\ \text{s.t. } H' \not\cong H}} \mu_H(H')\lambda_{H'}(H^-).$$

Consider a graph $H' \in \mathcal{S}_H$ with $H' \not\cong H$ and $H' \not\cong H^-$. H' is a non-empty loop-hereditary connected subgraph of H and not isomorphic to H or H^-. Note that H^- is not isomorphic to any graph in $\mathcal{S}_{H'}$ which gives $\lambda_{H'}(H^-) = 0$. Furthermore, $\mu_H(H^-) \geq 1$. Thus, we proceed

$$\begin{aligned}\lambda_H(H^-) &= -\mu_H(H^-)\lambda_{H^-}(H^-) \\ &\leq -1.\end{aligned}$$ ∎

We now have most of the tools at hand to classify the complexity of $\#\mathrm{Comp}(H)$. Tractability results come from Lemma 3.1. If H has a component that is not a reflexive clique or an irreflexive biclique then hardness will be lifted from Dyer and Greenhill's Theorem 1.1 via Theorem 3.4. The most difficult case is when all components of H are reflexive cliques or irreflexive bicliques, but some component is not an irreflexive star or a reflexive clique of size at most 2.

If H is connected then hardness will come from the following lemma, whose proof builds on the weighted graph set technology (Corollary 3.9) using Theorem 3.12 and Lemma 3.13 (using the stronger hardness result of Dyer and Greenhill, Theorem 2.1).

The remainder of the section generalises the connected case to the case in which H is not connected.

LEMMA 3.14. *If H is a reflexive clique of size at least 3 then $\#Comp^{\mathrm{C}}(H)$ is #P-hard. If H is an irreflexive biclique that is not a star then $\#Comp^{\mathrm{C}}(H)$ is #P-hard.*

Proof. Suppose that H is a reflexive clique of size at least 3 or an irreflexive biclique that is not a star. Recall the definitions of $\mathcal{S}_H$, λ_H and weighted graph sets (Definitions 3.5, 3.6 and 3.7). Note that $(\mathcal{S}_H, \lambda_H)$ is a weighted graph set. Let H^- be a graph obtained from H by deleting a non-loop edge. Note that H^- is connected and it is not a reflexive clique or an irreflexive biclique. Thus Theorem 2.1 states that $\#\mathrm{Hom}^{\mathrm{C}}(H^-)$ is #P-complete. We will complete the proof of the Lemma by showing $\#\mathrm{Hom}^{\mathrm{C}}(H^-) \leq \#\mathrm{Comp}^{\mathrm{C}}(H)$.

If H is a reflexive graph then the definition of $\mathcal{S}_H$ ensures that all graphs in $\mathcal{S}_H$ are reflexive. If H is an irreflexive bipartite graph, then the definition ensures that all graphs in $\mathcal{S}_H$ are irreflexive and bipartite. Since H^- is connected and therefore $\lambda_H(H^-) \neq 0$ by Lemma 3.13, we can apply Theorem 3.12 to the weighted graph set $(\mathcal{S}_H, \lambda_H)$ with $H^- \in \mathcal{S}_H$ to obtain $\#\mathrm{Hom}^{\mathrm{C}}(H^-) \leq \#\mathrm{GraphSetHom}^{\mathrm{C}}((\mathcal{S}_H, \lambda_H))$. By Corollary 3.9, $\#\mathrm{GraphSetHom}^{\mathrm{C}}((\mathcal{S}_H, \lambda_H)) \equiv \#\mathrm{Comp}^{\mathrm{C}}(H)$. The lemma follows.

We use the following two definitions in Lemmas 3.17 and 3.18 and in the proof of Theorem 1.2.

Definition 3.15. *Let H be a graph. Suppose that every connected component that has more than j vertices is an irreflexive star. Suppose further that some connected component has j vertices and is not an irreflexive star. Let $\mathcal{A}(H)$ be the set of reflexive components of H with j vertices and let $\mathcal{B}(H)$ be the set of irreflexive non-star components of H with j vertices.*

Definition 3.16. *Let $L(H)$ denote the set of loops of a graph H. We define the graph $H^0 = (V(H), E(H) \setminus L(H))$.*

Lemma 3.17. *Let H be a graph in which every component is a reflexive clique or an irreflexive biclique. If $J \in \mathcal{A}(H)$ then $\#Comp^{C}(J) \leq \#Comp(H)$.*

Proof. Let H be a graph in which every component is a reflexive clique or an irreflexive biclique. Let $\mathcal{A}(H) = \{A_1, \dots, A_k\}$. It follows from the definition of $\mathcal{A}(H)$ that all elements of $\mathcal{A}(H)$ are reflexive cliques of some size j (the same j for all graphs in $\mathcal{A}(H)$).

If $j \leq 2$, the statement of the lemma is trivially true, since Lemma 3.1 shows that $\#\mathrm{Comp}(A_i)$ is in FP, so the restricted problem $\#\mathrm{Comp}^{\mathrm{C}}(A_i)$ is also in FP.

Now assume $j \geq 3$. Suppose without loss of generality that $J = A_1$. Let G be a (connected) input to $\#\mathrm{Comp}^{\mathrm{C}}(J)$. For all $i \in [k]$, let $H \setminus A_i$ be the graph constructed from H by deleting the connected component A_i. Using Definition 3.16 we define the (irreflexive) graph $G' = (H \setminus J \oplus G)^0$ as an input to $\#\mathrm{Comp}(H)$. Intuitively, to form G' from H we replace the connected component J with the graph G, then we delete all loops. We will prove the following claim.

Claim: Let $h\colon V(G') \to V(H)$ be a compaction from G' to H. Then the restriction $h|_{V(G)}$ is a compaction from G onto an element of $\mathcal{A}(H)$.

Proof of the claim: As h is a homomorphism, it maps each connected component of G' to a connected component of H. As, furthermore, h is a compaction and G' and H have the same number of connected components, it follows that there exist connected components $C_1, \dots, C_k$ of G' such that for $i \in [k]$, $h|_{V(C_i)}$ is a compaction from C_i onto A_i. To prove the claim, we show that G is an element of $\mathcal{C} = \{C_1, \dots, C_k\}$. In order to use all vertices of a graph in $\mathcal{A}(H)$, i.e. a reflexive size-j clique, a graph in $\mathcal{C}$ has to have at least j vertices itself. Therefore and by the construction of G', an element of $\mathcal{C}$ can only be one of the following:

- a clique with j vertices,
- a biclique with j vertices,
- a star with at least j vertices
- or the copy of G.

Since $j \geq 3$, it is easy to see that there is no compaction from a star onto a clique with j vertices. In order to compact onto a reflexive clique of size j, an element of $\mathcal{C}$ also has to have at least $j(j-1)/2$ edges. Thus, $\mathcal{C}$ does not contain any bicliques. Finally, there are only $k-1$ connected components in G' that are j-vertex cliques other than (possibly) G. Therefore, G has to be an element of $\mathcal{C}$, which proves the claim. **(End of the proof of the claim.)**

Using the notation from Definition 3.16, the claim implies

$$N^{\text{comp}}\big(G' \to H\big) = \sum_{i=1}^{k} N^{\text{comp}}\big(G \to A_i\big) \cdot N^{\text{comp}}\big((H \setminus A_i)^0 \to H \setminus A_i\big). \tag{3.5}$$

We can simplify the expression (3.5) using the fact that all elements of $\mathcal{A}(H)$ are reflexive size-j cliques:

$$N^{\text{comp}}\big(G' \to H\big) = k \cdot N^{\text{comp}}\big(G \to J\big) \cdot N^{\text{comp}}\big((H \setminus J)^0 \to H \setminus J\big).$$

As $N^{\text{comp}}\big((H \setminus J)^0 \to H \setminus J\big)$ does not depend on G, it can be computed in constant time. Thus, using a single #Comp(H) oracle call we can compute $N^{\text{comp}}\big(G \to J\big)$ in polynomial time as required. ∎

Lemma 3.18. *Let H be a graph in which every component is a reflexive clique or an irreflexive biclique. If $\mathcal{A}(H)$ is empty but $\mathcal{B}(H)$ is non-empty, then there exists a component $J \in \mathcal{B}(H)$ such that #Comp$^C(J) \le$ #Comp(H).*

Proof. The proof is similar to that of Lemma 3.17. For completeness, we give the details. By Definition 3.15 the elements of $\mathcal{B}(H)$ are of the form $K_{a,b}$ with $a + b = j$ for some fixed j. As stars are excluded from $\mathcal{B}(H)$, we have $a, b \ge 2$. Let $\mathcal{B}^{\max}(H)$ denote the set of graphs with the maximum number of edges in $\mathcal{B}(H)$. The elements of $\mathcal{B}^{\max}(H)$ are pairwise isomorphic since the number of edges of a $K_{a,b}$ is $a \cdot b = a(j-a)$ and this function is strictly increasing for $a \le j/2$. For concreteness, fix a and b so that each $J \in \mathcal{B}^{\max}(H)$ is isomorphic to $K_{a,b}$. Let $\mathcal{B}^{\max}(H) = \{B_1, \ldots, B_k\}$. Take $J = B_1$.

For all $i \in [k]$, let $H \setminus B_i$ be the graph constructed from H by deleting the connected component B_i. Let $G' = (H \setminus J \oplus G)^0$ be an input to #Comp(H). We will prove the following claim.

Claim: Let $h\colon V(G') \to V(H)$ be a compaction from G' to H. Then the restriction $h|_{V(G)}$ is a compaction from G onto an element of $\mathcal{B}^{\max}(H)$.

Proof of the claim: As h is a homomorphism, it maps each connected component of G' to a connected component of H. As, furthermore, h is a compaction and G' and H have the same number of connected components, it follows that there exist connected components $C_1, \ldots, C_k$ of G' such that for $i \in [k]$, $h|_{V(C_i)}$ is a compaction from C_i onto B_i. To prove the claim, we show that G is an element of $\mathcal{C} = \{C_1, \ldots, C_k\}$. In order to compact onto a graph in $\mathcal{B}^{\max}(H)$, a graph in $\mathcal{C}$ has to have at least j vertices and $a \cdot b$ edges itself. By the construction of G' and the fact that $\mathcal{A}(H)$ is empty, a connected component in G' with at least j vertices and $a \cdot b$ edges can only be one of the following:

- a biclique $K_{a,b}$,
- a star with at least j vertices and at least $a \cdot b$ edges
- or the copy of G.

Since $a, b \ge 2$, it is easy to see that there is no compaction from a star onto a $K_{a,b}$. Finally, there are only $k - 1$ connected components in G' that are bicliques of the form $K_{a,b}$ other than (possibly) G. Therefore, G has to be an element of $\mathcal{C}$, which proves the claim. **(End of the proof of the claim.)**

Using the notation from Definition 3.16, the claim implies

$$N^{\text{comp}}\big(G' \to H\big) = \sum_{i=1}^{k} N^{\text{comp}}\big(G \to B_i\big) \cdot N^{\text{comp}}\big((H \setminus B_i)^0 \to H \setminus B_i\big). \tag{3.6}$$

We can simplify the expression (3.6) using the fact that all elements of $\mathcal{B}^{\max}(H)$ are of the form $K_{a,b}$:

$$N^{\text{comp}}\big(G' \to H\big) = k \cdot N^{\text{comp}}\big(G \to J\big) \cdot N^{\text{comp}}\big((H \setminus J)^0 \to H \setminus J\big).$$

As $N^{\text{comp}}\big((H \setminus J)^0 \to H \setminus J\big)$ does not depend on G, it can be computed in constant time. Thus, using a single #Comp(H) oracle call we can compute $N^{\text{comp}}\big(G \to J\big)$ in polynomial time as required. ∎

Finally, we prove the main theorem of this section, which we restate at this point.

THEOREM 1.2. *Let H be a graph. If every connected component of H is an irreflexive star or a reflexive clique of size at most* 2 *then #Comp(H) and #LComp(H) are in* FP. *Otherwise, #Comp(H) and #LComp(H) are* #P*-complete.*

Proof. The membership of #Comp(H) in #P is straightforward. We distinguish between a number of cases depending on the graph H.

Case 1: Suppose that every connected component of H is an irreflexive star or a reflexive clique of size at most 2. Then #LComp(H) is in FP by Lemma 3.1.

Case 2: Suppose that H contains a component that is not a reflexive clique or an irreflexive biclique. Then the hardness of #Hom(H) (from Theorem 1.1) together with the reduction #Hom(H) $\leq$ #Comp(H) (from Theorem 3.4) implies that #Comp(H) is #P-hard. The hardness of #LComp(H) follows from the trivial reduction from #Comp(H) to #LComp(H).

Case 3: Suppose that the components of H are reflexive cliques or irreflexive bicliques and that H contains at least one component that is not an irreflexive star or a reflexive clique of size at most 2. Every graph $J \in \mathcal{A}(H) \cup \mathcal{B}(H)$ is a reflexive clique of size at least 3 or an irreflexive biclique that is not a star. By Lemma 3.14, #Comp$^{\text{C}}$(J) is #P-complete. Finally, as $\mathcal{A}(H) \cup \mathcal{B}(H)$ is non-empty, we can use either Lemma 3.17 or Lemma 3.18 to obtain the existence of $J \in \mathcal{A}(H) \cup \mathcal{B}(H)$ with #Comp$^{\text{C}}$(J) $\leq$ #Comp(H). This implies that #Comp(H) is #P-hard. As in Case 2, the hardness of #LComp(H) follows from the trivial reduction from #Comp(H) to #LComp(H). ∎

4. Counting Surjective Homomorphisms.

The proof of Theorem 1.3 is divided into two sections. The first of these deals with tractable cases and the second deals with hardness results and also contains the proof of the final theorem. Taken together, Theorem 1.3 and Dyer and Greenhill's Theorem 1.1 show that the problem of counting surjective homomorphisms to a fixed graph H has the same complexity characterisation as the problem of counting all homomorphisms to H.

Section 4.3 shows that this equivalence disappears in the uniform case, where H is part of the input, rather than being a fixed parameter of the problem. Specifically, Theorem 4.4 demonstrates a setting in which counting surjective homomorphisms is more difficult than counting all homomorphisms (assuming FP $\neq$ #P).

4.1. Tractability Results.

THEOREM 4.1. *Let H be a graph. Then #LSHom(H) $\leq$ #LHom(H).*

Proof. Let H be fixed and $|V(H)| = q$. Let $(G, \mathbf{S})$ be an input instance of #LSHom(H). Let $(v_1, \ldots, v_n)$ be the vertices of G in an arbitrary but fixed order. With respect to this ordering and with respect to a homomorphism from G to H, let us denote by v_{i_1} the first vertex of G which is assigned the first new vertex of H ($v_{i_1} = v_1$),

v_{i_2} the first vertex of G which is assigned the second new vertex of H and so on. Every surjective homomorphism from G to H contains exactly one subsequence $\mathbf{v} = (v_{i_1}, \dots, v_{i_q})$ and every homomorphism containing such a subsequence is surjective. The number of subsequences is bounded from above by $\binom{n}{q}$. Let $\sigma\colon \mathbf{v} \to V(H)$ be an assignment of the vertices of H to the vertices in $\mathbf{v}$. There are $q!$ such assignments. We call $\psi = (\mathbf{v}, \sigma)$ a *configuration* of G and $\Psi(G)$ the set of all configurations for the given G. For every such configuration ψ we create a #LHom(H) instance $(G, \mathbf{S}^\psi)$ with $\mathbf{S}^\psi = \{S^\psi_{v_i} \subseteq V(H) \ : \ i \in [n]\}$ and

$$S^\psi_{v_i} = \begin{cases} S_{v_i} \cap \{\sigma(v_{i_j})\}, & \text{if } i = i_j \text{ for } j \in [q] \\ S_{v_i} \cap \{\sigma(v_{i_1}), \dots, \sigma(v_{i_j})\}, & \text{for } i_j < i < i_{j+1}. \end{cases}$$

Intuitively, we use lists to "pin" the vertices in $\mathbf{v}$ to the vertices assigned by σ and to prohibit the remainder of the vertices of G from being mapped to new vertices of H. Then

$$N^{\text{sur}}\big((G, \mathbf{S}) \to H\big) = \sum_{\psi \in \Psi(G)} N\big((G, \mathbf{S}^\psi) \to H\big)$$

We can compute $N^{\text{sur}}\big((G, \mathbf{S}) \to H\big)$ by making a #LHom(H) oracle call for every instance $(G, \mathbf{S}^\psi)$ and adding the results. The number of oracle calls $|\Psi(G)|$ is bounded from above by the polynomial $q!\binom{n}{q} \le n^q$. ∎

COROLLARY 4.2. *Let H be a graph. If every connected component of H is a reflexive clique or an irreflexive biclique then #LSHom(H) is in* FP.

Proof. The statement follows directly from Theorem 4.1 using Dyer and Greenhill's dichotomy from Theorem 1.1. ∎

4.2. Hardness Results. The following result and proof are very similar to that of Theorem 3.4 and Lemma 3.3, respectively. For completeness, we repeat the proof in detail.

THEOREM 4.3. *Let H be a graph. Then #Hom(H) $\le$ #SHom(H).*

Proof. Let $|V(H)| = q$ and G be an input to #Hom(H). We design a graph $G_t = G \oplus W_t$ as an input to the problem #SHom(H) by adding a set W_t of t new isolated vertices to the graph G.

We introduce some additional notation. Let $S^k(G)$ be the number of homomorphisms σ from G to H that use exactly k of the vertices of H. Let $\{w_1, \dots, w_k\}$ be a set of k arbitrary but fixed vertices from H. We define $N^k(W_t)$ as the number of homomorphisms τ from W_t to H such that $\{w_1, \dots, w_k\}$ are amongst the vertices used by τ. The particular choice of vertices $\{w_1, \dots, w_k\}$ is not important when counting homomorphisms from a set of isolated vertices—$N^k(W_t)$ only depends on the numbers k and t.

We observe that, for each surjective homomorphism $\gamma\colon V(G_t) \to V(H)$, the restriction $\gamma|_{V(G)}$ uses a subset $V' \subseteq V(H)$ of vertices and does not use any vertices outside of V'. Suppose that V' has cardinality $|V'| = q - k$ for some $k \in \{0, \dots, q\}$. Then $\gamma|_{W_t}$ uses at least the remaining k fixed vertices of H.

Therefore, we obtain the following linear equation for a fixed $t \ge 0$:

$$\underbrace{N^{\text{sur}}\big(G_t \to H\big)}_{b_t} = \sum_{k=0}^{q} \underbrace{S^{q-k}(G)}_{x_k} \underbrace{N^k(W_t)}_{a_{t,k}}.$$

By choosing $q+1$ different values for the parameter t we obtain a system of linear equations. Here, we choose $t = 0, \ldots, q$. Then the system is of the form $\mathbf{b} = \mathbf{A}\mathbf{x}$ for

$$\mathbf{b} = \begin{pmatrix} b_0 \\ \vdots \\ b_q \end{pmatrix} \qquad \mathbf{A} = \begin{pmatrix} a_{0,0} & \cdots & a_{0,q} \\ \vdots & \ddots & \vdots \\ a_{q,0} & \cdots & a_{q,q} \end{pmatrix} \qquad \text{and} \qquad \mathbf{x} = \begin{pmatrix} x_0 \\ \vdots \\ x_q \end{pmatrix}.$$

Note, that the vector $\mathbf{b}$ can be computed using $q+1$ #SHom(H) oracle calls. Further,

$$\sum_{k=0}^{q} x_k = \sum_{k=0}^{q} S^{q-k}(G) = \sum_{k=0}^{q} S^k(G) = N\big(G \to H\big).$$

Thus, determining $\mathbf{x}$ is sufficient for computing the sought-for $N\big(G \to H\big)$. It remains to show that the matrix $\mathbf{A}$ is of full rank and is therefore invertible.

For $t < k$, clearly $a_{t,k} = N^k(W_t) = 0$. Further, for the diagonal elements we have $a_{t,t} = N^t(W_t) = t!$ for $t \in \{0, \ldots, q\}$. Hence,

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ * & 1! & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ * & \cdots & * & q! \end{pmatrix}$$

is a triangular matrix with non-zero diagonal entries, which completes the proof. ◻

THEOREM 4.4. *Let H be a graph. If every connected component of H is a reflexive clique or an irreflexive biclique, then #SHom(H) and #LSHom(H) are in* FP. *Otherwise, #SHom(H) and #LSHom(H) are #*P*-complete.*

Proof. The easiness result follows from Corollary 4.2 using the trivial reduction #SHom(H) $\leq$ #LSHom(H). The hardness result follows from the same trivial reduction, along with Theorem 4.3 and the dichotomy for #Hom(H) from Theorem 1.1.

4.3. The Uniform Case. We have seen from Theorems 1.1 and 1.3 that the problem of counting homomorphisms to a fixed graph H has the same complexity as the problem of counting *surjective* homomorphisms to H.

Nevertheless, there are scenarios in which counting problems involving surjective homomorphisms are more difficult than those involving unrestricted homomorphisms. To illustrate this point, we consider the following *uniform* homomorphism-counting problems. Motivated by terminology from constraint satisfaction, we use "uniform" to indicate that the target graph H is part of the input, rather than being a fixed parameter.

Name. Uniform#HomToCliques.
Input. Irreflexive graph G whose components are cliques and reflexive graph H whose components are cliques.
Output. $N\big(G \to H\big)$.

Name. Uniform#SHomToCliques.
Input. Irreflexive graph G whose components are cliques and reflexive graph H whose components are cliques.
Output. $N^{\text{sur}}\big(G \to H\big)$.

The main result of this section is the following theorem.

THEOREM 4.4. *Uniform#HomToCliques is in* FP *but Uniform#SHomToCliques is* #P-*complete.*

In order to prove Theorem 4.4, we define a counting variant of the subset sum problem. Given a set of integers $\mathcal{A} = \{a_1, \dots, a_n\}$ and an integer b let $S(\mathcal{A}, b)$, be the number of subsets $\mathcal{A}' \subseteq \mathcal{A}$ such that the sum of the elements in $\mathcal{A}'$ is equal to b. The counting problem is stated as follows.

Name. #SubsetSum.
Input. A set of positive integers $\mathcal{A} = \{a_1, \dots, a_n\}$ and a positive integer b.
Output. $S(\mathcal{A}, b)$.

It is well known that #SubsetSum is #P-complete (see for instance the textbook by Papadimitriou [29, Theorems 9.9, 9.10 and 18.1]). Thus, Theorem 4.4 follows immediately from Lemmas 4.5 and 4.6.

LEMMA 4.5. *Uniform#HomToCliques is in* FP.

Proof. Let G and H be an input instance of Uniform#HomToCliques. Let k be the number of connected components of G and let $a_1, \dots, a_k$ be the number of vertices of these components, respectively. Let H have q connected components with $b_1, \dots, b_q$ vertices, respectively. Then, as all components are cliques and H is reflexive,

$$N\big(G \to H\big) = \prod_{i=1}^{k} \sum_{j=1}^{q} b_j^{a_i}.$$

Thus, it is easy to compute $N\big(G \to H\big)$. ◻

LEMMA 4.6. *#SubsetSum* $\leq$ *Uniform#SHomToCliques.*

Proof. Let $\mathcal{A} = \{a_1, \dots, a_k\}$, b be an input instance of #SubsetSum. We define $N = \sum_{i=1}^{k} a_i$. Now, we design a polynomial time algorithm to determine $S(\mathcal{A}, b)$ using an oracle for Uniform#SHomToCliques. If $N < b$, we have $S(\mathcal{A}, b) = 0$. Now assume $N \geq b$. We create an input of Uniform#SHomToCliques as follows. We set G to be an irreflexive graph with a connected component G_i for each $i \in [k]$, where G_i is a clique with a_i vertices. Furthermore, we set H to be a reflexive graph with two connected components H_1 and H_2. Let H_1 be a clique with b vertices and let H_2 be a clique with $N - b$ vertices. By $\left\{ {n \atop k} \right\}$ we denote the Stirling number of the second kind, i.e. the number of partitions of a set of n elements into k non-empty subsets. By definition, we have $\left\{ {n \atop k} \right\} = 0$ if $n < k$.

Let $h\colon V(G) \to V(H)$ be a homomorphism from G to H and let b' be the number of vertices of G that are mapped to the connected component H_1. Note that h has to map each connected component of G to a connected component of H. By the construction of G, this implies that there exists a subset $\mathcal{A}' \subseteq \mathcal{A}$ such that the sum of elements in $\mathcal{A}'$ is equal to b'. Furthermore, as all connected components of G and H are cliques and H is reflexive, the number of surjective homomorphisms from G to H that assign exactly b' fixed vertices to H_1 is equal to the number of surjective mappings from $[b']$ to $[b]$, which is $b!\left\{ {b' \atop b} \right\}$. Therefore, we can express $N^{\text{sur}}\big(G \to H\big)$ as follows.

$$N^{\text{sur}}\big(G \to H\big) = \sum_{b'=0}^{N} S(\mathcal{A}, b') \cdot b! \left\{ {b' \atop b} \right\} \cdot (N-b)! \left\{ {N-b' \atop N-b} \right\}, \tag{4.1}$$

where the factor $(N-b)!\left\{{N-b' \atop N-b}\right\}$ corresponds to the number surjective mappings from the remaining $N-b'$ fixed vertices of G to the component H_2. Finally, we use the fact that the summands in (4.1) are non-zero only if $b' \geq b$ and $N-b' \geq N-b$, which implies $b'=b$. Thus,

$$\begin{aligned} N^{\text{sur}}\big(G \to H\big) &= S(\mathcal{A}, b) \cdot b!\left\{{b \atop b}\right\} \cdot (N-b)!\left\{{N-b \atop N-b}\right\} \\ &= b!(N-b)! \cdot S(\mathcal{A}, b). \end{aligned}$$

□

5. Addendum: A Dichotomy for Approximately Counting Homomorphisms with Surjectivity Constraints. The following standard definitions are taken from [28, Definitions 11.1, 11.2, Exercise 11.3]. A randomised algorithm gives an (ϵ, δ)-approximation for the value V if the output X of the algorithm satisfies $\Pr(|X-V| \leq \epsilon V) \geq 1-\delta$. A *fully polynomial randomised approximation scheme* (FPRAS) for a problem V is a randomised algorithm which, given an input x and a parameter $\epsilon \in (0,1)$, outputs an $(\epsilon, 1/4)$-approximation to $V(x)$ in time that is polynomial in $1/\epsilon$ and the size of the input x. The concept of an approximation-preserving reduction (AP-reduction) between counting problems was introduced by Dyer, Goldberg, Greenhill and Jerrum [9]. We will not need the detailed definition here, but the definition has the property that if there is an AP-reduction from problem A to problem B (written as $A \leq_{\text{AP}} B$) then this reduction, together with an FPRAS for B, yields an FPRAS for A. The problem #BIS, which is the problem of counting the independent sets of a bipartite graph, comes up frequently in approximate counting because it is complete with respect to AP-reductions in an intermediate complexity class. It is not believed to have an FPRAS. Galanis, Goldberg and Jerrum [15] gave a dichotomy for the problem of *approximately* counting homomorphisms in the connected case, in terms of #BIS.

THEOREM 5.1 ([15]). *Let H be a connected graph. If H is a reflexive clique or an irreflexive biclique, then there is an FPRAS for #Hom(H). Otherwise, #BIS $\leq_{\text{AP}}$ #Hom(H).*

In this addendum we give a similar dichotomy for approximately counting homomorphisms with surjectivity constraints[3]. The tractability part of the following theorem follows from Theorem 1.3, Corollary 1.7 and from Lemma 5.3 below. The #BIS-hardness follows from Theorem 5.1 and from the reductions in Lemmas 5.4, 5.5 and 5.6.

THEOREM 5.2. *Let H be a connected graph. If H is a reflexive clique or an irreflexive biclique, then there is an FPRAS for #SHom(H), #Ret(H) and #Comp(H). Otherwise, each of these problems is #BIS-hard under approximation-preserving reductions.*

LEMMA 5.3. *Let H be a reflexive clique or an irreflexive biclique. Then there is an FPRAS for #Comp(H).*

Proof. Let H be a reflexive clique or an irreflexive biclique with q vertices and p edges. Our goal is give an FPRAS for #Comp(H).

First, we show that we can assume without loss of generality that every input G to #Comp(H) has no isolated vertices. To see this, suppose instead that G is of

[3]When H is not connected, the complexity of approximate counting is open even for counting homomorphisms. Hence we do not address this case here.

the form $G' \oplus I$ where I is the set of isolated vertices in G. As H is connected, we have $N^{\text{comp}}\big(G \to H\big) = q^{|I|} N^{\text{comp}}\big(G' \to H\big)$. Thus, an estimate of the number of compactions from G' to H will immediately enable us to approximately count compactions from G to H.

From now on we restrict attention to inputs G which have no isolated vertices. We use $\mathcal{H}(G,H)$ to denote the set of homomorphisms from G to H.

Case 1. H is a reflexive clique.

Let G be a size-n input to #Comp(H). Then $N\big(G \to H\big) = q^n$. If there is a compaction from G to H then there is a set $U \subseteq V(G)$ with $|U| \leq 2p$ and a compaction σ from $G[U]$ to H. Each assignment of the (at most $n-2p$) vertices in $V(G) \setminus U$ extends σ to a compaction from G to H. Thus, we have $N^{\text{comp}}\big(G \to H\big) \geq q^{n-2p} = N\big(G \to H\big)/q^{2p}$. Using this lower bound, it is straightforward to apply the naive Monte Carlo method (cf. [28, Theorem 11.1]). Hence Algorithm 5.1 with $c = q^{2p}$ and $\mathcal{H} = \mathcal{H}(G,H)$ gives an (ϵ,δ)-approximation for the number of compactions in $\mathcal{H}$.

Algorithm 5.1 If the number of compactions in $\mathcal{H}$ is at least $|\mathcal{H}|/c$ then by [28, Theorem 11.1] this algorithm gives an (ϵ,δ)-approximation for the number of compactions in $\mathcal{H}$.

Input: Irreflexive graph G, $\epsilon \in (0,1)$ and $\delta \in (0,1)$.

$m = \lceil c3\ln(2/\delta)/\epsilon^2 \rceil$.

Choose m samples independently and uniformly at random from $\mathcal{H}$.

Let $X_1,\ldots,X_m$ be the corresponding indicator random variables, where X_i takes value 1

if the ith sample is a compaction and 0 otherwise.

$Y = \dfrac{|\mathcal{H}|}{m}\sum_{i=1}^{m} X_i$.

Output: Y

If there are no compactions in $\mathcal{H}$ then the algorithm answers 0. Otherwise, the number of compactions in $\mathcal{H}$ is at least $|\mathcal{H}|/c$, so the algorithm gives an (ϵ,δ)-approximation.

When the algorithm is run with $\delta = 1/4$, the running time is at most a polynomial in n and $1/\epsilon$ because m is at most a polynomial in $1/\epsilon$ and the basic tasks (choosing a sample from $\mathcal{H}$, determining whether a sample is a compaction, and computing $|\mathcal{H}| = q^n$) can all be done in poly(n) time. Thus, the algorithm gives an FPRAS for #Comp(H).

Case 2. H is an irreflexive biclique.

Let the bipartition of $V(H)$ be (L_H, R_H) where $\ell_H = |L_H| \leq |R_H| = r_H$. We can assume that $\ell_H \geq 1$, otherwise counting compactions to H is trivial.

Without loss generality, we can assume that inputs G to #Comp(H) are bipartite (as well as having no isolated vertices). (If G is not bipartite, then $N^{\text{comp}}\big(G \to H\big) = 0$.)

Suppose that G is an input to #Comp(H). Let $C_1,\ldots,C_\kappa$ be the connected components of G. For each $i \in [\kappa]$, let (L_i, R_i) be a fixed bipartition of C_i such that $1 \leq \ell_i = |L_i| \leq |R_i| = r_i$. Then $N\big(G \to H\big) = \prod_{i=1}^{\kappa}\Big(\ell_H^{\ell_i} {r_H}^{r_i} + {\ell_H}^{r_i} {r_H}^{\ell_i}\Big) \leq 2\prod_{i=1}^{\kappa} {\ell_H}^{\ell_i} {r_H}^{r_i}$.

Let Ω be the set of functions $\omega\colon [\kappa] \to \{L_H, R_H\}$. Given $\omega \in \Omega$, we say that a homomorphism from G to H obeys ω if, for each $i \in [\kappa]$, the vertices of L_i are assigned to vertices in $\omega(i)$.

Case 2a. $\kappa \geq p$.

Let ω be the function in Ω that maps every $i \in [\kappa]$ to L_H. Since G has no isolated vertices, each of $C_1, \dots, C_\kappa$ has at least 2 vertices, so there is a compaction from G to H which obeys ω.

As in Case 1, there is a set $U \subseteq V(G)$ of size at most $2p$ such that there is a compaction σ from $G[U]$ to H that obeys the restriction of σ to U. Every assignment of the vertices in $V(G) \setminus U$ that obeys ω yields an ω-obeying compaction from G to H. Since $r_H \geq \ell_H$, we obtain the lower bound

$$N^{\mathrm{comp}}\big(G \to H\big) \geq \frac{1}{(r_H)^{2p}} \prod_{i=1}^{\kappa} {\ell_H}^{\ell_i} {r_H}^{r_i} \geq \frac{N\big(G \to H\big)}{2(r_H)^{2p}}.$$

By the same arguments as in Case 1, Algorithm 5.1 with $c = 2(r_H)^{2p}$ and $\mathcal{H} = \mathcal{H}(G, H)$ gives an (ϵ, δ)-approximation for the number of compactions in $\mathcal{H}$. When the algorithm is run with $\delta = 1/4$, the running time is at most a polynomial in $|V(G)|$ and $1/\epsilon$, so it can be used in an FPRAS for inputs G with $\kappa \geq p$.

Case 2b. $\kappa < p$.

For each $\omega \in \Omega$, let $\mathcal{H}_\omega(G, H)$ be the set of homomorphisms obeying ω, and let $N_\omega(G \to H)$ and $N_\omega^{\mathrm{comp}}(G \to H)$ be the number of homomorphisms and compactions obeying ω, respectively. Given a compaction that obeys ω we obtain a lower bound as before:

$$N_\omega^{\mathrm{comp}}(G \to H) \geq \frac{1}{(r_H)^{2p}} \prod_{i=1}^{\kappa} |\omega(i)|^{\ell_i} (|V(H)| - |\omega(i)|)^{r_i} = \frac{N_\omega(G \to H)}{(r_H)^{2p}}. \qquad \square$$

Now Algorithm 5.1 with $c = (r_H)^{2p}$ and $\mathcal{H} = \mathcal{H}_\omega(G, H)$ gives an (ϵ, δ)-approximation for the number of compactions in $\mathcal{H}_\omega(G, H)$. Taking $\delta = 1/(4 \cdot 2^\kappa)$ and summing over the $2^\kappa < 2^p$ functions $\omega \in \Omega$, we obtain an $(\epsilon, 1/4)$-approximation for the number of compactions in $\mathcal{H}(G, H)$. The running time of each call to Algorithm 5.1 is at most a polynomial in $|V(G)|$ and $1/\epsilon$. Thus, putting the cases together, we get an FPRAS for #Comp(H).

Lemma 5.4. *Let H be a graph. Then #Hom(H) $\leq_{\mathrm{AP}}$ #SHom(H).*

Proof. Let $q = |V(H)|$. Given any positive integer t, let $s_{t,q}$ denote the number of surjective functions from $[t]$ to $[q]$. Clearly, $s_{t,q} \geq q^t - 2^q (q-1)^t$, since the range of every non-surjective function from $[t]$ to $[q]$ is a proper subset of $[q]$, and there are most 2^q of these. Also, the number of functions from $[t]$ onto this subset is at most $(q-1)^t$.

Given any n-vertex input G to the problem #Hom(H), let

$$t = \lceil \log(5q^n 2^q) / \log(q/(q-1)) \rceil.$$

Clearly, $t = O(n)$, and t can be computed in time poly(n). Note that

$$\left(\frac{q}{q-1}\right)^t \geq 5q^n 2^q \geq 4q^n 2^q + 2^q. \tag{5.1}$$

Let G_t be the graph constructed from G by adding a set I_t of t isolated vertices that are distinct from the vertices in $V(G)$. We claim that

$$s_{t,q} N\big(G \to H\big) \leq N^{\mathrm{sur}}\big(G_t \to H\big) \leq s_{t,q} N\big(G \to H\big) + (q^t - s_{t,q}) q^n.$$

To see this, note that any homomorphism from G to H, together with a surjective homomorphism from the I_t to $V(H)$, constitutes a surjective homomorphism from G_t to H. Any other surjective homomorphism from G_t to H consists of a non-surjective homomorphism from I_t to H (and there are $q^t - s_{t,q}$ of these) together with some homomorphism from G to H (and there are at most q^n of these). Dividing through by $s_{t,q}$ and applying our lower bound for $s_{t,q}$ and then inequality (5.1), we have

$$\begin{aligned} N\big(G \to H\big) \le \frac{N^{\mathrm{sur}}\big(G_t \to H\big)}{s_{t,q}} &\le N\big(G \to H\big) + \left(\frac{q^t - s_{t,q}}{s_{t,q}}\right) q^n \\ &\le N\big(G \to H\big) + \frac{2^q (q-1)^t q^n}{q^t - 2^q (q-1)^t} \\ &= N\big(G \to H\big) + \frac{q^n}{\frac{q^t}{2^q (q-1)^t} - 1} \\ &\le N\big(G \to H\big) + \frac{1}{4}. \qquad (5.2) \end{aligned}$$

∎

Given Equation (5.2), the proof of [9, Theorem 3] shows that, in order to approximate $N\big(G \to H\big)$ with accuracy ε, we need only use the oracle to obtain an approximation $\widehat{S}$ for $N^{\mathrm{sur}}\big(G_t \to H\big)$ with accuracy $\epsilon/21$. We can then return the floor of $\widehat{S}/s_{t,q}$. The only remaining issue is how to compute $s_{t,q}$. However, it is easy to do this in time $\mathrm{poly}(t) = \mathrm{poly}(n)$ since $s_{t,q} = \left\{ {t \atop q} \right\} q! = \sum_{j=0}^{q} (-1)^{q-j} \binom{q}{j} j^t$, where $\left\{ {t \atop q} \right\}$ is a Stirling number of the second kind.

Lemma 5.5. *Let H be a connected graph. Then #Hom(H) $\le_{\mathrm{AP}}$ #Comp(H).*

Proof. If not explicitly defined otherwise, we use the same notation and observations as in the proof of Lemma 5.4. In addition let p be the number of non-loop edges in H and $c_{t,p} = 2^t s_{t,p}$. If G is an input to #Hom(H) of size n, G_t is the graph constructed from G by adding a set of t isolated edges distinct from the edges in G. If H is a graph of size 1 the statement of the lemma clearly holds. If otherwise H is a connected graph of size at least 2, every homomorphism that uses all non-loop edges of H is also surjective and therefore a compaction. Thus, we obtain

$$c_{t,p} N\big(G \to H\big) \le N^{\mathrm{comp}}\big(G_t \to H\big) \le c_{t,p} N\big(G \to H\big) + (2^t p^t - c_{t,p}) q^n.$$

Dividing through by $c_{t,p}$ gives

$$N\big(G \to H\big) \le \frac{N^{\mathrm{comp}}\big(G_t \to H\big)}{c_{t,p}} \le N\big(G \to H\big) + \left(\frac{p^t - s_{t,p}}{s_{t,p}}\right) q^n.$$

If we choose $t = \lceil \log(5q^n 2^p)/\log(p/(p-1)) \rceil$ the remainder of this proof is analogous to that of Lemma 5.4. ∎

Lemma 5.6. *Let H be a graph. Then #Hom(H) $\le_{\mathrm{AP}}$ #Ret(H).*

Proof. Let $q = |V(H)|$ and G be an input to #Hom(H). Further, let H' be a copy of H and $(u_1, \ldots, u_q)$ be the vertices of H' ordered in such a way that they induce a copy of H. Then $N\big(G \to H\big) = N^{\mathrm{ret}}\big((G \oplus H'; u_1, \ldots, u_q) \to H\big)$. ∎

Appendix A. Decomposition of $N^{\mathbf{comp}}\big(G \to K_{2,3}\big)$. In this appendix, we work through a long example to illustrate some of the definitions and ideas from Section 3.2. We do this by verifying the statement of Theorem 3.8 for the special case where $H = K_{2,3}$.

Of course, the theorem is already proved in the earlier sections of this paper, but we work through this example in order to help the reader gain familiarity with the definitions. For $H = K_{2,3}$ and a non-empty, irreflexive and connected graph G we want to prove

$$N^{\mathrm{comp}}\big(G \to H\big) = \sum_{J \in \mathcal{S}_H} \lambda_H(J) N\big(G \to J\big). \tag{A.1}$$

First, we set $\mathcal{S}_H = \{H_1, \ldots, H_{10}\}$, cf. Figure 3, as defined in Definition 3.6.

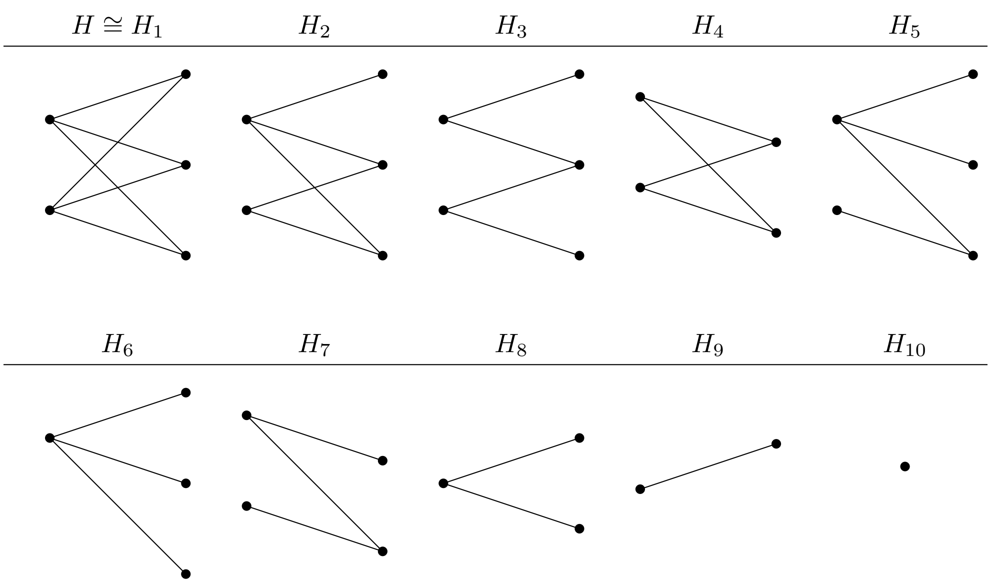


FIG. 3. $\mathcal{S}_H = \{H_1, \ldots, H_{10}\}$

Next, we recall the definitions of μ_H and λ_H from Definitions 3.6 and 3.7. For $J \in \mathcal{S}_H$, $\mu_H(J)$ is the number of non-empty connected subgraphs of H that are isomorphic to J. Also, $\lambda_H(J) = 1$ if $J \cong H$. If otherwise J is isomorphic to some graph in $\mathcal{S}_H$ but $J \ncong H$, we have

$$\lambda_H(J) = -\sum_{\substack{H' \in \mathcal{S}_H \\ \text{s.t. } H' \ncong H}} \mu_H(H') \lambda_{H'}(J). \tag{A.2}$$

In order to verify (A.1), we have to determine $\lambda_H(J)$ for all $J \in S_H$. As $\lambda_H(J)$ is defined inductively by (A.2), we first determine $\lambda_{H'}(J)$ for all $H' \in \mathcal{S}_H$ with $H' \ncong H$.

We start with the graph H_{10} and determine $\lambda_{H_{10}}$. Clearly, H_{10} has only one connected subgraph and we can choose $\mathcal{S}_{H_{10}} = \{H_{10}\}$. Recall that $\lambda_{H_{10}}(J) = 0$ for all graphs J that are not isomorphic to any graph in $\mathcal{S}_{H_{10}}$, i.e. not isomorphic to H_{10} in this case. By definition we have

$$\mu_{H_{10}}(H_{10}) = 1 \quad \text{as well as} \quad \lambda_{H_{10}}(H_{10}) = 1, \text{ see Table 2.}$$

This conforms with our intuition as for the single vertex graph H_{10}, it clearly holds that

$$N^{\mathrm{comp}}\big(G \to H_{10}\big) = N\big(G \to H_{10}\big). \tag{A.3}$$

Thus, we have now verified (A.1) for $H = H_{10}$.

Using this information, we consider the graph H_9 next and determine μ_{H_9} and λ_{H_9} for $\mathcal{S}_{H_9} = \{H_9, H_{10}\}$, see Table 3. H_9 contains two connected subgraphs that are isomorphic to H_{10}, therefore $\mu_{H_9}(H_{10}) = 2$. Then, from (A.2) we obtain

$$\lambda_{H_9}(H_{10}) = -\sum_{H' \in \{H_{10}\}} \mu_{H_9}(H')\lambda_{H'}(H_{10}) = -2.$$

Plugging this into (A.1) for $H = H_9$, we get

$$\begin{aligned} N^{\mathrm{comp}}\big(G \to H_9\big) &= \sum_{J \in \mathcal{S}_{H_9}} \lambda_{H_9}(J) N\big(G \to J\big) \\ &= N\big(G \to H_9\big) - 2N\big(G \to H_{10}\big). \end{aligned} \tag{A.4}$$

Now let us verify this expression. Recall that G is connected. The central idea behind our approach is that every homomorphism from G to H_9 is a compaction onto some connected subgraph H' of H_9. Furthermore, $\mu_{H_9}(H')$ tells us how many such subgraphs there are that are isomorphic to H'. Thus,

$$\begin{aligned} N\big(G \to H_9\big) &= \mu_{H_9}(H_9) \cdot N^{\mathrm{comp}}\big(G \to H_9\big) + \mu_{H_9}(H_{10}) \cdot N^{\mathrm{comp}}\big(G \to H_{10}\big) \\ &= N^{\mathrm{comp}}\big(G \to H_9\big) + 2N^{\mathrm{comp}}\big(G \to H_{10}\big). \end{aligned}$$

Rearranging and using the fact that $N^{\mathrm{comp}}\big(G \to H_{10}\big) = N\big(G \to H_{10}\big)$ from (A.3):

$$\begin{aligned} N^{\mathrm{comp}}\big(G \to H_9\big) &= N\big(G \to H_9\big) - 2N^{\mathrm{comp}}\big(G \to H_{10}\big) \\ &= N\big(G \to H_9\big) - 2N\big(G \to H_{10}\big). \end{aligned}$$

Thus, we have now proved (A.4) which in turn proves (A.1) for $H = H_9$.

Using (A.3) and (A.4) we can now go on to find (see Table 4) that

$$N^{\mathrm{comp}}\big(G \to H_8\big) = N\big(G \to H_8\big) - 2N\big(G \to H_9\big) + N\big(G \to H_{10}\big)$$

and so on.

This gives the intuition behind the formal definitions of μ_H and λ_H. For completeness, we give the values for all graphs H_1 through H_{10} in Tables 2 through 11. From Table 11 we can conclude that for $H = K_{2,3}$ the statement of Theorem 3.8 gives

$$\begin{aligned} N^{\mathrm{comp}}\big(G \to K_{2,3}\big) = N\big(G \to K_{2,3}\big) &- 6N\big(G \to H_2\big) + 6N\big(G \to H_3\big) \\ &+ 3N\big(G \to H_4\big) + 6N\big(G \to H_5\big) - 2N\big(G \to H_6\big) \\ &- 12N\big(G \to H_7\big) + 3N\big(G \to H_8\big). \end{aligned}$$

Table 2
Decomposition of H_{10}

H'	H_{10}
$\mu_{H_{10}}(H')$	1
$\lambda_{H_{10}}(H')$	1

Table 3
Decomposition of H_9

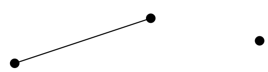
H'	H_9	H_{10}
		
$\mu_{H_9}(H')$	1	2
$\lambda_{H_9}(H')$	1	-2

Table 4
Decomposition of H_8

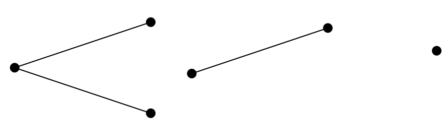
H'	H_8	H_9	H_{10}
			
$\mu_{H_8}(H')$	1	2	3
$\lambda_{H_8}(H')$	1	-2	1

Table 5
Decomposition of H_7

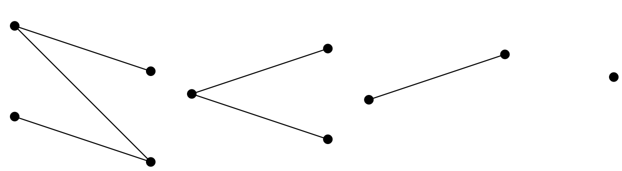
H'	H_7	H_8	H_9	H_{10}
				
$\mu_{H_7}(H')$	1	2	3	4
$\lambda_{H_7}(H')$	1	-2	1	0

TABLE 6
Decomposition of H_6

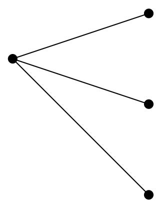
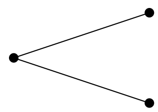
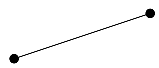
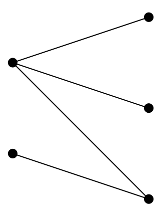
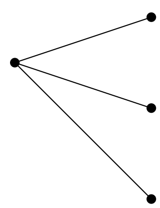
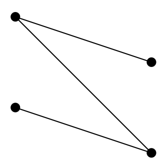
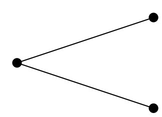
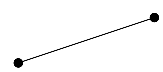
H'	H_6	H_8	H_9	H_{10}
				
$\mu_{H_6}(H')$	1	3	3	4
$\lambda_{H_6}(H')$	1	−3	3	−1

TABLE 7
Decomposition of H_5

H'	H_5	H_6	H_7	H_8	H_9
					
$\mu_{H_5}(H')$	1	1	2	4	4
$\lambda_{H_5}(H')$	1	−1	−2	3	−1

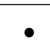
H'	H_{10}
	
$\mu_{H_5}(H')$	5
$\lambda_{H_5}(H')$	0

TABLE 8
Decomposition of H_4

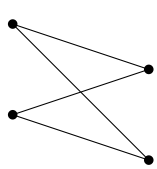
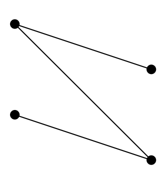
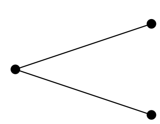
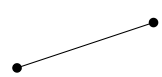
H'	H_4	H_7	H_8	H_9	H_{10}
					
$\mu_{H_4}(H')$	1	4	4	4	4
$\lambda_{H_4}(H')$	1	−4	4	0	0

TABLE 9
Decomposition of H_3

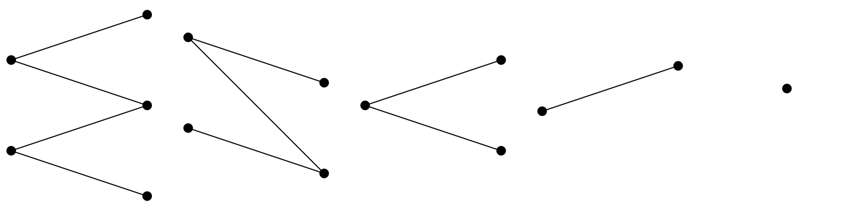
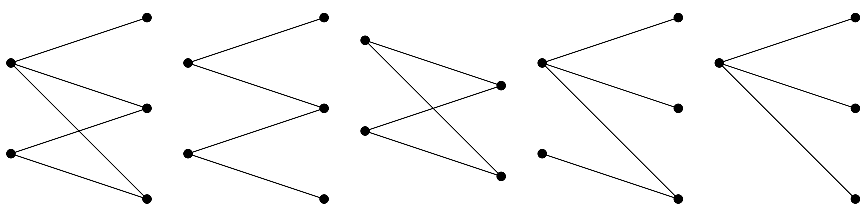
H'	H_3	H_7	H_8	H_9	H_{10}
					
$\mu_{H_3}(H')$	1	2	3	4	5
$\lambda_{H_3}(H')$	1	−2	1	0	0

TABLE 10
Decomposition of H_2

H'	H_2	H_3	H_4	H_5	H_6
					
$\mu_{H_2}(H')$	1	2	1	2	1
$\lambda_{H_2}(H')$	1	−2	−1	−2	1

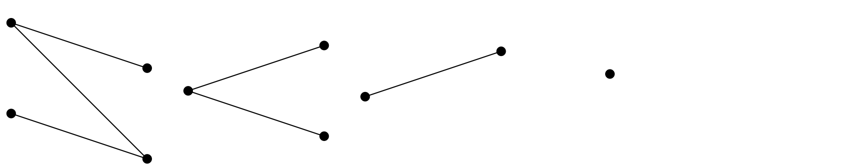
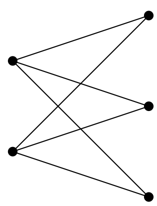
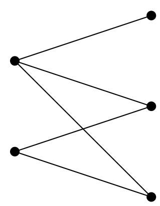
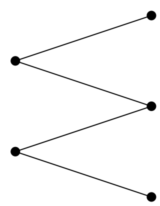
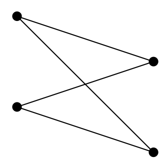
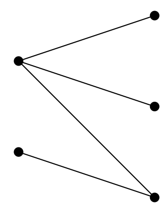
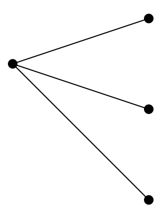
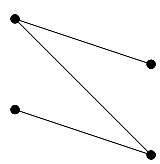
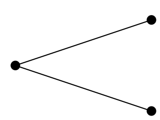
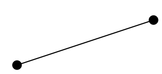
H'	H_7	H_8	H_9	H_{10}
				
$\mu_{H_2}(H')$	6	6	5	5
$\lambda_{H_2}(H')$	6	−3	0	0

TABLE 11
Decomposition of $H_1 = K_{2,3}$

H'	H_1	H_2	H_3	H_4	H_5
					
$\mu_{H_1}(H')$	1	6	6	3	6
$\lambda_{H_1}(H')$	1	−6	6	3	6

H'	H_6	H_7	H_8	H_9	H_{10}
					
$\mu_{H_1}(H')$	2	12	9	6	5
$\lambda_{H_1}(H')$	−2	−12	3	0	0

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