The Complexity of Boolean Constraint Isomorphism

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Abstract. We consider the Boolean constraint isomorphism problem, that is, the problem of determining whether two sets of Boolean constraint applications can be made equivalent by renaming the variables. We show that depending on the set of allowed constraints, the problem is either coNP-hard and GI-hard, equivalent to graph isomorphism, or polynomial-time solvable. This establishes a complete classification of the complexity of the problem, and moreover, it identifies exactly all those cases in which Boolean constraint isomorphism is polynomial-time many-one equivalent to graph isomorphism, the best-known and best-examined isomorphism problem in theoretical computer science.

1 Introduction

Constraint satisfaction problems (or, constraint networks) were introduced in 1974 by U. Montanari to solve computational problems related to picture processing [Mon74]. It turned out that they form a broad class of algorithmic problems that arise naturally in different areas [Kol03]. Today, they are ubiquitous in computer science (database query processing, circuit design, network optimization, planning and scheduling, programming languages), artificial intelligence (belief maintenance and knowledge based systems, machine vision, natural language understanding), and computational linguistics (formal syntax and semantics of natural languages).

A constraint satisfaction instance is given by a set of variables, a set of values that the variables may take (the so-called universe), and a set of constraints. A constraint restricts the possible assignments of values to variables; formally a \(k\)-place constraint is a \(k\)-ary relation over the universe. The most basic question one is interested in is to determine if there is an assignment of values to the variables such that all constraints are satisfied.

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This problem has been studied intensively in the past decade from a computational complexity point of view. In a particular case, that of 2-element universes, a remarkable complete classification was obtained, in fact already much earlier, by Thomas Schaefer [Sch78]. Note that in this case of a Boolean universe, the variables are propositional variables and the constraints are Boolean relations. A constraint satisfaction instance, thus, is a propositional formula in conjunctive normal form where, instead of the usual clauses, arbitrary Boolean relations may be used. In other words, the constraint satisfaction problem here is the satisfiability problem for generalized propositional formulas. Obviously the complexity of this problem depends on the set $C$ of constraints allowed, and is therefore denoted by CSP($C$) ($C$ will always be finite in this paper). In this way we obtain an infinite family of NP-problems, and Schaefer showed that each of them is either NP-complete or polynomial-time solvable. This result is surprising, since by Ladner’s Theorem [Lad75] there is an infinite number of complexity degrees between P and NP (assuming P $\neq$ NP), and consequently it is well conceivable that the members of an infinite family of problems may be located anywhere in this hierarchy. Schaefer showed that for the generalized satisfiability problem this is not the case: Each CSP($C$) is either NP-complete, that is in the highest degree, or in the lowest degree P. Therefore his result is called a dichotomy theorem.

For larger universes, much less is known. Satisfiability of constraint networks is always in NP, and for large families of allowed sets of constraints, NP-completeness was proven while for others, tractability (i.e., polynomial-time algorithms) was obtained. Research in this direction was strongly influenced by the seminal papers [JCG97, FV98], and many deep and beautiful results have been proven since then, see, e.g., [JCC98, KV98, JCG99, BJK00, BJK01, BBJK03]. Only recently, a dichotomy theorem for the complexity of satisfiability of constraint networks over 3-element universes was published [Bul02], but for larger domains such a complete classification still seems to be out of reach. For Boolean universes, however, a number of further computational problems have been addressed and in most cases, dichotomy theorems were obtained. These problems concern, among others, the problems to count how many satisfying solutions an instance has [CH96], to enumerate all satisfying solutions [CH97], to determine in certain ways optimal satisfying assignments [Cre95, KKK01a, RV03], to determine if there is a unique satisfying assignment [Jub99], learnability questions related to propositional formulas [Dal01], the inverse satisfiability problem [KS98], and the complexity of propositional circumscription [KK01b, DH03]. Results about approximability of optimization problems related to Boolean CSPs appeared in [Zwi98, KSTW01]. We point the reader to the monograph [CKS01] that discusses much of what is known about Boolean constraints.

In this paper, we address a problem that is not a variation of satisfiability, namely, the isomorphism problem for Boolean constraints. Perhaps the most prominent isomorphism problem in computational complexity theory is the graph isomorphism problem, GI, asking given two graphs if they are isomorphic. Graph isomorphism has been well studied because it is one of the very few problems
in NP neither known to be NP-complete nor known to be in P (in fact, there is strong evidence that GI is not NP-complete, see [KST93]); thus GI may be in one of the “intermediate degrees” mentioned above.

Another isomorphism problem studied intensively in the past few years is the propositional formula isomorphism. This problem asks, given two propositional formulas, if there is a renaming of the variables that makes both equivalent. The history of this problem goes back to the 19th century, where Jevons and Clifford, two mathematicians, were concerned with the task to construct formulas or circuits for all \( n \)-ary Boolean functions, but since there are too many \( (2^2)^n \) of them they wanted to identify a small set of Boolean circuits from which all others could then be obtained by some simple transformation. This problem has been referred to since as the “Jevons-Clifford-Problem.” One of the transformations they used was renaming of variables (producing an isomorphic circuit), another one was first renaming the variables and then negating some of them (producing what has been called a congruent circuit). Hence it is important to know how many equivalence classes for isomorphism and congruence there are, and how to determine if two circuits or formulas are isomorphic or congruent. (A more detailed discussion of these developments can be found in [Thi00, pp. 6–8].) However, the exact complexity of the isomorphism problem for Boolean circuits and formulas (the congruence problem turns out to be of the same computational complexity; technically: both problems are polynomial-time many-one equivalent) is still unknown: It is trivially hard for the class coNP (of all complements of NP-problems) and in \( \Sigma^p_2 \) (the second level of the polynomial hierarchy), and Agrawal and Thierauf showed that it is most likely not \( \Sigma^p_2 \)-hard (that is, unless the polynomial hierarchy collapses, an event considered very unlikely by most complexity-theorists) [AT00].

In this paper we study the Boolean formula isomorphism problem restricted to formulas in the Schaefer sense, in other words: the isomorphism problem for Boolean constraints. In a precursor, the present authors showed that this problem is either coNP-hard (the hard case, the same as for general formula isomorphism) or reducible to the graph isomorphism problem (the easy case) [BHRV02]. This result is not satisfactory, since it leaves the most interesting questions open: Are there “really easy” cases for which the isomorphism problem is tractable (that is, in P)? What exactly are these? And are the remaining cases which reduce to graph isomorphism actually equivalent to GI?

The present paper answers these questions affirmatively. To state precisely our main result (Theorem 7) already here (formal definitions of the relevant classes of constraints will be given in the next section), constraint isomorphism is coNP-hard and GI-hard for classes \( C \) of constraints that are neither Horn nor anti-Horn nor affine nor bijunctive, it is in in P if \( C \) is both affine and bijunctive, and in all other cases, the isomorphism problem is equivalent to graph isomorphism. This classification holds for constraint applications with as well as without constants. As in the case of Schaefer’s dichotomy, we thus obtain simple criteria to determine, given \( C \), which of the three cases holds. This theorem gives a complete classification of the computational complexity of Boolean constraint
isomorphism. Moreover, it determines exactly all those cases of the Boolean constraint isomorphism problem that are equivalent to graph isomorphism, the most prominent and probably most studied isomorphism problem so far.

The next section formally introduces constraint satisfaction problems and the relevant properties of constraints. Section 4 then contains the proof of our main theorem: In Section 3.1 we identify those classes of constraints for which isomorphism is in P and Section 3.2 contains the main technical contribution of this paper proving GI-hardness for all other cases.

2 Preliminaries

We start by formally introducing constraint problems. The following section is essentially from [BHRV02], following the standard notation developed in [CKS01].

Definition 1. 1. A constraint $C$ (of arity $k$) is a Boolean function from $\{0, 1\}^k$ to $\{0, 1\}$. 2. If $C$ is a constraint of arity $k$, and $x_1, x_2, \ldots, x_k$ are (not necessarily distinct) variables, then $C(x_1, x_2, \ldots, x_k)$ is a constraint application of $C$. In this paper, we view a constraint application as a Boolean function on a specific set of variables. Thus, for example, $x_1 \lor x_2 = x_2 \lor x_1$. 3. If $C$ is a constraint of arity $k$, and for $1 \leq i \leq k$, $x_i$ is a variable or a constant (0 or 1), then $C(x_1, x_2, \ldots, x_k)$ is a constraint application of $C$ with constants. 4. If $A$ is a constraint application [with constants], and $X$ a set of variables that includes all variables that occur in $A$, we say that $A$ is a constraint application [with constants] over variables $X$. Note that we do not require that every element of $X$ occurs in $A$.

The complexity of Boolean constraint problems depends on those properties of constraints that we define next.

Definition 2. Let $C$ be a constraint.

- $C$ is 0-valid if $C(0) = 1$. Similarly, $C$ is 1-valid if $C(1) = 1$.
- $C$ is Horn (or weakly negative) [anti-Horn (or weakly positive)] if $C$ is equivalent to a CNF formula where each clause has at most one positive [negative] literal.
- $C$ is bijunctive if $C$ is equivalent to a 2CNF formula.
- $C$ is affine if $C$ is equivalent to an XOR-CNF formula.
- $C$ is 2-affine (or, affine with width 2) if $C$ is equivalent to a XOR-CNF formula such that every clause contains at most two literals.

Let $\mathcal{C}$ be a finite set of constraints. We say $\mathcal{C}$ is 0-valid, 1-valid, Horn, anti-Horn, bijunctive, or affine if every constraint $C \in \mathcal{C}$ is 0-valid, 1-valid, Horn, anti-Horn, bijunctive, or affine, respectively. Finally, we say that $\mathcal{C}$ is Schaefer if $\mathcal{C}$ is Horn or anti-Horn or affine or bijunctive.
The question studied in this paper is that of whether a set of constraint applications can be made equivalent to a second set of constraint applications using a suitable renaming of its variables. We need some definitions.

**Definition 3.**
1. Let $S$ be a set of constraint applications with constants over variables $X$ and let $\pi$ be a permutation of $X$. By $\pi(S)$ we denote the set of constraint applications that results when we replace simultaneously all variables $x$ in $S$ by $\pi(x)$.
2. Let $S$ be a set of constraint applications over variables $X$. The number of satisfying assignments of $S$, $\#_1(S)$, is defined as $||\{ I \mid I$ is an assignment to all variables in $X$ that satisfies every constraint application in $S\}||$.

The isomorphism problem for Boolean constraints, first defined and examined in [BHRV02] is formally defined as follows.

**Definition 4.**
1. $ISO(C)$ is the problem of, given two sets $S$ and $U$ of constraint applications of $C$ over variables $X$, to decide whether $S$ and $U$ are isomorphic, i.e., whether there exists a permutation $\pi$ of $X$ such that $\pi(S)$ is equivalent to $U$.
2. $ISO_c(C)$ is the problem of, given two sets $S$ and $U$ of constraint applications of $C$ with constants over variables $X$, to decide whether $S$ and $U$ are isomorphic.

Böhm et al. obtained results about the complexity of the just-defined problem that, interestingly, pointed out relations to another isomorphism problem: the graph isomorphism problem (GI).

**Definition 5.** GI is the problem of, given two graphs $G$ and $H$, to determine whether $G$ and $H$ are isomorphic, i.e., whether there exists a bijection $\pi: V(G) \rightarrow V(H)$ such that for all $v, w \in V(G)$, $\{v, w\} \in E(G)$ if and only if $\{\pi(v), \pi(w)\} \in E(H)$. Our graphs are undirected, and do not contain self-loops. We also assume a standard enumeration of the edges, and will write $E(G) = \{e_1, \ldots, e_m\}$.

GI is a problem that is in NP, not known to be in P, and not NP-complete unless the polynomial hierarchy collapses. For details, see, for example, [KST93]. Recently, Torán showed that GI is hard for NL, PL, Mod_kL, and DET under logspace many-one reductions [Tor00]. Arvind and Kurur showed that GI is in the class SPP [AK02], and thus, for example in $\oplus P$.

The main result from [BHRV02] can now be stated as follows.

**Theorem 6.** Let $C$ be a set of constraints. If $C$ is Schaefer, then $ISO(C)$ and $ISO_c(C)$ are polynomial-time many-one reducible to GI, otherwise, $ISO(C)$ and $ISO_c(C)$ are coNP-hard.

Note that if $C$ is Schaefer the isomorphism problems $ISO(C)$ and $ISO_c(C)$ cannot be coNP-hard, unless NP = coNP. (This follows from Theorem 6 and the fact that GI is in NP.) Under the (reasonable) assumption that NP $\neq$ coNP,
and that GI is neither in P, nor NP-complete. Theorem 8 thus distinguishes a hard case (coNP-hard) and an easier case (many-one reducible to GI).

Böhler et al. also pointed out that there are some bijunctive, Horn, or affine constraint sets C for which actually ISO(C) and ISO_c(C) are equivalent to graph isomorphism. On the other hand, certainly there are C for which ISO(C) and ISO_c(C) are in P. In the upcoming section we will completely classify the complexity of ISO(C) and ISO_c(C), obtaining for which C exactly we are equivalent to GI and for which C we are in P.

3 A Classification of Boolean Constraint Isomorphism

The main result of the present paper is a complete complexity-theoretic classification of the isomorphism problem for Boolean constraints.

**Theorem 7.** Let C be a finite set of constraints.

1. If C is not Schaefer, then ISO(C) and ISO_c(C) are coNP-hard and GI-hard.
2. If C is Schaefer and not 2-affine, then ISO(C) and ISO_c(C) are polynomial-time many-one equivalent to GI.
3. Otherwise, C is 2-affine and ISO(C) and ISO_c(C) are in P.

The rest of this section is devoted to a proof of this theorem and organized as follows. The coNP lower-bound part from Theorem 7 follows from Theorem 6. In Section 3.1 we will prove the polynomial-time upper bound if C is 2-affine (Theorem 10). The GI upper bound if C is Schaefer again is part of Theorem 6. In Section 3.2 we will show that ISO_c(C) is GI-hard if C is not 2-affine (Theorems 15 and 17). Theorem 23 finally shows that ISO(C) is GI-hard if C is not 2-affine.

### 3.1 Upper Bounds

A central step in our way of obtaining upper bounds is to bring sets of constraint applications into a unique normal form. This approach is also followed in the proof of the coIP[2][2] upper bound\(^1\) for the isomorphism problem for Boolean formulas [AV00] and the GI upper bound from Theorem 6 [BHRV02].

**Definition 8.** Let C be a set of constraints. nf is a normal form function for C if and only if for all sets S and U of constraint applications of C with constants over variables X, and for all permutations \(\pi\) of \(X\),

1. \(nf(S, X)\) is a set of Boolean functions over variables \(X\),
2. \(S \equiv nf(S, X)\) (here we view \(S\) as a set of Boolean functions, and define equivalence for such sets as logical equivalence of corresponding propositional formulas),
3. \(nf(\pi(S), X) = \pi(nf(S, X))\), and

\(^1\) Here IP[2] means an interactive proof system where there are two messages exchanged between the verifier and the prover.
4. if \( S \equiv U \), then \( nf(S, X) = nf(U, X) \) (here, “=” is equality between sets of Boolean functions).

It is important to note that \( nf(S, X) \) is not necessarily a set of constraint applications of \( C \) with constants.

An easy property of the definition is that \( S \equiv U \) iff \( nf(S, X) = nf(U, X) \).

Also, it is not too hard to observe that using normal forms removes the need to check whether two sets of constraint applications with constants are equivalent, more precisely: \( S \) is isomorphic to \( U \) iff there exists a permutation \( \pi \) of \( X \) such that \( \pi(nf(S)) = nf(U) \).

There are different possibilities for normal forms. The one used by BHRV02 is the maximal equivalent set of constraint applications with constants, defined by \( nf(S, X) \) to be the set of all constraint applications \( A \) of \( C \) with constants over variables \( X \) such that \( S \rightarrow A \). For the upper bound for 2-affine constraints, we use the normal form described in the following lemma, whose proof can be found in Appendix A. Note that this normal form is not necessarily a set of 2-affine constraint applications with constants.

**Lemma 9.** Let \( C \) be a set of 2-affine constraints. There exists a polynomial-time computable normal form function \( nf \) for \( C \) such that for all sets \( S \) of constraint applications of \( C \) with constants over variables \( X \), the following hold:

1. If \( S \equiv 0 \), then \( nf(S, X) = \{0\} \).
2. If \( S \not\equiv 0 \), then \( nf(S, X) = \{Z, O\} \cup \bigcup_{i=1}^{\ell} \{(X_i \land Y_i) \lor (\overline{X_i} \land Y_i)\} \), where \( Z, O, X_1, Y_1, \ldots, X_\ell, Y_\ell \) are pairwise disjoint subsets of \( X \) such that \( X_i \cup Y_i \neq \emptyset \) for all \( 1 \leq i \leq \ell \), and for \( W \) a set of variables, \( W \) in a formula denotes \( \bigwedge W \), and \( \overline{W} \) denotes \( \neg \bigvee W \).

Making use of the normal form, it is not too hard to prove our claimed upper bound.

**Theorem 10.** Let \( C \) be a set of constraints. If \( C \) is 2-affine, then \( \text{ISO}(C) \) and \( \text{ISO}_{\cup}(C) \) are in \( P \).

**Proof.** Let \( S \) and \( U \) be two sets of constraint applications of \( C \) and let \( X \) be the set of variables that occur in \( S \cup U \). Use Lemma 9 to bring \( S \) and \( U \) into normal form. Using the first point in that lemma, it is easy to check whether \( S \) or \( U \) are equivalent to 0. For the remainder of the proof, we now suppose that neither \( S \) nor \( U \) is equivalent to 0. Let \( Z, O, X_1, Y_1, \ldots, X_\ell, Y_\ell \) and \( Z', O', X'_1, Y'_1, \ldots, X'_k, Y'_k \) be subsets of \( X \) such that:

1. \( Z, O, X_1, Y_1, \ldots, X_\ell, Y_\ell \) are pairwise disjoint and \( Z', O', X'_1, Y'_1, \ldots, X'_k, Y'_k \) are pairwise disjoint,
2. \( X_i \cup Y_i \neq \emptyset \) for all \( 1 \leq i \leq \ell \) and \( X'_i \cup Y'_i \neq \emptyset \) for all \( 1 \leq i \leq k \),
3. \( nf(S, X) = \{Z, O\} \cup \bigcup_{i=1}^{\ell} \{(X_i \land Y_i) \lor (\overline{X_i} \land Y_i)\} \), and \( nf(U, X) = \{Z', O'\} \cup \bigcup_{i=1}^{k} \{(X'_i \land Y'_i) \lor (\overline{X'_i} \land Y'_i)\} \).
We need to determine whether $S$ is isomorphic to $U$. Since $nf$ is a normal form function for $C$, it suffices to check if there exists a permutation $\pi$ on $X$ such that $\pi(nf(S, X)) = nf(U, X)$. Note that

$$
\pi(nf(S, X)) = \{\pi(Z), \pi(O)\} \cup \bigcup_{i=1}^{\ell} \{(\pi(X_i) \land \pi(Y_i)) \lor (\overline{\pi(X_i)} \land \pi(Y_i))\}.
$$

It is immediate that $\pi(nf(S, X)) = nf(U, X)$ if and only if

- $\ell = k$, $\pi(Z) = Z'$, $\pi(O) = O'$, and
- $\{\{\pi(X_1), \pi(Y_1)\}, \ldots, \{\pi(X_k), \pi(Y_k)\}\} = \{\{X'_1, Y'_1\}, \ldots, \{X'_k, Y'_k\}\}$.

Since $Z, O, X_1, Y_1, \ldots, X_k, Y_k$ are pairwise disjoint subsets of $X$, and since $Z', O', X'_1, Y'_1, \ldots, X'_k, Y'_k$ are pairwise disjoint subsets of $X$, it is easy to see that there exists a permutation $\pi$ on $X$ such that $nf(\pi(S), X) = nf(U, X)$ if and only if

- $\ell = k$, $||Z|| = ||Z'||$, $||O|| = ||O'||$, and
- $\{||X_1||, ||Y_1||, \ldots, ||X_k||, ||Y_k||\} = \{||X'_1||, ||Y'_1||, \ldots, ||X'_k||, ||Y'_k||\}$; here $\{\cdots\}$ denotes a multi-set.

It is easy to see that the above conditions can be verified in polynomial time. It follows that $\text{ISO}(C)$ and $\text{ISO}_c(C)$ are in $P$. \qed

### 3.2 GI-hardness

In this section, we will prove that if $C$ is not 2-affine, then GI is polynomial-time many-one reducible to $\text{ISO}_c(C)$ and $\text{ISO}(C)$. As in the upper bound proofs of the previous section, we will often look at certain normal forms. In this section, it is often convenient to avoid constraint applications that allow duplicates.

**Definition 11.** Let $C$ be a set of constraints.

1. $A$ is a constraint application of $C$ **without duplicates** if there exists a constraint $C \in C$ of arity $k$ such that $A = C(x_1, \ldots, x_k)$, where $x_i \neq x_j$ for all $i \neq j$.
2. Let $S$ be a set of constraint applications of $C$ [without duplicates] over variables $X$. We say that $S$ is a maximal set of constraint applications of $C$ [without duplicates] over variables $X$ if for all constraint applications $A$ of $C$ [without duplicates] over variables $X$, if $S \rightarrow A$, then $A \in S$.

If $X$ is the set of variables occurring in $S$, we will say that $S$ is a maximal set of constraint applications of $C$ [without duplicates].

The following lemma is easy to see.

**Lemma 12.** Let $C$ be a set of constraints. Let $S$ and $U$ be maximal sets of constraint applications of $C$ over variables $X$ [without duplicates]. Then $S$ is isomorphic to $U$ iff there exists a permutation $\pi$ of $X$ such that $\pi(S) = U$. 


Note that if $C$ is not 2-affine, then $C$ is not affine, or $C$ is affine and not bijunctive. We will first look at some very simple non-affine constraints.

**Definition 13 ([CKS01, p. 20]).**
1. OR$_0$ is the constraint $\lambda xy.x \lor y$.
2. OR$_1$ is the constraint $\lambda xy.x \lor y$.
3. OR$_2$ is the constraint $\lambda xy.x \lor \neg y$.
4. OneInThree is the constraint $\lambda xyz.(x \land \neg y \land z) \lor (\neg x \land y \land z) \lor (\neg x \land \neg y \land z)$.

As a first step in the general GI-hardness proof, we show that GI reduces to some particular constraints. The reduction of GI to ISO($\{\text{OR}_0\}$) already appeared in [BRS98]. Reductions in the other cases follow similar patterns. The proofs can be found in Appendix C.

**Lemma 14.** 1. GI is polynomial-time many-one reducible to ISO($\{\text{OR}_i\}$), $i \in \{0, 1, 2\}$.
2. Let $h$ be the 4-ary constraint $h(x,y,x',y') = (x \lor y) \land (x \oplus x') \land (y \oplus y')$. GI is polynomial-time many-one reducible to ISO($\{h\}$).
3. Let $h$ be a 6-ary constraint $h(x,y,z,x',y',z') = \text{OneInThree}(x,y,z) \land (x \oplus x') \land (y \oplus y') \land (z \oplus z')$. Then GI is polynomial-time many-one reducible to ISO($\{h\}$).

The constraints OR$_0$, OR$_1$, and OR$_2$ are the simplest non-affine constraints. However, it is not enough to show that GI reduces to the isomorphism problem for these simple cases. In order to prove that GI reduces to the isomorphism problem for all sets of constraints that are not affine, we need to show that all such sets can “encode” a finite number of simple cases.

Different encodings are used in the lower bound proofs for different constraint problems. All encodings used in the literature however, allow the introduction of auxiliary variables. In [CKS01], Lemma 5.30, it is shown that if $C$ is not affine, then $C$ plus constants can encode OR$_0$, OR$_1$, or OR$_2$. This implies that, for certain problems, lower bounds for OR$_0$, OR$_1$, or OR$_2$ transfer to $C$ plus constants. However, their encoding uses auxiliary variables, which means that lower bounds for the isomorphism problem don’t automatically transfer. For sets of constraints that are not affine, we will be able to use part of the proof of [CKS01], Lemma 5.30, but we will have to handle auxiliary variables explicitly, which makes the constructions much more complicated.

**Theorem 15.** If $C$ is not affine, then GI is polynomial-time many-one reducible to ISO$_c(C)$.

**Proof.** First suppose that $C$ is weakly negative and weakly positive. Then $C$ is bijunctive [CH90]. From the proof of [CKS01] Lemma 5.30 it follows that there exists a constraint application $A(x,y,z)$ of $C$ with constants such that $A(0,0,0) = A(0,1,1) = A(1,0,1) = 1$ and $A(1,1,0) = 0$. Since $C$ is weakly positive, we also have that $A(1,1,1) = 1$. Since $C$ is bijunctive, we have that $A(0,0,1) = 1$. The following truth-table summarizes all possibilities (this is a simplified version of [CKS01], Claim 5.31).
Thus we obtain $A(x, y, z) = (x \lor y)$, and the result follows from Lemma 14.

So, suppose that $C$ is not weakly negative or not weakly positive. We follow the proof of [CKS01], Lemma 5.30. From the proof of [CKS01], Lemma 5.26, it follows that there exists a constraint application $A$ of $C$ with constants such that $A(x, y) = OR_0(x, y)$, $A(x, y) = OR_2(x, y)$, or $A(x, y) = x \lor y$. In the first two cases, the result follows from Lemma 14.

Consider the last case. From the proof of [CKS01], Lemma 5.30, there exist a set $S(x, y, z, x', y', z')$ of $C$ constraint applications with constants and a ternary function $h$ such that $S(x, y, z, x', y', z') = h(x, y, z) \land (x \lor x') \land (y \lor y') \land (z \lor z')$, $h(000) = h(011) = h(101) = 1$, and $h(110) = 0$.

The following truth-table summarizes all possibilities:

| $xyz$ | $000$ | $001$ | $010$ | $011$ | $100$ | $101$ | $110$ | $111$ |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| $h(x, y, z)$ | $1$ | $a$ | $b$ | $1$ | $c$ | $1$ | $0$ | $d$ |

We will first show that in most cases, there exists a set $U$ of constraint applications of $C$ with constants such that $U(x, y, x', y') = (x \lor y) \land (x \lor x') \land (y \lor y')$. In all these cases, the result follows from Lemma 14 above.

- $b = 0, d = 1$. In this case, $S(x, y, x, x', y', x') = (x \lor y') \land (x \lor x') \land (y \lor y') = (x \lor y') \land (x \lor x') \land (y \lor y')$.
- $b = 1, d = 0$. In this case, $S(x, y, x, x', y', x') = (x' \lor y') \land (x \lor x') \land (y \lor y')$.
- $c = 0, d = 1$. In this case, $S(x, y, y, x', y', y') = (x' \lor y) \land (x \lor x') \land (y \lor y')$.
- $c = 1, d = 0$. In this case, $S(x, y, y, x, y', y') = (x' \lor y') \land (x \lor x') \land (y \lor y')$.
- $b = c = 1$. In this case, $S(x, y, 0, x', y', 1) = (x' \lor y') \land (x \lor x') \land (y \lor y')$.
- $b = c = d = 0; a = 1$. In this case, $S(0, y, z, 1, y', z') = (y' \lor z) \land (y \lor y') \land (z \lor z')$.

The previous cases are analogous to the cases from the proof of [CKS01], Claim 5.31. However, we have to explicitly add the $\lor$ conjuncts to simulate the negated variables used there, which makes Lemma 14 necessary.

The last remaining case is the case where $a = b = c = d = 0$. In the proof of [CKS01], Claim 5.31, it suffices to note that $(y' \lor z) = \exists x h(x, y, z)$. But, since we are looking at isomorphism, we cannot ignore auxiliary variables. Our result uses a different argument and follows from Lemma 14 above and the observation that $S(x, y, z, x', y', z') = OneInThree(x, y, z') \land (x \lor x') \land (y \lor y') \land (z \lor z')$.

In the case where $C$ is affine but not 2-affine, we first show GI-hardness of a particular constraint and then turn to the general result. (The proofs, using similar constructions as in the proofs of Lemma 14 and Theorem 15, is given in Appendix [L] and [L].)

**Lemma 16.** Let $h$ be the 6-ary constraint such that $h(x, y, z, x', y', z') = (x \lor y \lor z) \land (x \lor x') \land (y \lor y') \land (z \lor z')$. GI is polynomial-time many-one reducible to $ISO\{\{h\}\}$.
Theorem 17. If $C$ is affine and not bijunctive, then GI is polynomial-time many-one reducible to $\text{ISO}_c(C)$.

Finally, to finish the proof of statement 2 of Theorem 7, it remains to show GI-hardness of $\text{ISO}(C)$ for $C$ not 2-affine. In Appendix H we show that it is possible to remove the introduction of constants in the previous constructions of this section.

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A Proof of Lemma 9

Let $S$ be a set of constraint applications of $C$ with constants over variables $X$. Since $C$ is 2-affine, we can in polynomial time check whether $S \equiv 0$. If so, $nf(S, X) = \{0\}$. Now suppose that $S$ is not equivalent to 0. Let $D$ be the set of all unary and binary 2-affine constraints, i.e., $D = \{\lambda a.a, \lambda a.\overline{a}, \lambda a.b, \lambda b.\overline{(a \oplus b)}\}$.

Let $S''$ be the set of all constraint applications $A$ of $D$ with constants over variables $X$ such that $S \rightarrow A$. In other words, we are using the maximal equivalent set normal form used in $\text{[BHRV02]}$, that we described in the paragraph preceding Lemma 9. It follows from $\text{[BHRV02]}$ that $S''$ is computable in polynomial time. Certainly, $S = S''$, since every constraint application in $S$ can be written as the conjunction of constraint applications of $D$. We will now show how to compute $nf(S, X)$.

Let $Z$ be the set of those variables in $X$ that, when set to 1, make $S''$ equivalent to 0. Let $O$ be the set of those variables in $X$ that, when set to 0, make $S''$ equivalent to 0. Note that $S'' \rightarrow \overline{Z} \land O$. Let $S'$ be the set of constraint applications that is obtained from $S''$ by setting all elements of $Z$ to 0 and all elements of $O$ to 1. Note that $S'' \equiv \overline{Z} \land O \land S'$.

Let $\widehat{S}$ be the set of all constraint applications from $S'$ that do not contain constants. We claim that $\widehat{S} \equiv S'$. For suppose that $\alpha$ is an assignment that satisfies $\widehat{S}$, but $\alpha$ does not satisfy $S'$. Then there is a constraint application with constants $A \in S' \setminus \widehat{S}$ such that $\alpha$ does not satisfy $A$. Note that $A$ must contain a constant, since $A \notin \widehat{S}$. $A$ must contain a variable, since $A$ is satisfiable (since $S$ is satisfiable). But then $A$ contains exactly one occurrence of exactly one variable, and thus $A$ is equivalent to $x$ or $\overline{y}$ for some variable $x$. But then $x$ would have been put in $Z$ or $O$, and $x$ would not occur in $S'$.

So, $S \equiv \overline{Z} \land O \land \widehat{S}$, and every element of $\widehat{S}$ is of the form $x \oplus y$ where $x, y \in X$ and $x \neq y$ or of the form $\neg(x \oplus y)$, where $x, y \in X$ and $x \neq y$ or of the form $\neg(x \oplus x)$, where $x \in X$. Note that it is possible that $\widehat{S} = \emptyset$ and that all variables in $X$ occur in $S$.

Also note that, since $S''$ contains all of its implicates that are of the right form, for every three distinct variables $x, y,$ and $z$,

- if $(x \oplus y) \in \widehat{S}$ and $(y \oplus z) \in \widehat{S}$, then $\neg(x \oplus z) \in \widehat{S}$,
- if $\neg(x \oplus y) \in \widehat{S}$ and $(y \oplus z) \in \widehat{S}$, then $(x \oplus z) \in \widehat{S}$, and
- if $(x \oplus y) \in \widehat{S}$ and $\neg(y \oplus z) \in \widehat{S}$, then $\neg(x \oplus z) \in \widehat{S}$.

So, $\widehat{S}$ is closed under a form of transitivity.

Partition $\widehat{S}$ into $S_1, \ldots, S_\ell$, where $S_1, \ldots, S_\ell$ are minimal sets that are pairwise disjoint with respect to occurring variables. Since the $S_i$s are minimal, and not equivalent to 0, it follows from the observation above about the closure of $\widehat{S}$, that for every pair of distinct variables $x, y$ in $S_i$, exactly one of $(x \oplus y)$ and $\neg(x \oplus y)$ is in $S_i$. For every $i$, $1 \leq i \leq \ell$, let $x_i$ be an arbitrary variable that occurs in $S_i$. Let $X_i = \{y \mid \neg(x_i \oplus y) \in S_i\}$ and let $Y_i = \{y \mid x_i \oplus y \in S_i\}$. Then $X_i \cap Y_i = \emptyset$ and $X_i \cup Y_i = \text{the variables that occur in } S_i$. 

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It is easy to see that $S_i \equiv \{(X_i \land Y_i) \lor (X_i \land Y_i)\}$.
We claim that
\[ \text{nf}(S, X) = \{Z, O\} \cup \bigcup_{i=1}^{\ell} \{(X_i \land Y_i) \lor (X_i \land Y_i)\} \]
fulfills the criteria of Lemma 9.

First of all, it is clear that $\text{nf}$ is computable in polynomial time. From the observations above, it follows that $Z, O, X_1, \ldots, X_\ell, Y_1$ are pairwise disjoint subsets of $X$ such that
1. $X = Z \cup O \cup \bigcup_{i=1}^{\ell} (X_i \cup Y_i)$, and
2. $X_i \cup Y_i \neq \emptyset$ for all $1 \leq i \leq \ell$.

that $\text{nf}(S, X) \equiv S$, and that $\text{nf}(\pi(S), X) = \pi(\text{nf}(S), X)$, for all permutations $\pi$ of $X$.

It remains to show that if $U$ is a set of constraint applications of $C$ with constants, and $S \equiv U$, then $\text{nf}(S, X) = \text{nf}(U, X)$.

Let $Z', O', X'_1, Y'_1, \ldots, X'_\ell, Y'_\ell$ be subsets of $X$ such that:
1. $Z', O', X'_1, Y'_1, \ldots, X'_\ell, Y'_\ell$ are pairwise disjoint,
2. $X = Z' \cup O' \cup \bigcup_{i=1}^{\ell} (X'_i \cup Y'_i)$,
3. $X'_i \cup Y'_i \neq \emptyset$ for all $1 \leq i \leq \ell$,
4. $\text{nf}(U, X) = \{Z', O'\} \cup \bigcup_{i=1}^{\ell} \{(X'_i \land Y'_i) \lor (X'_i \land Y'_i)\}$.

Since $S \equiv \text{nf}(S, X)$, $U \equiv \text{nf}(U, X)$, and $S \equiv U$, it follows that $\text{nf}(S, X) \equiv \text{nf}(U, X)$. From this, it is immediate that $Z = Z'$ and that $O = O'$. In addition, for any two variables $x, y \in X$:
- $(\{x, y\} \in X_i$ or $\{x, y\} \in Y_i$ for some $i$) iff $(S$ is satisfiable iff $x \equiv y$) iff $(\{x, y\} \in X'_j$ or $\{x, y\} \in Y'_j$ for some $j$), and
- $(\{x, y\} \cap X_i \neq \emptyset$ and $\{x, y\} \cap Y_i \neq \emptyset$ for some $i$) iff $(S$ is satisfiable iff $x \not\equiv y$) iff $(\{x, y\} \cap X'_j \neq \emptyset$ and $\{x, y\} \cap Y'_j \neq \emptyset$ for some $j$).

This implies that $\text{nf}(U, X) = \text{nf}(S, X)$, which completes the proof.

**B Graph Isomorphism for Restricted Graphs**

When reducing from GI, it is often useful to assume that the graphs have certain properties. The following lemma (whose proof is given in Appendix B) shows that the complexity of GI for certain restricted classes of graphs does not decrease.

**Lemma 18.** GI is polynomial-time many-one reducible to the graph isomorphism problem for pairs of graphs $G$ and $H$ such that for some $n$, $G$ and $H$ have the same set of vertices $\{1, \ldots, n\}$, $G$ and $H$ have the same number of edges, every vertex in $G$ and $H$ has degree at least two (i.e., is incident with at least two edges), and $G$ and $H$ do not contain triangles.
Proof. Let $G$ and $H$ be graphs. If $G$ and $H$ do not contain the same number of vertices, or if $G$ and $H$ do not contain the same number of edges, or if $G$ and $H$ do not contain the same number of isolated vertices, then $G$ is not isomorphic to $H$.

So suppose that $G$ and $H$ have the same number of vertices, the same number of edges, and the same number of isolated vertices. Let $G_1$ be the graph that results if we remove all isolated vertices from $G$. Let $H_1$ be the graph that results if we remove all isolated vertices from $H$. Then $G_1$ and $H_1$ have the same number of vertices and the same number of edges, all vertices in $G_1$ and $H_1$ have degree at least one, and $G$ is isomorphic to $H$ iff $G_1$ is isomorphic to $H_1$. Without loss of generality, assume that $G_1$ has at least 3 vertices.

We will now ensure that no vertex has degree less than two. Let $v_0$ be a new vertex. Define $G_2$ as follows: $V(G_2) = V(G_1) \cup \{v_0\}$, $E(G_2) = E(G_1) \cup \{\{v_0, v\} \mid v \in V(G_1)\}$. Define $H_2$ in the same way, i.e., $V(H_2) = V(H_1) \cup \{v_0\}$, $E(H_2) = E(H_1) \cup \{\{v_0, v\} \mid v \in V(H_1)\}$. Note that $G_2$ and $H_2$ have the same number of vertices and the same number of edges, and that all vertices in $G_2$ and $H_2$ have degree at least two. In addition, it is easy to see that $G_1$ is isomorphic to $H_1$ iff $G_2$ is isomorphic to $H_2$: If $\pi$ is an isomorphism from $G_2$ to $H_2$, then we can define an isomorphism $\rho$ from $G_1$ to $H_1$ as follows: For all $v \in V(G_1)$, $\rho(v) = \pi(v)$ if $\pi(v) \neq v_0$, and $\rho(v) = \pi(v_0)$ if $\pi(v) = v_0$.

Next, we will remove triangles. Define $G_3$ as follows: $V(G_3) = V(G_2) \cup E(G_2)$, $E(G_3) = \{\{v, w\} \mid v \in V(G_2), w \in E(G_2), v \in w\}$. Define $H_3$ in the same way, i.e., $V(H_3) = V(H_2) \cup E(H_2)$, $E(H_3) = \{\{v, w\} \mid v \in V(H_2), w \in E(H_2), v \in w\}$. Note that $G_3$ and $H_3$ are triangle-free graphs with the same number of vertices and the same number of edges, and that all vertices in $G_3$ and $H_3$ have degree at least two. We claim that $G_2$ is isomorphic to $H_2$ iff $G_3$ is isomorphic to $H_3$. The left-to-right direction is immediate. The right-to-left direction follows since an isomorphism from $G_3$ to $H_3$ maps $V(G_2)$ to $V(H_2)$, since these are exactly the vertices at even distance from a vertex of degree greater than two. (Here we use the fact that the degree of $v_0$ is greater than 2.)

Let $n$ be the number of vertices of $G_3$ and $H_3$. Rename the vertices in $G_3$ and $H_3$ to $\{1, 2, \ldots, n\}$. This proves Lemma \ref{lem:3}.

\section{Proof of Lemma \ref{lem:4}}

1. As mentioned, the polynomial-time many-one reduction of GI to ISO($\{\text{OR}_0\}$) was already published in \cite{bresar2003}. We will first recall this proof, since the proofs of the other cases will be similar though more complicated. Let $G$ be a graph and let $V(G) = \{1, 2, \ldots, n\}$. We encode $G$ in the obvious way as a set of constraint applications $S(G) = \{x_i \lor x_j \mid \{i, j\} \in E(G)\}$. It is easy to see that $S(G)$ is a maximal set of constraint applications of OR$_0$. If $G$ and $H$ are two graphs without isolated vertices and with vertex set $\{1, 2, \ldots, n\}$, then $G$ is isomorphic to $H$ if and only if there exists a permutation $\pi$ of $\{x_1, \ldots, x_n\}$ such that $\pi(S(G)) = S(H)$. By Lemma \ref{lem:2} it follows that $G$ is isomorphic to $H$ if and only if $S(G)$ is isomorphic to $S(H)$.
If we negate all occurring variables in $S(\hat{G})$, i.e., $S(\hat{G}) = \{x_i \lor x_j \mid \{i, j\} \in E(\hat{G})\}$, we obtain a reduction from GI to ISO(\{OR\}).

It remains to show that GI is reducible to ISO(\{OR\}). Note that the obvious encoding \{\{x_i \lor \overline{x_j} \mid \{i, j\} \in E(\hat{G})\} does not work, since a 3-vertex graph with edges \{1, 2\} and \{1, 3\} will be indistinguishable from a 3-vertex graph with edges \{1, 2\}, \{1, 3\}, and \{2, 3\}.

We solve this problem by using a slightly more complicated encoding. Let $E(\hat{G}) = \{e_1, \ldots, e_m\}$. Define $S(\hat{G}) = \{x_i \lor \overline{y_k}, x_j \lor \overline{y_k} \mid e_k = \{i, j\}\}$. We claim that if $G$ and $H$ are two graphs without isolated vertices with vertex set \{1, 2, \ldots, n\}, then $G$ is isomorphic to $H$ if and only if $S(\hat{G})$ is isomorphic to $S(H)$.

The left-to-right direction is immediate. For the converse, note that for all $\hat{G}$, $S(\hat{G})$ is a maximal set of constraint applications of OR. Thus, by Lemma 12 if $S(\hat{G})$ is isomorphic to $S(H)$, there exists a permutation $\pi$ of the variables such that $\pi(S(\hat{G})) = S(H)$. Since the $x_i$ variables are exactly those variables that occur positively in $S(\hat{G})$ and $S(H)$, $\pi$ maps $x$-variables to $y$-variables, and thus induces an isomorphism from $G$ to $H$.

2. We use a similar encoding as in the first case above. Let $\hat{G}$ be a graph and let $V(\hat{G}) = \{1, 2, \ldots, n\}$. We encode $\hat{G}$ as the following set of constraint applications of $h$: $S(\hat{G}) = \{h(x_i, x_j, x'_i, x'_j) \mid \{i, j\} \in E(\hat{G})\}$.

Let $X = \{x_1, \ldots, x_n, x'_1, \ldots, x'_n\}$. Note that for all variables $x, y \in X$, $(S(\hat{G}) \rightarrow (x \lor y)$ and $S(\hat{G}) \not\rightarrow (x \lor y)$) iff there exists an edge $\{i, j\} \in E$ such that $\{x, y\} = \{x_i, x_j\}$.

Let $G$ and $H$ be two graphs without isolated vertices with vertex set \{1, 2, \ldots, n\}. We claim that $G$ is isomorphic to $H$ if and only if $S(\hat{G})$ is isomorphic to $S(H)$. The left-to-right direction is immediate, since an isomorphism $\pi$ from $G$ to $H$ induces an isomorphism $\rho$ from $S(G)$ to $S(H)$, by letting $\rho(x_i) = x_{\pi(i)}$ and $\rho(x'_i) = x'_{\pi(i)}$.

For the converse, suppose that $\rho$ is a permutation of $X$ such that $\rho(S(\hat{G})) = S(H)$. As noted above, for all $\{i, j\} \in E(\hat{G})$, it holds that $S(H) \rightarrow (\rho(x_i) \lor \rho(x_j))$ and $S(H) \not\rightarrow (\rho(x_i) \lor \rho(x_j))$. Again by the observation above, there exists an edge $\{k, \ell\} \in E(H)$ such that $\{\rho(x_k), \rho(x_\ell)\} = \{x_k, x_\ell\}$. Thus, $\rho$ maps $x$-variables to $x$-variables. Let $\pi(i) = j$ iff $\rho(x_i) = x_j$. It is easy to see that $\pi$ is an isomorphism from $G$ to $H$.

3. Let $\hat{G}$ be a graph such that $V(\hat{G}) = \{1, 2, \ldots, n\}$ and $E(\hat{G}) = \{e_1, \ldots, e_m\}$. Define $S(\hat{G})$ as follows: $S(\hat{G}) = \{h(x_i, x_j, y_k, x'_i, x'_j, y'_k) \mid e_k = \{i, j\}\} \cup \{x_i \oplus x'_i \mid 1 \leq i \leq n\} \cup \{y_i \oplus y'_i \mid 1 \leq i \leq m\}$.

Define $U(\hat{G})$ as follows: $U(\hat{G}) = \{\{x_i, x_j, y_k\} \mid e_k = \{i, j\}\} \cup \{x_i \oplus x'_i \mid 1 \leq i \leq n\} \cup \{y_i \oplus y'_i \mid 1 \leq i \leq m\}$. Clearly, $U(\hat{G})$ is equivalent to $S(\hat{G})$. Let $X$ be the set of all variables that occur in $U(\hat{G})$.

We will use the following claim whose proof will be given in Appendix E.

**Claim 19** The set of all constraint applications of OneInThree without duplicates that occur in $U(\hat{G})$ is a maximal set of constraint applications of OneInThree over variables $X$ without duplicates, where $X$ is the set of all variables that occur in $U(\hat{G})$. 

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Let $G$ and $H$ be graphs without isolated vertices, with vertex set $\{1, 2, \ldots, n\}$, and with the same number of edges. Also assume that every vertex in $G$ and $H$ is incident with at least two edges (see Lemma 13). Let $E(G) = \{e_1, \ldots, e_m\}$ and let $E(H) = \{e'_1, \ldots, e'_n\}$.

We claim that $G$ is isomorphic to $H$ iff $S(G)$ is isomorphic to $S(H)$. It suffices to show that $G$ is isomorphic to $H$ iff $U(G)$ is isomorphic to $U(H)$.

The left-to-right direction is trivial, since an isomorphism between the graphs induces an isomorphism between sets of constraint applications as follows. If $\pi : V \to V$ is an isomorphism from $G$ to $H$, then we can define an isomorphism $\rho$ from $U(G)$ to $U(H)$ as follows:

- $\rho(x_i) = x_{\pi(i)}$, $\rho(x'_i) = x'_{\pi(i)}$, for $i \in V$.
- For $e_k = \{i, j\}$, $\rho(y_k) = y_i$, and $\rho(y'_k) = y'_j$, where $e'_i = \{\pi(i), \pi(j)\}$.

For the converse, suppose that $\rho$ is an isomorphism from $U(G)$ to $U(H)$. Let $U'(G)$ and $U'(H)$ be the sets of all constraint applications of OneInThree without duplicates that occur in $U(G)$ and $U(H)$, respectively.

From Claim 19 and Lemma 12 it follows that $\rho(U'(G)) = U'(H)$. Note that the $x$-variables in $U'(G)$ and $U'(H)$ are exactly those variables that occur in at least two constraint applications of OneInThree without constants. Thus, $\rho$ maps $x$-variables to $x$-variables. Likewise, $\rho$ maps $y$-variables to $y$-variables. Let $\pi$ be the bijection on $\{1, 2, \ldots, n\}$ defined by $\pi(i) = j$ iff $\rho(x_i) = x_j$. We claim that $\pi$ is an isomorphism from $G$ to $H$. First let $e_k = \{i, j\}$. Thus, OneInThree($x_i, x_j, y_k$) is in $U'(G)$. Then, OneInThree($\rho(x_i), \rho(x_j), \rho(y_k)$) is in $U'(H)$. Thus, OneInThree($x_{\pi(i)}, x_{\pi(j)}, \rho(y_k)$) is in $U'(H)$. This implies that $\{i, j\}$ is an edge in $H$. For the converse, suppose that $e'_k = \{\pi(i), \pi(j)\}$ is an edge in $H$. Then OneInThree($x_{\pi(i)}, x_{\pi(j)}, y_k$) is in $U'(H)$. Thus we conclude OneInThree($\rho(x_i), \rho(x_j), y_k$) is in $U'(H)$ and hence OneInThree($x_i, x_j, \rho^{-1}(y_k)$) is in $U'(G)$. It follows that $\{i, j\}$ is an edge in $G$.

D Proof of Lemma 16

Following [CKS01] p. 20, we use XOR2 to denote the constraint $\lambda xy.x \oplus y$, and XOR3 to denote $\lambda xyz.x \oplus y \oplus z$.

Let $\hat{G}$ be a graph such that $V(\hat{G}) = \{1, 2, \ldots, n\}$, and $E(\hat{G}) = \{e_1, e_2, \ldots, e_m\}$. We will use a similar encoding as in the proof of Lemma 13. Again, propositional variable $x_i$ will correspond to vertex $i$ and propositional variable $y_i$ will correspond to edge $e_i$.

Define $S(\hat{G})$ as follows: $S(\hat{G}) = \{h(x_i, x_j, y_k, x'_i, x'_j, y'_k) \mid e_k = \{i, j\}\} \cup \{x_i \oplus x'_i \mid 1 \leq i \leq n\} \cup \{y_i \oplus y'_i \mid 1 \leq i \leq m\}$.

Define $U(\hat{G})$ as follows: $U(\hat{G}) = \{(x_i \oplus x_j \oplus y_k), (x'_i \oplus x'_j \oplus y'_k), (x_i \oplus x'_i) \mid e_k = \{i, j\}\} \cup \{x_i \oplus x'_i \mid 1 \leq i \leq n\} \cup \{y_i \oplus y'_i \mid 1 \leq i \leq m\}$. Clearly, $U(G)$ is equivalent to $S(G)$. Let $X$ be the set of variables occurring in $U(\hat{G})$. 

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The proof relies on the following claim, which shows that \( U(\hat{G}) \) is a maximal set of constraint applications of \{XOR_2, XOR_3\} without duplicates (a proof can be found in Appendix C):

**Claim 20** Let \( \hat{G} \) be a triangle-free graph such that \( V(\hat{G}) = \{1, 2, \ldots, n\}, E(\hat{G}) = \{e_1, e_2, \ldots, e_m\} \), and every vertex has degree at least two. Then \( U(\hat{G}) \) is a maximal set of constraint applications of \{XOR_2, XOR_3\} without duplicates.

Let \( G \) and \( H \) be graphs such that \( V(G) = V(H) = \{1, \ldots, n\}, E(G) = \{e_1, \ldots, e_m\}, E(H) = \{e'_1, \ldots, e'_m\} \), all vertices in \( G \) and \( H \) have degree at least two, and \( G \) and \( H \) do not contain triangles.

We will show that \( G \) is isomorphic to \( H \) if and only if \( S(G) \) is isomorphic to \( S(H) \). It suffices to show that \( G \) is isomorphic to \( H \) if and only if \( U(G) \) is isomorphic to \( U(H) \).

The left-to-right direction is trivial, since an isomorphism between the graphs induces an isomorphism between sets of constraint applications as follows. If \( \pi : V \to V \) is an isomorphism from \( G \) to \( H \), then we can define an isomorphism \( \rho \) from \( U(G) \) to \( U(H) \) as follows:

- \( \rho(x_i) = x_{\pi(i)}, \rho(x'_i) = x'_{\pi(i)}, \) for \( i \in V \).
- For \( e_k = \{i, j\} \), \( \rho(y_k) = y_{\ell}, \) and \( \rho(y'_k) = y'_{\ell}, \) where \( e'_{\ell} = \{\pi(i), \pi(j)\} \).

For the converse, suppose that \( \rho \) is an isomorphism from \( U(G) \) to \( U(H) \). By Lemma 12 and Claim 20, \( \rho(U(G)) = U(H) \). Note that every \( y_k \) and \( y'_k \) variable occurs in exactly two constraint applications of XOR_3 in \( U(G) \) and \( U(H) \), while every \( x_i \) and \( x'_i \) variable occurs in at least four constraint applications of XOR_3 in \( U(G) \) and \( U(H) \) (since every vertex in \( G \) and \( H \) has at least two variables). From the XOR_2 constraint applications, it is also immediate that for all \( a \in \{x_1, \ldots, x_n, y_1, \ldots, y_m\} \), there exists a \( \rho(a) \) such that \( \{\rho(a), \rho(a')\} = \{b, b'\} \).

Define \( \pi \) as follows: \( \pi(i) = j \) if and only if \( \{\rho(x_i), \rho(x'_i)\} = \{x_j, x'_j\} \). By the observations above, \( \pi \) is total and 1-1. It remains to show that \( \{i, j\} \in E(G) \) iff \( \{\pi(i), \pi(j)\} \in E(H) \).

Let \( e_k = \{i, j\} \). Then \( x_i \oplus x_j \oplus e_k \in E(G) \). Thus, \( \rho(x_i) \oplus \rho(x_j) \oplus \rho(y_k) \in U(H) \). That is, \( a \oplus b \oplus \rho(y_k) \in U(H) \) for some \( a \in \{x_{\pi(i)}, x'_{\pi(i)}\} \) and \( b \in \{x_{\pi(j)}, x'_{\pi(j)}\} \).

But that implies that \( \rho(y_k) \in \{y_{\ell}, y'_{\ell}\} \) where \( e'_{\ell} = \{\pi(i), \pi(j)\} \). This implies that \( \{\pi(i), \pi(j)\} \in E(H) \). For the converse, suppose that \( \{\pi(i), \pi(j)\} \in E(H) \). Then \( x_{\pi(i)} \oplus x_{\pi(j)} \oplus y_{\ell} \in U(H) \) for \( e'_{\ell} = \{\pi(i), \pi(j)\} \). It follows that \( a \oplus b \oplus \rho^{-1}(y_k) \in U(G) \) for some \( a \in \{x_i, x'_i\} \) and \( b \in \{x_j, x'_j\} \). By the form of \( U(G) \), it follows that \( \{i, j\} \in E(G) \).

### E Proof of Theorem 17

Schaef er characterized classes of Boolean constraints in terms of closure properties. Important for us will be his characterization of bijunctive constraints.
Lemma 21 ([Sch78]). Let $f$ be a Boolean function of arity $k$. $f$ is bijunctive if and only if for all assignments $s, t, u \in \{0, 1\}^k$ that satisfy $f$, $\text{majority}(s, t, u)$ (the vector obtained from $s, t, u$ by bitwise majority) satisfies $f$.

Proof. (of Theorem 17)
Recall from the proof of Theorem 15 that if $C$ is not bijunctive, then $C$ is not weakly positive or not weakly negative. As in the proof of that theorem, it follows from the proof of [CXS01], Lemma 5.26 that there exists a constraint application $A$ of $C$ with constants such that $A(x, y) = \text{OR}_0(x, y)$, $A(x, y) = \text{OR}_2(x, y)$, or $A(x, y) = x \oplus y$. Since $A$ is affine, and $\text{OR}_0$ and $\text{OR}_2$ are not affine, the first two cases cannot occur.

Consider the last case. Let $B \in C$ be a constraint that is not bijunctive. Let $k$ be the arity of $B$. Following Schauer’s characterization of bijunctive functions (see Lemma 21), there exist assignments $s, t, u \in \{0, 1\}^k$ such that $B(s) = B(t) = B(u) = 1$ and $B(\text{majority}(s, t, u)) = 0$. In addition, since $C$ is affine, using Schauer’s characterization of affine functions, $B(s \oplus t \oplus u) = 1$.

Let $\tilde{B}(x, y, z, x', y', z') = B(x_1, \ldots, x_k)$ be the constraint application of $B$ with constants that results if for all $1 \leq i \leq k$, $x_i =$

- 1 if $s_i = t_i = u_i = 1$,
- 0 if $s_i = t_i = u_i = 0$,
- $x$ if $s_i = t_i = 0$ and $u_i = 1$,
- $x'$ if $s_i = t_i = 1$ and $u_i = 0$,
- $y$ if $s_i = u_i = 0$ and $t_i = 1$,
- $y'$ if $s_i = u_i = 1$ and $t_i = 0$,
- $z$ if $s_i = 0$ and $t_i = u_i = 1$,
- $z'$ if $s_i = 1$ and $t_i = u_i = 0$.

Note that

- $\tilde{B}(0, 0, 0, 1, 1, 1) = B(s) = 1$,
- $\tilde{B}(0, 1, 1, 1, 0, 0) = B(t) = 1$,
- $\tilde{B}(1, 0, 1, 0, 1, 0) = B(u) = 1$,
- $\tilde{B}(1, 1, 0, 0, 0, 1) = B(s \oplus t \oplus u) = 1$,
- and $\tilde{B}(0, 0, 1, 1, 1, 0) = B(\text{majority}(s, t, u)) = 0$.

Let $S = \{ \tilde{B}(x, y, z, x', y', z'), A(x, x'), A(y, y'), A(z, z') \}$. Then $S$ is a set of constraint applications of $C$ with constants such that there exists a ternary function $h$ such that $S(x, y, z, x', y', z') = h(x, y, z) \land (x \oplus x') \land (y \oplus y') \land (z \oplus z')$ and $h(000) = h(011) = h(101) = h(110) = 1$ and $h(001) = 0$.

The following table summarizes the possibilities we have.

| $xyz$ | $000$ | $001$ | $010$ | $011$ | $100$ | $101$ | $110$ | $111$ |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| $h(x, y, z)$ | $1$ | $0$ | $a$ | $b$ | $1$ | $1$ | $c$ |

We will analyze all cases.

- $a = 1$. In this case, $S(0, y, z, 1, y', z') = (y \lor z') \land (y \oplus y') \land (z \oplus z')$, and the result follows from Lemma 14.2.
- $b = 1$. In this case, $S(x, 0, z, x', 1, z') = (x \lor z') \land (x \oplus x') \land (z \oplus z')$, and the result follows from Lemma 14.2.
- $b = 0$ and $c = 1$. In this case, $S(1, y, z, 0, y', z') = (y \lor z) \land (y \oplus y') \land (z \oplus z')$, and the result follows from Lemma 14.2.
- $a = b = c = 0$. In this case, $S(x', y, z, x', y', z') = (x \oplus y \oplus z) \land (x \oplus x') \land (y \oplus y') \land (z \oplus z')$, and the result follows from Lemma 10.

$\square$

## F Proof of Claim 19

Suppose for a contradiction that $a$, $b$, and $c$ are three distinct variables in $X$ such that $U(\hat{G}) \rightarrow \text{OneInThree}(a, b, c)$ and $\text{OneInThree}(a, b, c) \not\in U(\hat{G})$.

First note that that it cannot be the case that $\{a, b, c\}$ contains $\{x_i, x'_i\}$ or $\{y_i, y'_i\}$ for some $i$, since that would imply that $U(\hat{G}) \rightarrow \neg d$ for some variable $d \in X$. But clearly, there exists a satisfying assignment for $U(\hat{G})$ such that the value of $d$ is 1.

Secondly, note that if we set all $x'$-variables and all $y$-variables to 1, and all other variables in $X$ to 0, we obtain a satisfying assignment for $U(\hat{G})$. It follows that exactly one variable in $\{a, b, c\}$ is an $x'$-variable or a $y$-variable. The proof consists of a careful analysis of the different cases. We will show that in each case, there exists an assignment that satisfies $U(\hat{G})$ but that does not satisfy $\text{OneInThree}(a, b, c)$, which contradicts the assumption that $U(\hat{G}) \rightarrow \text{OneInThree}(a, b, c)$.

1. If $\{a, b, c\} = \{x_i, x_j, y_k\}$, then, since $\text{OneInThree}(a, b, c) \not\in U(\hat{G})$, $e_k \neq \{i, j\}$.

   Without loss of generality, let $j \not\in e_k$. It is easy to see that there is a satisfying assignment for $U(\hat{G})$ such that $y_k$ and $x_j$ are set to 1. (Set all other $x$-variables to 0 and set $y_k$ to 1 if $j \not\in e_k$.) Thus, we have an assignment that satisfies $U(\hat{G})$ but not $\text{OneInThree}(a, b, c)$.

2. If $\{y'_i, y'_j\} \subseteq \{a, b, c\}$, note that $k \neq \ell$, by the observation made above. Let $i$ be such that $i \in e_\ell$ and $i \not\in e_k$. Set $x_i$ to 1, and set all other $x$-variables to 0. This can be extended to a satisfying assignment for $S(\hat{G})$, and in this assignment, $y_{\ell} = 0$ (and thus $y'_\ell = 1$), and $y_k = 1$.

3. If $\{x'_i, x_j\} \subseteq \{a, b, c\}$. Then $i \neq j$. Set $x_j$ to 1 and all other $x$-variables to 0. It is easy to see that this can be extended to a satisfying assignment for $U(\hat{G})$.

4. If $\{a, b, c\} = \{x'_i, y'_j, y'_k\}$, then, if $i \not\in e_\ell$ and $i \not\in e_k$, then set $x_i$ to 1, set all other $x$-variables to 0, set $y_r$ to 1 if $i \not\in e_r$, and extend this to a satisfying assignment for $U(\hat{G})$. If $i \in e_\ell$ or $i \in e_k$, assume without loss of generality that $i \in e_k$, set $x_i$ to 0, set $y_k$ to 0, and extend this to a satisfying assignment for $U(\hat{G})$. 

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G  Proof of Claim [20]

Suppose that $a$ and $b$ are two distinct variables in $X$ such that $U(\hat{G}) \rightarrow (a \oplus b)$ and $a \oplus b \notin U(\hat{G})$. It is easy to see that we can set $a$ and $b$ to 0, and extend this to a satisfying assignment of $U(\hat{G})$, which is a contradiction.

Next, let $a, b, c$ be three distinct variables in $X$ such that $U(\hat{G}) \rightarrow (a \oplus b \oplus c)$ and $a \oplus b \oplus c \notin U(\hat{G})$. Let $\hat{X} = \{x_1, \ldots, x_n, y_1, \ldots, y_m\}$. Any assignment that sets all variables in $\hat{X}$ to 1, and all variables not in $\hat{X}$ to 0, satisfies $U(\hat{G})$. It follows that either exactly one or exactly three elements of $\{a, b, c\}$ are in $\hat{X}$.

If exactly one of $\{a, b, c\}$ is in $\hat{X}$, assume without loss of generality that $a \in \hat{X}$. If $a' \in \{b, c\}$, then, without loss of generality, let $a' = b$. In this case, $U(\hat{G}) \rightarrow 1$. But this is a contradiction, since it is immediate that we can set $c$ to 1 and extend this to a satisfying assignment of $U(\hat{G})$. Next, let $d, e \in \hat{X}$ be such that $d' = b$ and $e' = c$. In that case, $a, d$, and $e$ are distinct variables in $\hat{X}$ such that $U(\hat{G}) \rightarrow a \oplus d \oplus e$ and $a \oplus d \oplus e \notin U(\hat{G})$. This falls under the next case.

Finally, suppose that $a, b, c$ are three distinct variables in $\hat{X}$ such that $U(\hat{G}) \rightarrow a \oplus b \oplus c$ and $a \oplus b \oplus c \notin U(\hat{G})$. Let $\hat{\hat{U}}(\hat{G}) = \{(x_i \oplus x_j \oplus y_k) \mid e_k = \{i, j\}\}$, i.e., $\hat{\hat{U}}(\hat{G})$ consists of all constraint applications in $U(\hat{G})$ whose variables are in $\hat{X}$. Since any assignment on $\hat{X}$ that satisfies $\hat{\hat{U}}(\hat{G})$ can be extended to a satisfying assignment of $U(\hat{G})$ (by letting $a' = \pi$ for all $a \in \hat{X}$), the desired result follows immediately from the following claim.

Claim 22 $\hat{\hat{U}}(\hat{G})$ is a maximal set of constraint applications of $\text{XOR}_3$ without duplicates over variables $\hat{X}$.

Proof. Suppose that $a, b, c$ are three distinct variables in $\hat{X}$ such that $\hat{\hat{U}}(\hat{G}) \rightarrow a \oplus b \oplus c$ and $a \oplus b \oplus c \notin \hat{\hat{U}}(\hat{G})$. The proof consists of a careful analysis of the different cases. We will show that in each case, there exists an assignment on $\hat{X}$ that satisfies $\hat{\hat{U}}(\hat{G})$ but not $(a \oplus b \oplus c)$, which contradicts the assumption that $\hat{\hat{U}}(\hat{G}) \rightarrow a \oplus b \oplus c$.

It is important to note that any assignment to $\{x_1, \ldots, x_n\}$ can be extended to a satisfying assignment of $\hat{\hat{U}}(\hat{G})$.

1. If $a, b$, and $c$ are in $\{x_1, \ldots, x_n\}$, then set $a$, $b$, and $c$ to 0. This assignment can be extended to an assignment on $\hat{X}$ that satisfies $x_i \oplus x_j \oplus y_k$ for $e_k = \{i, j\}$.

2. If exactly two of $\{a, b, c\}$ are in $\{x_1, \ldots, x_n\}$, then without loss of generality, let $c = y_k$ for $e_k = \{i, j\}$. By the assumption that $a \oplus b \oplus c$ is not in $\hat{\hat{U}}(\hat{G})$, at least one of $a$ and $b$ is not in $\{x_i, x_j\}$.

Without loss of generality, let $a \notin \{x_i, x_j\}$. Set $a$ to 0 and set $\{x_1, \ldots, x_m\} \setminus \{a\}$ to 1. This assignment can be extended to a satisfying assignment for $\hat{\hat{U}}(\hat{G})$. Note that such an assignment will set $y_k$ to 1. It follows that this assignment does not satisfy $a \oplus b \oplus c$. 

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3. If exactly one of \( \{a, b, c\} \) are in \( \{x_1, \ldots, x_n\} \), without loss of generality, let \( a \in \{x_1, \ldots, x_n\} \). Set \( a \) to 0 and \( b \) and \( c \) to 1. It is easy to see that this can be extended to a satisfying assignment for \( \hat{U}(\hat{G}) \).

4. If \( a, b, \) and \( c \) are in \( \{y_1, \ldots, y_m\} \), let \( a = y_{k_1}, b = y_{k_2}, c = y_{k_3} \) such that \( c_{k_\ell} = \{i_\ell, j_\ell\} \) for \( \ell \in \{1, 2, 3\} \). First suppose that for every \( \ell \in \{1, 2, 3\} \), for every \( x \in \{x_{i_\ell}, x_{j_\ell}\} \), there exists an \( \ell' \in \{1, 2, 3\} \) with \( \ell' \neq \ell \) and a constraint application \( A \) in \( \hat{U}(\hat{G}) \) such that \( x \) and \( y_{k_{\ell'}} \) occur in \( A \). This implies that every vertex in \( \{i_1, j_1, i_2, j_2, i_3, j_3\} \) is incident with at least 2 of the edges in \( e_{k_1}, e_{k_2}, e_{k_3} \). Since these three edges are distinct, it follows that the edges \( e_{k_1}, e_{k_2}, e_{k_3} \) form a triangle in \( \hat{G} \), which contradicts the assumption that \( \hat{G} \) is triangle-free.

So, let \( \ell \in \{1, 2, 3\} \), \( x \in \{x_{i_\ell}, x_{j_\ell}\} \) be such that for all \( \ell' \in \{1, 2, 3\} \) with \( \ell' \neq \ell \), \( x \) and \( y_{k_{\ell'}} \) do not occur in the same constraint application in \( \hat{U}(\hat{G}) \).

Set \( x \) to 0 and set \( \{x_1, \ldots, x_n\} \setminus \{x\} \) to 1. This can be extended to a satisfying assignment of \( \hat{U}(\hat{G}) \) and such a satisfying assignment must have the property that \( y_{k_\ell} = 0 \) and \( y_{k_{\ell'}} = 1 \) for all \( \ell' \in \{1, 2, 3\} \) such that \( \ell' \neq \ell \).

\(\square\)

H Removing Constants

In Section 3.2 we showed that for all \( \mathcal{C} \) that are not 2-affine, GI \( \leq^p_m \) ISO\(_\ell\)(\( \mathcal{C} \)).

In this section, we will show that we can get the same result without using constants.

**Theorem 23.** If \( \mathcal{C} \) is not 2-affine, then GI \( \leq^p_m \) ISO\(_\ell\)(\( \mathcal{C} \)).

This completes the proof of Theorem 7.

Note that constants are used a lot in the proofs in the previous section. It is known that removing constants can be a lot of work, see, for example Dalmau’s work to remove constants from quantified constraint applications [Dal97].

Part of the problem is that there are far more cases to consider than in the case with constants. Recall that in the case with constants, if sufficed to prove GI-hardness for 6 constraints (namely, the constraints from Lemma 14 and Lemma 16), since it follows from the proofs of Theorems 15 and 17 that for all \( \mathcal{C} \) that are not 2-affine, there exists a set of constraint applications with constants that is equivalent to one of these 6 constraints. Now look at one of the simplest of these 6 constraints, namely, OR\(_0\). If there exists a set of constraint applications \( S(0, 1, x, y) \) of \( \mathcal{C} \) such that \( S(0, 1, x, y) \equiv \text{OR}\(_0\)(x, y) \), and we can use constants, it suffices to show GI-hardness for OR\(_0\). But if we cannot use constants, we need to show GI-hardness for all 2\(^{12}\) constraints \( A \) of arity 4 such that \( A(0, 1, x, y) \equiv \text{OR}\(_0\)(x, y) \). For the most complicated of the 6 constraints from the previous section, which has arity 6, we will now have 2\(^{192}\) cases to consider.

Clearly, handling each of these constraints separately is not an option. We need a way to uniformly transform the GI-hardness reductions for the case with constants from the previous section into GI-hardness reductions to the corresponding constant-free isomorphism problems.
A crucial tool in this transformation will be the following lemma, Lemma 24. This lemma does not immediately imply the result, but it will enable us to transform the GI-hardness reductions from the previous section into GI-hardness reductions to the corresponding case without constants.

Say that a constraint $C$ is complementative (or $C$-closed) if for every $s \in \{0,1\}^k$, $C(s) = \overline{C(\overline{s})}$, where $k$ is the arity of $C$ and $\overline{s} \in \{0,1\}^k = \text{def } 1 - s$, i.e., $\overline{s}$ is obtained by flipping every bit of $s$. A set of constraints is complementative if each of its elements is.

Often, we will want to be explicit about the variables and/or constants that occur in a set of constraint applications (with constants). In such cases, we will write (sets of) constraint applications as $S(x_1, \ldots, x_k)$ or $S(0,1,x_1,\ldots,x_k)$. It is important to recall that in our terminology, a set of constraint applications of $C$ does not contain constants.

**Lemma 24.** If $C$ is not 2-affine, then

- there exists a set $S(x,y)$ of constraint applications of $C$ such that $S(x,y)$ is equivalent to $\overline{x} \land y$, $\overline{x} \lor y$, $x \lor y$, or $x \leftrightarrow y$; or
- there exists a set $S(t,x,y)$ of constraint applications of $C$ such that $S(t,x,y)$ is equivalent to $t \land (\overline{x} \lor y)$, $t \land (x \leftrightarrow y)$, or $t \land (x \lor y)$; or
- there exists a set $S(f,x,y)$ of constraint applications of $C$ such that $S(f,x,y)$ is equivalent to $\overline{t} \land (\overline{x} \lor y)$, $\overline{t} \land (x \leftrightarrow y)$, or $\overline{t} \land (\overline{x} \land \overline{y})$.

**Proof.** Let $A(0,1,x,y)$ be a constraint application of $C$ with constants such that $A(0,1,x,y)$ is equivalent to $\text{OR}_0(x,y)$, $\text{OR}_1(x,y)$, $\text{OR}_2(x,y)$, or $\text{XOR}_2(x,y)$. The existence of $A(0,1,x,y)$ follows immediately from the proof of Theorem 15 and from the first paragraph of the proof of Theorem 17.

As is usual in proofs of dichotomy theorems for Boolean constraints, our proof uses case distinctions. The main challenge of the proof is to keep the number of cases in check.

**A is not 0-valid, not 1-valid, and not complementative** In this case, there exists a constraint application of $A$ that is equivalent to $\overline{x} \land y$ [CH96], see also [CKS01] Lemma 5.25.

**A is 0-valid, 1-valid, and not complementative** In this case, there exists a constraint application of $A$ that is equivalent to $\overline{x} \lor y$ [CH96] Lemma 4.13, see also [CKS01] Lemma 5.25.

**A is not 0-valid, not 1-valid, and complementative** In this case, there exists a constraint application of $A$ that is equivalent to $x \lor y$ [CKS01], proof of Lemma 5.24.

**A is 0-valid, 1-valid, and complementative** Let $\alpha$ be an assignment that does not satisfy $A(x_1,x_2,x_3,x_4)$. Such an assignment exists, since $A(x_1,x_2,x_3,x_4)$ is not a tautology. Let $B(x,y)$ be the constraint application of $A$ that results when replacing all variables in $A(x_1,x_2,x_3,x_4)$ whose value is true in $\alpha$ by $x$, and replacing all variables in $A(x_1,x_2,x_3,x_4)$ whose value is false in $\alpha$ by $y$. Note that $B(0,0) = B(1,1) = 1$, since $B$ is 0-valid and 1-valid; $B(1,0) = 0$ by construction; and $B(0,1) = 0$, since $B$ is complementative. It follows that $B$ is equivalent to $x \leftrightarrow y$. 

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A is 1-valid and not 0-valid  In this case we can force a variable $z$ to be true by adding the constraint application $A(z, z, z, z)$.

Let $B$ be the 3-ary constraint such that $B(f, x, y) \equiv A(f, 1, x, y)$. Then $B$ is 1-valid, since $A$ is 1-valid. If $B$ is 0-valid, then, by the cases handled above, there exists a constraint application of $B$ that is equivalent to $\overline{t} \lor y$ or to $x \leftrightarrow y$. Since $\{A(f, t, x, y), A(t, t, t)\}$ is equivalent to $t \land B(f, x, y)$, it follows that there exists a set of constraint applications of $A$ that is equivalent to $t \land (\overline{t} \lor y)$ or to $t \land (x \leftrightarrow y)$.

It remains to handle the case that $B$ is not 0-valid, i.e., the case that $A(0, 1, 0, 0) = 0$. Since $A(0, 1, 0, 0) = 0$, we have that $A(0, 1, x, y) \equiv \text{OR}_0(x, y)$ or $A(0, 1, x, y) \equiv \text{XOR}_2(x, y)$.

First consider the case that $A(0, 1, x, y) \equiv \text{OR}_0(x, y)$. If $A(1, 1, 0, 1) = 0$, then consider the set

$$S(t, x, y) = \{A(x, t, y, t), A(t, t, t)\}.$$  

This set is equivalent to $t \land (\overline{t} \lor y)$, since $A(0, 1, 0, 1) = 1$; $A(0, 1, 1, 1) = 1$; $A(1, 1, 0, 1) = 0$; and $A(1, 1, 1, 1) = 1$.

If $A(1, 1, 0, 1) = 1$, then consider the set

$$S(t, x, y) = \{A(x, t, y, x), A(t, t, t)\}.$$  

This set is equivalent to $t \land (x \lor y)$, since $A(0, 1, 0, 0) = 0$; $A(0, 1, 1, 0) = 1$; $A(1, 1, 0, 1) = 1$; and $A(1, 1, 1, 1) = 1$.

Finally, consider the case that $A(0, 1, x, y) \equiv \text{XOR}_2(x, y)$. We are in the following situation: $A(0, 1, 0, 0) = 0$, $A(0, 1, 0, 1) = 1$, $A(0, 1, 1, 0) = 1$, $A(0, 1, 1, 1) = 0$, and $A(1, 1, 1, 1) = 1$. Consider the following set

$$S(t, x, y) = \{A(t, t, t), A(x, t, y, t)\}.$$  

If $A(1, 1, 0, 1) = 1$, then $S(t, x, y) \equiv t \land (x \lor y)$. If $A(1, 1, 0, 1) = 0$, then $S(t, x, y) \equiv t \land (x \leftrightarrow y)$.

A is 0-valid and not 1-valid  In this case we can force a variable $z$ to be false by adding the constraint application $A(z, z, z, z)$.

Let $B$ be the 3-ary constraint such that $B(t, x, y) \equiv A(0, t, x, y)$. Then $B$ is 0-valid, since $A$ is 0-valid. If $B$ is 1-valid, then, by the cases handled above, there exists a constraint application of $B$ that is equivalent to $\overline{t} \lor y$ or to $x \leftrightarrow y$. Since $\{A(f, t, x, y), A(f, f, f, f)\}$ is equivalent to $\overline{t} \land B(f, x, y)$, it follows that there exists a set of constraint applications of $A$ that is equivalent to $\overline{t} \land (\overline{t} \lor y)$ or to $\overline{t} \land (x \leftrightarrow y)$.

It remains to handle the case that $B$ is not 1-valid, i.e., the case that $A(0, 1, 1, 1) = 0$. Since $A(0, 1, 1, 1) = 0$, $A(0, 1, x, y) \equiv \text{OR}_2(x, y)$.

If $A(0, 1, 0, 0) = 0$, then consider the set

$$S(f, x, y) = \{A(f, x, y, f), A(f, f, f, f)\}.$$  

This set is equivalent to $\overline{t} \land (x \lor y)$, since $A(0, 0, 0, 0) = 1$; $A(0, 1, 0, 0) = 1$; $A(0, 0, 1, 0) = 0$; and $A(0, 1, 1, 0) = 1$.  

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If \( A(0,0,1,0) = 1 \), then consider the set
\[
S(f,x,y) = \{ A(f,x,y,x), A(f,f,f,f) \}.
\]
This set is equivalent to \( \overline{7} \land (\pi \lor \overline{\pi}) \), since \( A(0,0,0,0) = 1; A(0,0,1,0) = 1; A(0,1,0,1) = 1; \) and \( A(0,1,1,1) = 0 \). \( \square \)

When we look at Lemma 24, some of the cases will give us the required reduction immediately or almost immediately.

**Lemma 25.** GI is polynomial-time many-one reducible to

1. ISO(\( \{ \lambda xy.(\pi \lor y) \} \)),
2. ISO(\( \{ \lambda txy.(t \land (\overline{\pi} \lor y)) \} \)),
3. ISO(\( \{ \lambda txy.(t \land (x \lor y)) \} \)),
4. ISO(\( \{ \lambda fxy.(\overline{f} \land (\pi \lor y)) \} \)), and
5. ISO(\( \{ \lambda fxy.(\overline{f} \land (\pi \lor y)) \} \)).

**Proof.** The first case follows from Lemma 14. For the remaining cases, we will adapt the reductions of of the proof of Lemma 14.

Let \( \hat{G} \) be a graph and let \( V(\hat{G}) = \{ 1, 2, \ldots, n \} \). Let \( E(\hat{G}) = \{ e_1, \ldots, e_m \} \).

Define
\[
S_2(\hat{G}) = \{ t \land (x_i \lor \overline{y_k}), t \land (x_j \lor \overline{y_k}) \mid e_k = \{ i, j \} \}
\]
\[
S_3(\hat{G}) = \{ t \land (x_i \lor x_j) \mid \{ i, j \} \in E(\hat{G}) \}
\]
\[
S_4(\hat{G}) = \{ \overline{f} \land (x_i \lor \overline{y_k}), \overline{f} \land (x_j \lor \overline{y_k}) \mid e_k = \{ i, j \} \}
\]
\[
S_5(\hat{G}) = \{ \overline{f} \land (\overline{x_i} \lor \overline{x_j}) \mid \{ i, j \} \in E(\hat{G}) \}
\]

Let \( G \) and \( H \) be two graphs without isolated vertices and with vertex set \( \{ 1, 2, \ldots, n \} \). We will show that for \( 2 \leq i \leq 5 \), \( G \) is isomorphic to \( H \) if and only if \( S_i(G) \) is isomorphic to \( S_i(H) \).

For \( i = 2, 3 \), it follows from the proof of Lemma 14 that \( G \) is isomorphic to \( H \) if and only if \( S_i(G)[t := 1] \) is isomorphic to \( S_i(H)[t := 1] \).

Note that \( S_1(G) \equiv (S_1(G)[t := 1] \land t) \) and \( S_1(H) \equiv (S_1(H)[t := 1] \land t) \). Thus, if \( S_i(G)[t := 1] \) is isomorphic to \( S_i(H)[t := 1] \), then \( S_i(G) \) is isomorphic to \( S_i(H) \).

For the converse, note that if \( S_i(G) \) is isomorphic to \( S_i(H) \), then the isomorphism must map \( t \) to \( t \), since \( t \) is the unique variable \( z \) such that \( S_i(G) \rightarrow z \) and the unique variable \( z \) such that \( S_i(H) \rightarrow z \). It follows immediately that \( S_i(G)[t := 1] \) is isomorphic to \( S_i(H)[t := 1] \), by the same isomorphism.

For \( i = 4, 5 \), it follows from the proof of Lemma 14 that \( G \) is isomorphic to \( H \) if and only if \( S_i(G)[f := 0] \) is isomorphic to \( S_i(H)[f := 0] \).

Note that \( S_i(G) \equiv (S_i(G)[f := 0] \land \overline{f}) \) and \( S_i(H) \equiv (S_i(H)[f := 0] \land \overline{f}) \). Thus, if \( S_i(G)[f := 0] \) is isomorphic to \( S_i(H)[f := 0] \), then \( S_i(G) \) is isomorphic to \( S_i(H) \).

For the converse, note that if \( S_i(G) \) is isomorphic to \( S_i(H) \), then the isomorphism must map \( f \) to \( f \), since \( f \) is the unique variable \( z \) such that \( S_i(G) \rightarrow \pi \)
and the unique variable $z$ such that $S_i(H) \rightarrow z$. It follows immediately that $S_i(G)[f := 0]$ is isomorphic to $S_i(H)[f := 0]$, by the same isomorphism. \hfill \Box

To complete the proof of Theorem 28, it remains to show the following claim.

**Claim 26** If $C$ is not 2-affine, and

- there exists a set $U(x, y)$ of constraint applications of $C$ such that $U(x, y)$ is equivalent to $\exists y, x \oplus y$, or $x \leftrightarrow y$; or
- there exists a set $U(t, x, y)$ of constraint applications of $C$ such that $U(t, x, y)$ is equivalent to $t \land (x \leftrightarrow y)$, or
- there exists a set $U(f, x, y)$ of constraint applications of $C$ such that $U(f, x, y)$ is equivalent to $\exists f \land (x \leftrightarrow y)$,

then $GI \leq_m ISO(C)$.

These cases will be handled by transforming the GI-hardness reductions from the previous section into GI-hardness reductions to the corresponding constant-free isomorphism problems using the set of constraint applications $U$ from Claim 26.

We first restate some of the definitions and results from the previous section in a way that is explicit about the occurrences of constants.

**Definition 27.**

1. $D_1$ is the set of 4-ary constraints $D$ such that $D(0, 1, x, y) \equiv OR_0(x, y)$.
2. $D_2$ is the set of 4-ary constraints $D$ such that $D(0, 1, x, y) \equiv OR_1(x, y)$.
3. $D_3$ is the set of 4-ary constraints $D$ such that $D(0, 1, x, y) \equiv OR_2(x, y)$.
4. $D_4$ is the set of 6-ary constraints $D$ such that $D(0, 1, x, y, x', y') \equiv (x \lor y) \land (x \oplus x') \land (y \oplus y')$.
5. $D_5$ is the set of 8-ary constraints $D$ such that $D(0, 1, x, y, z, x', y', z') \equiv OneInThree(x, y, z) \land (x \lor x') \land (y \lor y') \land (z \lor z')$.
6. $D_6$ is the set of 8-ary constraints $D$ such that $D$ is affine and $D(0, 1, x, y, z, x', y', z') \equiv (x \lor y \lor z) \land (x \lor x') \land (y \lor y') \land (z \lor z')$.

From the previous section, we know the following fact.

**Fact 28** If $C$ is not 2-affine, then there exists a set of constraint applications $S(x_1, \ldots, x_k)$ of $C$ such that $S(x_1, \ldots, x_k) \equiv D(x_1, \ldots, x_k)$ for some $D \in \bigcup_{1 \leq i \leq 6} D_i$.

- For $1 \leq i \leq 6$, and for all $D \in D_i$, $GI \leq_m ISO_e(\{D\})$.

**Proof.** The second part follows immediately from Lemmas 23 and 26. For the first part, it follows from the proofs of Theorems 10 and 11 that there exist an $i$ such that $1 \leq i \leq 6$, a constraint $D' \in D_i$, and a set $S(0, 1, x_3, \ldots, x_k)$ of constraint applications of $C$ with constants such that $S(0, 1, x_3, \ldots, x_k)$ is equivalent to $D'(0, 1, x_3, \ldots, x_k)$. By definition of $D_i$, there exists a constraint $D \in D_i$ such that $S(x_1, x_2, x_3, \ldots, x_k)$ is equivalent to $D(x_1, x_2, x_3, \ldots, x_k)$. \hfill \Box

Our goal is to remove the constants and show that for $1 \leq i \leq 6$, and for all $D \in D_i$, $GI \leq_m ISO(\{D\})$. 27
In order to do this, we will transform the reduction for the case with constants into a reduction for the case without constants. We will need some properties from the case with constants.

**Definition 29.** Let \( \hat{G} \) be a graph.

1. For \( D \in \mathcal{D}_1 \), \( S_{1,D}(\hat{G}) = \{D(f, t, x_i, x_j) \mid \{i, j\} \in E(\hat{G})\} \).
2. For \( D \in \mathcal{D}_2 \), \( S_{2,D}(\hat{G}) = \{D(f, t, y_k, x_i), D(f, t, y_k, x_j) \mid e_k = \{i, j\}\} \).
3. For \( D \in \mathcal{D}_3 \), \( S_{3,D}(\hat{G}) = \{D(f, t, x_i, x_j) \mid \{i, j\} \in E(\hat{G})\} \).
4. For \( D \in \mathcal{D}_4 \), \( S_{4,D}(\hat{G}) = \{D(f, t, x_i, x_j, x'_i, x'_j) \mid \{i, j\} \in E(\hat{G})\} \).
5. For \( D \in \mathcal{D}_5 \), \( S_{5,D}(\hat{G}) = \{D(f, t, x_i, y_k, x'_i, y'_k) \mid e_k = \{i, j\}\} \).
6. For \( D \in \mathcal{D}_6 \), \( S_{6,D}(\hat{G}) = \{D(f, t, x_i, y_k, x'_i, y'_k) \mid e_k = \{i, j\}\} \).

From the proofs of Lemmas 14 and 16 we have the following fact, which witnesses the GI-hardness for the case with constants.

**Fact 30** Let \( G \) and \( H \) be graphs such that \( V(G) = V(H) = \{1, \ldots, n\} \), \( E(G) = \{e_1, \ldots, e_m\} \), \( E(H) = \{e'_1, \ldots, e'_m\} \), all vertices in \( G \) and \( H \) have degree at least two, and \( G \) and \( H \) do not contain triangles.

For all \( 1 \leq i \leq 6 \) and for all \( D \in \mathcal{D}_i \), \( G \) is isomorphic to \( H \) if and only if \( S_{i,D}(G)[f := 0, t := 1] \) is isomorphic to \( S_{i,D}(H)[f := 0, t := 1] \).

The following simple observation is also useful.

**Observation 31.** Let \( G \) and \( H \) be graphs such that \( V(G) = V(H) = \{1, \ldots, n\} \), \( E(G) = \{e_1, \ldots, e_m\} \), \( E(H) = \{e'_1, \ldots, e'_m\} \), all vertices in \( G \) and \( H \) have degree at least two, and \( G \) and \( H \) do not contain triangles.

For all \( 1 \leq i \leq 6 \) and for all \( D \in \mathcal{D}_i \), if \( G \) is isomorphic to \( H \), then \( S_{i,D}(G) \) is isomorphic to \( S_{i,D}(H) \) by an isomorphism that maps \( f \) to \( f \) and \( t \) to \( t \).

**Proof.** Let \( \pi \) be an isomorphism from \( G \) to \( H \). Then \( S_{i,D}(G) \) is isomorphic to \( S_{i,D}(H) \), by an isomorphism that maps \( x_i \) to \( x_{\pi(i)} \), \( x'_i \) to \( x'_{\pi(i)} \), \( y_k \) to \( y_{ \ell} \) and \( y'_k \) to \( y'_{ \ell} \) for \( e_k = \{i, j\}, e'_k = \{ \pi(i), \pi(j)\} \), \( f \) to \( f \), and \( t \) to \( t \). Note that this isomorphism even makes the sets of constraints equal, rather than merely equivalent. \( \square \)

In order to remove the constants, we need to use the set \( U \) from Claim 28 as well as certain properties of \( S_{i,D} \).

**Lemma 32.** Let \( \hat{G} \) be a graph such that \( V(\hat{G}) = \{1, \ldots, n\} \), \( E(\hat{G}) = \{e_1, \ldots, e_m\} \), all vertices in \( \hat{G} \) have degree at least two, and \( \hat{G} \) does not contain triangles. Let \( 1 \leq i \leq 6 \), let \( D \in \mathcal{D}_i \), and let \( z \) and \( z' \) be any two distinct variables. If

\[
S_{i,D}(\hat{G}) \cup \{f, f_1, f_2, t, t_1\} \rightarrow (z \leftrightarrow z'),
\]

then \( \{z, z'\} = \{f, f_1\}, \{f, f_2\}, \{f_1, f_2\}, \text{ or } \{t, t_1\} \).

**Proof.** If \( S_{i,D}(\hat{G}) \cup \{f, f_1, f_2, t, t_1\} \rightarrow (z \leftrightarrow z') \), then \( S_{i,D}(\hat{G}) \cup \{f, f_1, f_2, t, t_1\} \) \([f, f_1, f_2 := 0, t, t_1 := 1] \rightarrow (z \leftrightarrow z') \). Since \( f_1, f_2 \), and
For all $i$ and all $j \neq i$, $S(\hat{G})[x_i := 1], S(\hat{G})[x_i := 0], S(\hat{G})[x_i := 0, x_j := 1]$ are satisfiable by setting all (remaining) variables to 1.

2. In this case, $S(\hat{G})$ is equivalent to $\{x_i \lor x_j \mid \{i, j\} \in E(\hat{G})\}$. For all $i$ and all $j \neq i$, $S(\hat{G})[x_i := 1], S(\hat{G})[x_i := 0], S(\hat{G})[x_i := 0, x_j := 1]$ are satisfiable by setting all (remaining) variables to 1.

3. In this case, $S(\hat{G})$ is equivalent to $\{\bar{x}_i \lor \bar{x}_j \mid \{i, j\} \in E(\hat{G})\}$. For all $i$ and all $j \neq i$, $S(\hat{G})[x_i := 1], S(\hat{G})[x_i := 0], S(\hat{G})[x_i := 0, x_j := 1]$ are satisfiable by setting all (remaining) variables to 1.

4. In this case, $S(\hat{G})$ is equivalent to $\{x_i \lor x_j \} \land (x_i \lor x_j) \land (x_j \lor x_j) \mid \{i, j\} \in E(\hat{G})\}$. For all $i, j$, $S(\hat{G})[x_i := 1], S(\hat{G})[x_j := 1], S(\hat{G})[x_i := 1, x_j := 1]$ are satisfiable by setting all (remaining) variables to 1.

5. In this case, $S(\hat{G})$ is equivalent to $\{\text{OneHThree}(x_i, x_j, y_k) \land (x_i \lor x_j) \land (x_j \lor x_j) \land (y_k \lor y_k) \mid \{i, j, k\}\}$. For all $i, j, k, \ell$, $S(\hat{G})[x_i := 0], S(\hat{G})[x_j := 1], S(\hat{G})[y_k := 1], S(\hat{G})[y_\ell := 0], S(\hat{G})[x_i := 0, x_j := 1], S(\hat{G})[y_k := 1, y_\ell := 0], S(\hat{G})[x_i := 0, y_k := 1], S(\hat{G})[x_i := 1, y_k := 1, y_\ell := 0], S(\hat{G})[x_i := 1, y_\ell := 0], S(\hat{G})[x_i := 0, x_j := 1]$, and $S(\hat{G})[x_i := 1, x_j := 1, x_\ell := 0]$ are satisfiable by setting all $x$-variables and $y$-variables to 0, and all $y$-variables and $x$-variables to 1.
Proof of Claim 26.

Let $C$ be not $2$-affine. Let $U(X)$ be a set of constraint applications of $C$ fulfilling the statement of Claim 26, i.e.,

- $U(x, y)$ is equivalent to $\overline{x} \land y$, $x \lor y$, or $x \leftrightarrow y$; or
- $U(t, x, y)$ is equivalent to $t \land (x \leftrightarrow y)$, or
- $U(f, x, y)$ is equivalent to $\overline{f} \land (x \leftrightarrow y)$.

Let $D$ be a constraint and $1 \leq i \leq 6$ be such that $D \in D_1$ and there exists a set of constraint applications $S(x_1, \ldots, x_k)$ of $C$ such that $S(x_1, \ldots, x_k) \equiv D(x_1, \ldots, x_k)$. For $\hat{G}$ a graph, we will write $S(\hat{G})$ for $S_{i,D}(\hat{G})$.

Let $\hat{G}$ be a graph such that $V(\hat{G}) = \{1, \ldots, n\}$ and $E(\hat{G}) = \{e_1, \ldots, e_m\}$. For each of the cases for $U$, we will define a polynomial-time computable set $\hat{S}(\hat{G})$ of constraint applications of $C$.

1. If $U(x, y) \equiv \overline{x} \land y$, define $\hat{S}(\hat{G})$ as $S(\hat{G}) \cup \{U(f, t), U(f_1, t), U(f_2, t_1)\}$. Then $\hat{S}(\hat{G})$ is equivalent to $S(\hat{G}) \cup \{\overline{f}, \overline{f_1}, \overline{f_2}, t, t_1\}$.
2. If $U(x, y) \equiv x \lor y$, define $\hat{S}(\hat{G})$ as $S(\hat{G}) \cup \{(U(f, t), U(f_1, t), U(f_2, t), U(f, t_1))\}$. Then $\hat{S}(\hat{G})$ is equivalent to $S(\hat{G}) \cup \{f \land t, f_1 \land t, f_2 \land t, f \land t_1\}$.
3. If $U(x, y) \equiv x \leftrightarrow y$, define $\hat{S}(\hat{G})$ as $S(\hat{G}) \cup \{(U(f, f_1), U(f, f_2), U(t, t_1))\}$. Then $\hat{S}(\hat{G})$ is equivalent to $S(\hat{G}) \cup \{f \leftrightarrow f_1, f \leftrightarrow f_2, t \leftrightarrow t_1\}$.
4. If $U(t, x, y) \equiv t \land (x \leftrightarrow y)$, define $\hat{S}(\hat{G})$ as $S(\hat{G}) \cup \{(U(t, f, f_1), U(t_1, f, f_2))\}$. Then $\hat{S}(\hat{G})$ is equivalent to $S(\hat{G}) \cup \{t, t_1, (f \leftrightarrow f_1), (f \leftrightarrow f_2)\}$.
5. If $U(f, x, y) \equiv \overline{f} \land (x \leftrightarrow y)$, define $\hat{S}(\hat{G})$ as $S(\hat{G}) \cup \{(U(f, f, f_1), U(f_2, t, t_1))\}$. Then $\hat{S}(\hat{G})$ is equivalent to $S(\hat{G}) \cup \{\overline{f}, \overline{f_1}, \overline{f_2}, (t \leftrightarrow t_1)\}$.

Finally, we are ready to prove Claim 26 which completes the proof of Theorem 26.
Let $G$ and $H$ be graphs such that $V(G) = V(H) = \{1, \ldots, n\}$, $E(G) = \{e_1, \ldots, e_m\}$, $E(H) = \{e'_1, \ldots, e'_m\}$, all vertices in $G$ and $H$ have degree at least two, and $G$ and $H$ do not contain triangles. By Lemma 18, it suffices to show that $G$ is isomorphic to $H$ if and only if $\hat{S}(G)$ is isomorphic to $\hat{S}(H)$.

If there exists an isomorphism from $G$ to $H$, then, by Observation 31, there exists an isomorphism from $S(G)$ to $S(H)$ that maps $f$ to $f$ and $t$ to $t$. We can easily extend this to an isomorphism from $\hat{S}(G)$ to $\hat{S}(H)$, by mapping $f_1$ to $f_1$, $f_2$ to $f_2$, and $t_1$ to $t_1$.

For the converse, note that, in all cases, $\hat{S}(\hat{G}) \rightarrow (f \leftrightarrow f_1) \land (f \leftrightarrow f_2) \land (t \leftrightarrow t_1)$. Also note that in all cases, $S(\hat{G}) \cup \{f, f_1, f_2, t, t_1\} \rightarrow \hat{S}(\hat{G})$.

Now suppose that $\hat{S}(G)$ is isomorphic to $\hat{S}(H)$. By Lemma 32 and the observations made above, for $\hat{G} \in \{G, H\}$, $\{f, f_1, f_2\}$ is the unique triple of equivalent distinct variables. It follows that the isomorphism maps $\{f, f_1, f_2\}$ to $\{f, f_1, f_2\}$. It also follows from Lemma 32 and the observations made above that among the remaining variables, $\{t, t_1\}$ is the unique pair of equivalent distinct variables. Thus, the isomorphism maps $\{t, t_1\}$ to $\{t, t_1\}$. It follows that $\hat{S}(G)[f, f_1, f_2 := 0, t, t_1 := 1]$ is isomorphic to $\hat{S}(H)[f, f_1, f_2 := 0, t, t_1 := 1]$.

For $\hat{G} \in \{G, H\}$, $\hat{S}(\hat{G})[f, f_1, f_2 := 0, t, t_1 := 1]$ is equivalent to $S(\hat{G})[f := 0, t := 1]$. It follows that $S(G)[f := 0, t := 1]$ is isomorphic to $S(H)[f := 0, t := 1]$. By Fact 30 it follows that $G$ is isomorphic to $H$. \qed