Datalog-Expressibility for Monadic and Guarded Second-Order Logic

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- Abstract

We characterise the sentences in Monadic Second-order Logic (MSO) that are over finite structures equivalent to a Datalog program, in terms of an existential pebble game. We also show that for every class \mathcal{C} of finite structures that can be expressed in MSO and is closed under homomorphisms, and for all $\ell, k \in \mathbb{N}$, there exists a *canonical* Datalog program Π of width (ℓ, k) , that is, a Datalog program of width (ℓ, k) which is sound for \mathcal{C} (i.e., Π only derives the goal predicate on a finite structure \mathfrak{A} if $\mathfrak{A} \in \mathcal{C}$) and with the property that Π derives the goal predicate whenever *some* Datalog program of width (ℓ, k) which is sound for \mathcal{C} derives the goal predicate. The same characterisations also hold for Guarded Second-order Logic (GSO), which properly extends MSO. To prove our results, we show that every class \mathcal{C} in GSO whose complement is closed under homomorphisms is a finite union of constraint satisfaction problems (CSPs) of ω -categorical structures.

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1 Introduction

- 31 Monadic Second-order Logic (MSO) is an important logic in theoretical computer science.
- By Büchi's theorem, a formal language can be defined in MSO if and only if it is regular (see,
- e.g., [24]). MSO sentences can be evaluated in polynomial time on classes of structures whose
- treewidth is bounded by a constant; this is known as Courcelle's theorem [16]. The latter
- $_{35}$ $\,$ result even holds for the more expressive logic of $\it Guarded~Second\mbox{-}order~Logic~(GSO)~[21,~18],$
- which extends First-order Logic by second-order quantifiers over guarded relations. Guarded
- Second-order Logic contains *Guarded First-order Logic* (which itself captures many description logics [20]).
- Another fundamental formalism in theoretical computer science, which is heavily studied in database theory, is *Datalog* (see, e.g., [24]). Every Datalog program can be evaluated on
- finite structures in polynomial time. Like MSO, Datalog strikes a good balance between
- expressivity and good mathematical and computational properties. Two important parameters
- of a Datalog program Π are the maximal arity ℓ of its auxiliary predicates (IDBs), and the

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maximal number k of variables per rule in Π . We then say that Π has width (ℓ, k) , following the terminology of Feder and Vardi [19]. These parameters are important both in theory and in practice: ℓ closely corresponds to the exponent of the size of the memory space and k to the exponent of the number of computation steps needed when evaluating Π on a given structure (see, e.g., [4]).

In some scenarios we are interested in having the good computational properties of expressibility in Datalog and having the good computational properties of expressibility in MSO. A wide variety of popular query formalisms (among them (unions of) conjunctive queries, (2-way conjunctive) regular path queries, monadic Datalog, guarded Datalog, monadically defined queries, or nested monadically defined queries) are known to be both in Datalog and GSO [25]. Also, all these formalisms have favourable properties when it comes to static analysis, most notably decidable query containment [25]. Note that on the contrary, query containment in unrestricted Datalog is undecidable, as is query containment in unrestricted MSO / GSO. So it is really the interplay of the restrictions imposed by both formalisms that is required to ensure decidability of a central task in databases and that makes this fragment interesting and worthwhile investigating.

In this paper we investigate two questions that (perhaps surprisingly) turn out to be closely related:

- 1. Which classes of finite structures are simultaneously expressible in MSO and in Datalog?
- **2.** Which constraint satisfaction problems (CSPs) can be expressed in MSO, or, more generally, in GSO?

For a structure \mathfrak{B} with a finite relational signature τ , the constraint satisfaction problem for \mathfrak{B} is the class of all finite τ -structures that homomorphically map to \mathfrak{B} . Every finite-domain constraint satisfaction problem can already be expressed in monotone monadic SNP (MMSNP; [19]), which is a small fragment of MSO. On the other hand, the constraint satisfaction problem for $(\mathbb{Q}; <)$, which is the class of all finite acyclic digraphs (V; E), cannot be expressed in MMSNP [6], but can be expressed in MSO by the sentence

$$\forall X \neq \emptyset \ \exists x \in X \ \forall y \in X : \neg E(x, y).$$

The class of CSPs of arbitrary infinite structures \mathfrak{B} is quite large; it is easy to see that a class \mathcal{D} of finite structures with a finite relational signature τ is a CSP of a countably infinite structure if and only if

- es it is closed under disjoint unions, and
- $\mathfrak{A} \in \mathcal{D}$ for any \mathfrak{A} that maps homomorphically to some $\mathfrak{A}' \in \mathcal{D}$.

The second item can equivalently be rephrased as the complement of \mathcal{D} (meant within the class of all finite τ -structures; this comment applies throughout and will be omitted in the following) being closed under homomorphisms: a class \mathcal{C} is closed under homomorphisms if for any structure $\mathfrak{A} \in \mathcal{C}$ that maps homomorphically to some \mathfrak{C} we have $\mathfrak{C} \in \mathcal{C}$. Examples of classes of structures that are closed under homomorphisms naturally arise from Datalog. We say that a class \mathcal{C} of finite τ -structures is definable in Datalog¹ if there exists a Datalog program Π with a distinguished predicate nullary goal such that Π derives goal on a finite τ -structure if and only if the structure is in \mathcal{C} ; in this case, we write Π for \mathcal{C} . Every class of τ -structures in Datalog is closed under homomorphisms. However, not every class of finite structures in Datalog describes the complement of a CSP: consider for example, for unary predicates R and R, the class $\mathcal{C}_{R,R}$ of finite R structures R such that $R^{\mathfrak{A}}$ is empty or

Warning: Feder and Vardi [19] say that a CSP is in Datalog if its *complement* in the class of all finite τ -structures is in Datalog.

 $B^{\mathfrak{A}}$ is empty. Clearly, $\mathcal{C}_{R,B}$ is not closed under disjoint unions. However, a finite structure is in $\mathcal{C}_{R,B}$ if and only if the Datalog program that consists of just one rule

$$goal := R(x), B(y)$$

does not derive goal on that structure.

An important class of CSPs is the class of CSPs for structures $\mathfrak B$ that are countably infinite and ω -categorical. A structure $\mathfrak B$ is ω -categorical if all countable models of the first-order theory of $\mathfrak B$ are isomorphic. A well-known example of an ω -categorical structure is $(\mathbb Q;<)$, which is a result due to Cantor [15]. Constraint satisfaction problems of ω -categorical structures can be evaluated in polynomial time on classes of treewidth bounded by some constant $k\in\mathbb N$, by a result of Bodirsky and Dalmau [7]. The polynomial-time algorithm presented by Bodirsky and Dalmau is in fact a Datalog program of width (k-1,k). A Datalog program Π is called sound for a class of τ -structures $\mathcal C$ if Π $\subseteq \mathcal C$. Bodirsky and Dalmau showed that if $\mathcal C$ is the complement of the CSP of an ω -categorical τ -structure $\mathfrak B$ then there exists for all $\ell, k \in \mathbb N$ a canonical Datalog program of width (ℓ, k) for $\mathcal C$, i.e., a Datalog program Π of width (ℓ, k) such that

 \blacksquare II is sound for \mathcal{C} , and

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 \blacksquare $\llbracket\Pi'\rrbracket \subseteq \llbracket\Pi\rrbracket$ for every Datalog program Π' of width (ℓ,k) which is sound for \mathcal{C} .

Moreover, whether the canonical Datalog program of width (ℓ, k) for \mathcal{C} derives goal on a given τ -structure \mathfrak{A} can be characterised in terms of the existential pebble game from finite 85 model theory, played on $(\mathfrak{A},\mathfrak{B})$ [7]. The existential ℓ,k pebble game is played by two players, called Spoiler and Duplicator (see, e.g., [17, 19, 23]). Spoiler starts by placing k pebbles on 87 elements a_1, \ldots, a_k of \mathfrak{A} , and Duplicator responds by placing k pebbles b_1, \ldots, b_k on \mathfrak{B} . If 88 the map that sends a_1, \ldots, a_k to b_1, \ldots, b_k is not a partial homomorphism from \mathfrak{A} to \mathfrak{B} , then the game is over and Spoiler wins. Otherwise, Spoiler removes all but at most ℓ pebbles from \mathfrak{A} , and Duplicator has to respond by removing the corresponding pebbles from \mathfrak{B} . Then 91 Spoiler can again place all his pebbles on \mathfrak{A} , and Duplicator must again respond by placing her pebbles on \mathfrak{B} . If the game continues forever, then Duplicator wins. If \mathfrak{B} is a finite, or 93 more generally a countable ω -categorical structure then Spoiler has a winning strategy for the existential ℓ, k pebble game on $(\mathfrak{A}, \mathfrak{B})$ if and only if the canonical Datalog program for $CSP(\mathfrak{B})$ derives goal on \mathfrak{A} (Theorem 19). This connection played an essential role in proving Datalog inexpressibility results, for example for the class of finite-domain CSPs [2] (leading 97 to a complete classification of those finite structures \mathfrak{B} such that the complement of $\mathrm{CSP}(\mathfrak{B})$ can be expressed in Datalog [3]).

Results and Consequences

We present a characterisation of those GSO sentences Φ that are over finite structures equivalent to a Datalog program. Our characterisation involves a variant of the existential pebble game from finite model theory, which we call the (ℓ, k) -game. This game is defined for a homomorphism-closed class \mathcal{C} of finite τ -structures, and it is played by the two players Spoiler and Duplicator on a finite τ -structure \mathfrak{A} as follows.

Duplicator picks a countable τ -structure \mathfrak{B} such that $CSP(\mathfrak{B}) \cap \mathcal{C} = \emptyset$.

The game then continues as the existential (ℓ, k) pebble game played by Spoiler and Duplicator on $(\mathfrak{A}, \mathfrak{B})$.

In Section 4 we show that a GSO sentence Φ is over finite structures equivalent to a Datalog program of width (ℓ, k) if and only if

 \blacksquare $\llbracket \Phi \rrbracket$ is closed under homomorphisms, and

Spoiler wins the existential (ℓ, k) -game for $\llbracket \Phi \rrbracket$ on $\mathfrak A$ if and only if $\mathfrak A \models \Phi$. We also show that for every GSO sentence Φ whose class of finite models $\mathcal C$ is closed under homomorphisms and for all $\ell, k \in \mathbb{N}$ there exists a canonical Datalog program Π of width 114 (ℓ, k) for C (Theorem 22). To prove these results, we first show that every class of finite structures in GSO whose complement is closed under homomorphisms is a finite union of 116 CSPs that can also be expressed in GSO (Lemma 16; an analogous statement holds for MSO). 117 Moreover, every CSP in GSO is the CSP of a countable ω -categorical structure (Corollary 10); 118 this allows us to use results from [7] to make the link to existential pebble games. We also 119 present an example of such a CSP which is even expressible in MSO and coNP-complete, and hence not the CSP of a reduct of a finitely bounded homogeneous structure, unless NP=coNP 121 (Proposition 23). Note that our results imply that every class of finite structures that can be expressed both in in GSO and in Datalog is a finite intersection of the complements of CSPs for ω -categorical structures. In general, it is not true that a Datalog program describes a 124 finite intersection of complements of CSPs (we present a counterexample in Example 18). 125

2 Preliminaries

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In the entire text, τ denotes a finite signature containing relation symbols and sometimes also constant symbols. If $R \in \tau$ is a relation symbol, we write ar(R) for its arity. If $\mathfrak A$ is a τ -structure we use the corresponding capital roman A letter to denote the domain of $\mathfrak A$; the domains of structures are assumed to be non-empty. If $R \in \tau$, then $R^{\mathfrak A} \subseteq A^{ar(R)}$ denotes the corresponding relation of $\mathfrak A$.

A primitive positive τ -formula (in database theory also conjunctive query) is a first-order τ -formula without disjunction, negation, and universal quantification. Every primitive positive formula is equivalent to a formula of the form

$$\exists x_1, \ldots, x_n (\psi_1 \land \cdots \land \psi_m)$$

where ψ_1, \ldots, ψ_m are atomic τ -formulas, i.e., formulas built from relation symbols in τ or equality. An existential positive τ -formula is a first-order τ -formula without negation and universal quantification. We write $\psi(x_1, \ldots, x_n)$ if the free variables of ψ are from x_1, \ldots, x_n . If \mathfrak{A} is a τ -structure and $\psi(x_1, \ldots, x_n)$ is a τ -formula, then the relation

$$R := \{(a_1, \dots, a_n) \mid \mathfrak{A} \models \psi(a_1, \dots, a_n)\}$$

is called the relation defined by ψ over \mathfrak{A} ; if ψ can be chosen to be primitive positive (or existential positive) then R is called *primitively positively definable* (or existentially positively definable, respectively).

For all logics over the signature τ considered in this text, we say that two formulas $\Phi(x_1, \ldots, x_n)$ and $\Psi(x_1, \ldots, x_n)$ are equivalent (over finite structures) if for all (finite) τ -structures $\mathfrak A$ and all $a_1, \ldots, a_n \in A$ we have

$$\mathfrak{A} \models \Phi(a_1,\ldots,a_n) \Leftrightarrow \mathfrak{A} \models \Psi(a_1,\ldots,a_n).$$

It is easy to see that every existential positive τ -formula is a disjunction of primitive positive τ -formulas (and hence referred to as a *union of conjunctive queries* in database theory). Formulas without free variables are called *sentences*; in database theory, formulas are often called *queries* and sentences are often called *Boolean queries*. If Φ is a sentence, we write $\llbracket \Phi \rrbracket$ for the class of all finite models of Φ .

A reduct of a relational structure $\mathfrak A$ is a structure $\mathfrak A'$ obtained from $\mathfrak A$ by dropping some of the relations, and $\mathfrak A$ is called an *expansion* of $\mathfrak A'$.

2.1 Datalog

In this section we refer to the finite set of relation and constant symbols τ as EDBs (for extensional database predicates). Let ρ be a finite set of new relation symbols, called the IDBs (for intensional database predicates). A Datalog program is a set of rules of the form

$$\psi_0 := \psi_1, \dots, \psi_n$$

where ψ_0 is an atomic ρ -formula and ψ_1, \ldots, ψ_n are atomic $(\rho \cup \tau)$ -formulas; we also assume that every variable that appears in the head also appears in the body. If $\mathfrak A$ is a τ -structure, and Π is a Datalog program with EDBs τ and IDBs ρ , then a $(\tau \cup \rho)$ -expansion $\mathfrak A'$ of $\mathfrak A$ is called a *fixed point of* Π *on* $\mathfrak A$ if $\mathfrak A'$ satisfies the sentence

$$\forall \bar{x}(\psi_0 \vee \neg \psi_1 \vee \dots \vee \neg \psi_n)$$

for each rule $\psi_0 := \psi_1, \dots, \psi_n$. If \mathfrak{A}_1 and \mathfrak{A}_2 are two $(\rho \cup \tau)$ -structures with the same domain 143 A, then $\mathfrak{A}_1 \cap \mathfrak{A}_2$ denotes the $(\rho \cup \tau)$ -structure with domain A such that $R^{\mathfrak{A}_1 \cap \mathfrak{A}_2} := R^{\mathfrak{A}_1} \cap R^{\mathfrak{A}_2}$. 144 Note that if \mathfrak{A}_1 and \mathfrak{A}_2 are two fixed points of Π on \mathfrak{A} , then $\mathfrak{A}_1 \cap \mathfrak{A}_2$ is a fixed point of Π on 145 \mathfrak{A} , too. Hence, there exists a unique smallest (with respect to inclusion) fixed point of Π on \mathfrak{A} , which we denote by $\Pi(\mathfrak{A})$. It is well-known that if \mathfrak{A} is a finite structure then $\Pi(\mathfrak{A})$ can be computed in polynomial time in the size of \mathfrak{A} [24]. If $R \in \rho$, we also say that Π defines 148 $R^{\Pi(\mathfrak{A})}$ on \mathfrak{A} . A Datalog program together with a distinguished predicate $R \in \rho$ may also be viewed as a formula, which we also call a Datalog query, and which over a given τ -structure 150 \mathfrak{A} denotes the relation $R^{\Pi(\mathfrak{A})}$. If the distinguished predicate has arity 0, we often call it 151 the goal predicate; we say that Π derives goal on \mathfrak{A} if goal $\Pi(\mathfrak{A}) = \{()\}$. The class \mathcal{C} of finite au-structures $\mathfrak A$ such that Π derives goal on $\mathfrak A$ is called the class of finite au-structures defined 153 by Π , and denoted by Π . Note that this class \mathcal{C} is definable in universal second-order logic 154 (we have to express that in every expansion of the input by relations for the IDBs that satisfies all the rules of the Datalog program the goal predicate is non-empty). 156

2.2 Second-Order Logic

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Second-order logic is the extension of first-order logic which additionally allows existential and universal quantification over relations; that is, if R is a relation symbol and ϕ is a second-order $\tau \cup \{R\}$ -formula, then $\exists R : \phi$ and $\forall R : \phi$ are second-order τ -formulas. If $\mathfrak A$ is a τ -structure and Φ is a second-order τ -sentence, we write $\mathfrak A \models \Phi$ (and say that $\mathfrak A$ is a model of Φ) if $\mathfrak A$ satisfies Φ , which is defined in the usual Tarskian style. We write $\llbracket \Phi \rrbracket$ for the class of all finite models of Φ . A second-order formula is called monadic if all second-order variables are unary. We use syntactic sugar and also write $\forall x \in X : \psi$ instead of $\forall x(X(x) \Rightarrow \psi)$ and $\exists x \in X : \psi$ instead of $\exists x(X(x) \land \psi)$.

2.3 Guarded Second-Order Logic

Guarded Second-order Logic (GSO), introduced by Grädel, Hirsch, and Otto [21], is the
extension of guarded first-order logic by second-order quantifiers. Guarded (first-order)
τ-formulas are defined inductively by the following rules [1]:

- 1. all atomic τ -formulas are guarded τ -formulas;
- 2. if ϕ and ψ are guarded τ -formulas, then so are $\phi \wedge \psi$, $\phi \vee \psi$, and $\neg \phi$.
- 3. if $\psi(\bar{x}, \bar{y})$ is a guarded τ -formula and $\alpha(\bar{x}, \bar{y})$ is an atomic τ -formula such that all free variables of ψ occur in α then $\exists \bar{y} \big(\alpha(\bar{x}, \bar{y}) \land \psi(\bar{x}, \bar{y}) \big)$ and $\forall \bar{y} \big(\alpha(\bar{x}, \bar{y}) \Rightarrow \psi(\bar{x}, \bar{y}) \big)$ are guarded τ -formulas.

$$w_{1} \xrightarrow{N} w_{2} \xrightarrow{N} w_{3} \xrightarrow{N} w_{4}$$

$$S \stackrel{\downarrow}{:} R \stackrel{\uparrow}{\mid} R \stackrel{\uparrow}{\mid} T \stackrel{\downarrow}{\mid}$$

$$v_{1} \xrightarrow{N} v_{2} \xrightarrow{N} v_{3} \xrightarrow{N} v_{4}$$

$$w_{1} < w_{2} < w_{3} < w_{4}$$

$$v_{1} < w_{2} < v_{3} < w_{4}$$

$$v_{1} < v_{2} < v_{3} < v_{4}$$

$$P_{a} \qquad P_{a} \qquad P_{a}$$

$$P_{b} \qquad P_{b} \qquad P_{b} \qquad P_{b}$$

$$w_{1} < w_{2} < w_{3} < w_{4}$$

$$v_{1} < v_{2} < v_{3} < v_{4}$$

$$P_{a} \qquad P_{a} \qquad P_{a} \qquad P_{a}$$

$$P_{a} \qquad P_{a} \qquad P_{a}$$

$$(c) \text{ Word } w_{3}$$

Figure 1 An example of an $\{S, T, R, N\}$ -structure \mathfrak{B} in the class \mathcal{C} of Proposition 3.

Guarded second-order formulas are defined similarly, but we additionally allow (unrestricted) second-order quantification; GSO generalises Courcelle's logic MSO₂ from graphs to general relational structures.

▶ **Definition 1.** A second-order τ -formula is called guarded if it is defined inductively by the rules (1)-(3) for guarded first-order logic and additionally by second-order quantification.

There are many semantically equivalent ways of introducing GSO [21]. Let \mathfrak{B} be a τ -structure. Then $(t_1,\ldots,t_n)\in B^n$ is called guarded in \mathfrak{B} if there exists an atomic τ -formula ϕ and b_1,\ldots,b_k such that $\mathfrak{B}\models\phi(b_1,\ldots,b_k)$ and $\{t_1,\ldots,t_n\}\subseteq\{b_1,\ldots,b_k\}$. Note that (for n=1) every element of B is guarded (because of the atomic formula x=x). A relation $R\subseteq B^n$ is called guarded if all tuples in R are guarded. Note that all unary relations are guarded. If Ψ is an arbitrary second-order sentence, we say that a finite structure \mathfrak{A} satisfies Ψ with guarded semantics, in symbols $\mathfrak{A}\models_g \Phi$, if all second-order quantifiers in Ψ are evaluated over guarded relations only. Note that for MSO sentences, the usual semantics and the guarded semantics coincide.

▶ Proposition 2 (see [21]). Guarded Second-order Logic and full Second-order Logic with guarded semantics are equally expressive.

It follows that GSO is at least as expressive as MSO. There are Datalog programs that are equivalent to a GSO sentence, but not to an MSO sentence. The proof is based on a variant of an example of a Datalog query in GSO given in [13] (Example 2).

▶ Proposition 3. There is a Datalog query that can be expressed in GSO but not in MSO.

Proof. Let τ be the signature consisting of the binary relation symbols S, T, R, N, and let \mathcal{C} be the class of finite τ -structures such that the following Datalog program with one binary IDB U derives goal.

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\begin{split} U(x,y) := & S(x,y) \\ U(x',y') := & U(x,y), N(x,x'), N(y,y'), R(x',y') \\ \text{goal} := & U(x,y), T(x,y) \end{split}
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On the left of Figure 1 one can find an example of a $\{S, T, R, N\}$ -structure \mathfrak{B} where the given Datalog program derives goal. To show that \mathcal{C} is not MSO definable, suppose for contradiction that there exists an MSO sentence Φ such that $\llbracket \Phi \rrbracket = \mathcal{C}$. We use Φ to construct an MSO sentence Ψ which holds on a finite word $w \in \{a,b\}^*$ (represented as a structure with signature $P_a, P_b, <$ in the usual way [24]) if and only if $w \in \{a^n b^n \mid n \geq 1\}$; this contradicts the theorem of Büchi-Elgot-Trakhtenbrot (see, e.g., [24]). Let Φ' be the MSO sentence obtained from Φ by replacing all subformulas of Φ of the form

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S(x,y) by a formula $\phi_S(x,y)$ that states that x is the smallest element with respect to 209 <, that $P_b(y)$, and that there is no z < y in P_b ; 210

T(x,y) by a formula $\phi_T(x,y)$ that states that $P_a(x)$, that there is no z>x in P_a , and 211 that y is the largest element with respect to <; 212

R(x,y) by the formula $\phi_R(x,y)$ given by x < y;

N(x,y) by a formula $\phi_N(x,y)$ stating that y is the next element after x with respect to <. 215

The resulting MSO sentence Ψ_1 has the signature $\{P_a, P_b, <\}$; let Ψ be the conjunction of Ψ_1 with the sentence Ψ_2 which states that for all $x, y \in A$, if x < y and $P_a(y)$ then $P_a(x)$. We first show that if \mathfrak{A} is a $\{<, P_a, P_b\}$ -structure that represents a word $w_{\mathfrak{A}} \in \{a, b\}^*$, then $\mathfrak{A} \models \Psi$ if and only if $w_{\mathfrak{A}}$ is of the form a^nb^n for some $n\geq 1$. Let \mathfrak{B} be the $\{S,T,R,N\}$ -structure such that for $X \in \{S, T, R, N\}$ we have $X^{\mathfrak{B}} := \{(x, y) \mid \mathfrak{A} \models \phi_X(x, y)\}$. See Figure 1 for an example of a structure \mathfrak{A} such that $w_{\mathfrak{A}} = a^4 b^4$ and the corresponding $\{S, T, R, N\}$ -structure \mathfrak{B} .

If $w_{\mathfrak{A}}$ is of the form $a^n b^n$ for some $n \geq 1$, then \mathfrak{A} clearly satisfies Ψ_2 . To show that it also satisfies Ψ_1 , let $v_1, \ldots, v_n, w_1, \ldots, w_n \in A$ be such that $\{v_1, \ldots, v_n\} = P_a^{\mathfrak{A}}$ and $\{w_1, \ldots, w_n\} = P_b^{\mathfrak{A}}$ such that for all $i, j \in \{1, \ldots, n\}$, if i < j then $v_i <^{\mathfrak{A}} v_j$ and $w_i <^{\mathfrak{A}} w_j$.

$$(v_1, w_1) \in S^{\mathfrak{B}}, \qquad (v_n, w_n) \in T^{\mathfrak{B}},$$

 $(v_i, w_i) \in R^{\mathfrak{B}} \text{ for all } i \in \{2, \dots, n-1\},$
 $(v_i, v_{i+1}), (w_i, w_{i+1}) \in N^{\mathfrak{B}} \text{ for all } i \in \{1, \dots, n-1\}.$ (1)

It follows that \mathfrak{B} satisfies Φ and therefore $\mathfrak{A} \models \Psi$.

For the converse direction, suppose that $\mathfrak{A} \models \Psi$. Clearly, $w_{\mathfrak{A}} \in a^*b^*$ because $\mathfrak{A} \models \Psi_2$. Moreover, since $\mathfrak{A} \models \Psi_1$ we have that $\mathfrak{B} \models \Phi$, and hence there exist $n \in \mathbb{N}$ and elements $v_1, \ldots, v_n, w_1, \ldots, w_n \in A$ such that \mathfrak{B} satisfies (1). We first prove that $P_a^{\mathfrak{A}} = \{v_1, \ldots, v_n\}$ and $|P_a^{\mathfrak{A}}| = n$. Since $(v_n, w_n) \in T^{\mathfrak{B}}$ we have $\phi_T(v_n, w_n)$ and hence $v_n \in P_a^{\mathfrak{A}}$. Since $\mathfrak{B} \models N(v_1, v_2), \ldots, N(v_{n-1}, v_n)$ we have that $v_1 < v_2 < \cdots < v_{n-1} < v_n$ holds in \mathfrak{A} and it also follows that $|P_a^{\mathfrak{A}}| = n$. Then for every $i \in n$ we have that $v_i \in P_a^{\mathfrak{A}}$ because $v_i \leq v_n, v_n \in P_a^{\mathfrak{A}}$, and $w_{\mathfrak{A}} \in a^*b^*$. Now suppose for contradiction that there exists $x \in P_a^{\mathfrak{A}} \setminus \{v_1, \dots, v_n\}$; choose x largest with respect to $<^{\mathfrak{A}}$. Since $(v_n, w_n) \in T^{\mathfrak{B}}$ and $x \in P_a^{\mathfrak{A}}$ we must have $x \leq v_n$, and hence $x < v_n$ since $x \notin \{v_1, \dots, v_n\}$. Then there exists $y \in A$ such that $\phi_N(x,y)$ holds in \mathfrak{A} . Since $y \leq v_n$, $v_n \in P_a^{\mathfrak{A}}$, and $w_{\mathfrak{A}} \in a^*b^*$, we must have $P_a^{\mathfrak{A}}$. By the maximal choice of x we get that $y = v_i$ for some $i \in \{1, ..., n\}$. But then $\phi_N(x, v_i)$ implies that $x \in \{v_1, \dots, v_{n-1}\}$, a contradiction. Similarly, one can prove that $P_b^{\mathfrak{A}} = \{w_1, \dots, w_n\}$ and that $|P_h^{\mathfrak{A}}| = n$. This implies that $w_{\mathfrak{A}} = a^n b^n$.

We finally have to prove that \mathcal{C} is in GSO. Let Φ be the GSO $\{S, T, R, N\}$ sentence with existentially quantified unary relations V, W, and existentially quantified binary relations $R' \subseteq R$ and $N' \subseteq N$, which states that

there are elements $v_1, v_n \in V$ and $w_1, w_n \in W$ such that $S(v_1, w_1)$ and $T(v_n, w_n)$ hold;

for every $x \in V \setminus \{v_1\}$ there exists a unique element $y \in V \setminus \{v_n\}$ such that N'(y,x)249 250

for every $x \in V \setminus \{v_n\}$ there exists a unique element $y \in V \setminus \{v_1\}$ such that N'(x,y)252

for every $x \in W \setminus \{w_1\}$ there exists a unique element $y \in W \setminus \{w_n\}$ such that N'(y,x)253 254

for every $x \in W \setminus \{w_n\}$ there exists a unique element $y \in W \setminus \{w_1\}$ such that N'(x,y)255 holds; 256

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for all v \in V and w \in W we have that N'(v_1, v) \wedge N'(w_1, w) implies R'(v, w).

for all v, v' \in V \setminus \{v_1, v_n\} and w, w' \in W \setminus \{w_1, w_n\} we have that R'(v, w) \wedge N'(v, v') \wedge N'(w, w') implies R'(v, w).

For all v \in V and v \in W we have that N'(v, v_n) \wedge N'(w, w_n) implies R'(v, w).

Then \Phi holds on a finite \{S, T, R, N\}-structure \mathfrak B if and only if B has elements v_1, \ldots, v_n, w_1, \ldots, w_n satisfying (1), which is the case if and only if \mathfrak B \in \mathcal C.
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Sometimes, we will also use the term GSO (MSO, Datalog) to denote all problems (i.e., all classes of structures) that can be expressed in the formalism. In particular, this justifies to say that a certain CSP is *in* GSO (MSO, Datalog).

3 Homomorphism-Closed GSO

We prove that the class of finite models of a GSO sentence is a finite union of CSPs of ω -categorical structures whenever its complement is closed under homomorphisms. In particular, every CSP in GSO (and therefore every CSP in MSO) is the CSP of an ω -categorical structure. CSPs that can be formulated as the CSP of an ω -categorical structure have been characterised [10]; this characterisation will be recalled in the next section.

3.1 CSPs for Countably Categorical Structures

By the theorem of Ryll-Nardzewski, a countable structure \mathfrak{B} is ω -categorical if and only if for every $n \in \mathbb{N}$ there are finitely many orbits of the componentwise action of the automorphism group of \mathfrak{B} on B^n (see, e.g., [22]). We now present a condition that characterises classes of structures that are CSPs of ω -categorical structures. Let \mathcal{C} be a class of finite τ -structures. Let Λ_n be the class of primitive positive τ -formulas with free variables x_1, \ldots, x_n whose canonical database is in \mathcal{C} . We define $\sim_n^{\mathcal{C}}$ to be the equivalence relation on Λ_n such that $\phi_1 \sim_n^{\mathcal{C}} \phi_2$ holds if for all primitive positive τ -formulas $\psi(x_1, \ldots, x_n)$ we have that $\phi_1(x_1, \ldots, x_n) \wedge \psi(x_1, \ldots, x_n)$ is satisfiable in a structure from \mathcal{C} if and only if $\phi_2(x_1, \ldots, x_n) \wedge \psi(x_1, \ldots, x_n)$ is satisfiable in a structure from \mathcal{C} . The *index* of an equivalence relation is the number of its equivalence classes.

- ▶ **Theorem 4** (Bodirsky, Hils, Martin [10], Theorem 4.27). Let \mathcal{C} be a constraint satisfaction problem. Then there is an ω -categorical structure \mathfrak{B} such that $\mathcal{C} = \mathrm{CSP}(\mathfrak{B})$ iff $\sim_n^{\mathcal{C}}$ has finite index for all n. Moreover, the structure \mathfrak{B} can be chosen so that for all $n \in \mathbb{N}$ the orbits of the componentwise action of the automorphism group of \mathfrak{B} on B^n are primitively positively definable in \mathfrak{B} .
- ▶ **Example 5.** The structure $\mathfrak{B}_1 := (\mathbb{Z}; <)$ is not ω -categorical. However, $\sim_n^{\mathrm{CSP}(\mathfrak{B}_1)}$ has finite index for all n, and indeed $\mathrm{CSP}(\mathbb{Z}; <) = \mathrm{CSP}(\mathbb{Q}; <)$ and $(\mathbb{Q}; <)$ is ω -categorical. On the other hand, for $\mathfrak{B}_2 := (\mathbb{Z}; \mathrm{Succ})$ we have that the index $\sim_2^{\mathrm{CSP}(\mathfrak{B}_2)}$ is infinite, and it follows that there is no ω -categorical structure \mathfrak{B} such that $\mathrm{CSP}(\mathfrak{B}_2) = \mathrm{CSP}(\mathfrak{B})$; see [6].

A rich source of examples of ω -categorical structures are structures with finite relational signature that are *homogeneous*, i.e., every isomorphism between finite substructures can be extended to an automorphism. There are uncountably many countable homogeneous digraphs with pairwise distinct CSP, and it follows that there are homogeneous digraphs with undecidable CSPs. A structure $\mathfrak B$ is called *finitely bounded* if there exists a finite set $\mathcal F$ of finite structures such that a finite structure $\mathfrak A$ embeds into $\mathfrak B$ if and only if no structure in $\mathcal F$ embeds into $\mathfrak A$.

It is well-known that if a structure is ω -categorical, then all of its reducts are ω -categorical as well [22]. Moreover, it is easy to see that the CSP of reducts of finitely bounded structures is in NP. It has been conjectured that the CSP of reducts of finitely bounded homogeneous structures is in P or NP-complete [12]; this conjecture generalises the finite-domain complexity dichotomy that was conjectured by Feder and Vardi [19] and proved by Bulatov [14] and by Zhuk [26].

3.2 Quantifier Rank 305

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In order to construct ω -categorial structures for a given CSP in GSO, we need to verify the condition given in Theorem 4; in this context, it will be convenient to work with signatures that also contain constant symbols. The quantifier rank of a second-order τ -formula Φ is the maximal number of nested (first-order or second-order) quantifiers in Φ ; for this definition, we view Φ as a second-order sentence with guarded semantics, just as in [5]. If $\mathfrak A$ and $\mathfrak B$ are τ -structures and $q \in \mathbb{N}$ we write $\mathfrak{A} \equiv_q^{\mathrm{GSO}} \mathfrak{B}$ if \mathfrak{A} and \mathfrak{B} satisfy the same GSO τ -sentences of quantifier rank at most q.

▶ **Lemma 6** (Proposition 3.3 in [5]). Let $q \in \mathbb{N}$ and τ be a finite signature with relation and constant symbols. Then \equiv_q^{GSO} is an equivalence relation with finite index on the class of all finite τ -structures. Moreover, every class of \equiv_q^{GSO} can be defined by a single GSO sentence with quantifier rank q. The analogous statements hold for MSO as well.

If \mathfrak{A} is a τ -structure and \bar{a} is a k-tuple of elements of A, then we write (\mathfrak{A}, \bar{a}) for a $\tau \cup \{c_1, \ldots, c_k\}$ -structure expanding \mathfrak{A} where c_1, \ldots, c_k denote fresh constant symbols being mapped to the corresponding entries of \bar{a} . If \mathfrak{A} and \mathfrak{B} are τ -structures and $\bar{a} \in A^k$, $\bar{b} \in B^k$, and when writing $(\mathfrak{A}, \bar{a}) \equiv_q^{\text{GSO}} (\mathfrak{B}, \bar{b})$ we implicitly assume that we have chosen the same constant symbols for \bar{a} and for \bar{b} .

▶ **Lemma 7** (Proposition 3.4 in [5]). Let $q \in \mathbb{N}$ and let \mathfrak{A} and \mathfrak{B} be τ -structures. Then 322 $\mathfrak{A} \equiv_{a+1}^{\mathrm{GSO}} \mathfrak{B}$ if and only if the following properties hold: 323

(first-order forth) For every $a \in A$, there exists $b \in B$ such that $(\mathfrak{A}, a) \equiv_q^{\mathrm{GSO}} (\mathfrak{B}, b)$. (first-order back) For every $b \in B$, there exists $a \in A$ such that $(\mathfrak{A}, a) \equiv_q^{\mathrm{GSO}} (\mathfrak{B}, b)$. 324

(second-order forth) For every expansion \mathfrak{A}' of \mathfrak{A} by a guarded relation, there exists an 326 expansion \mathfrak{B}' of \mathfrak{B} by a guarded relation such that $\mathfrak{A}' \equiv_q^{\text{GSO}} \mathfrak{B}'$. 327

(second-order back) For every expansion \mathfrak{B}' of \mathfrak{B} by a guarded relation, there exists an expansion \mathfrak{A}' of \mathfrak{A} by a guarded relation such that $\mathfrak{A}' \equiv_a^{\text{GSO}} \mathfrak{B}'$. 329

In the following, τ denotes a finite relational signature.

▶ **Definition 8.** Let $\rho := \{c_1, \ldots, c_n\}$ be a finite set of constant symbols. Then \mathcal{D}_n is defined 331 to be the set of all pairs $(\mathfrak{A},\mathfrak{B})$ of finite $(\tau \cup \rho)$ -structures such that

 $c^{\mathfrak{A}} = c^{\mathfrak{B}}$ for all constant symbols $c \in \rho$; 333

We write $\mathfrak{A} \oplus \mathfrak{B}$ for the structure with domain $A \cup B$ such that $R^{\mathfrak{A} \oplus \mathfrak{B}} := R^{\mathfrak{A}} \cup R^{\mathfrak{B}}$ for each 335 relation symbol $R \in \tau$ and $c^{\mathfrak{A} \uplus \mathfrak{B}} = c^{\mathfrak{A}} = c^{\mathfrak{B}}$ for each constant symbol $c \in \rho$. 336

The following theorem in the special case of n = 0 is Proposition 4.1 in [5].

▶ Theorem 9. Let $q, n, r, s \in \mathbb{N}$, let $(\mathfrak{A}_1, \mathfrak{B}_1), (\mathfrak{A}_2, \mathfrak{B}_2) \in \mathcal{D}_n$, and let $\bar{a}_1 \in (A_1)^r$, $\bar{a}_2 \in (A_2)^r$, $\bar{b}_1 \in (B_1)^s, \ \bar{b}_2 \in (B_2)^s \ be \ such \ that \ (\mathfrak{A}_1, \bar{a}_1) \equiv_q^{\rm GSO} (\mathfrak{A}_2, \bar{a}_2) \ and \ (\mathfrak{B}_1, \bar{b}_1) \equiv_q^{\rm GSO} (\mathfrak{B}_2, \bar{b}_2).$ Then

$$(\mathfrak{A}_1 \uplus \mathfrak{B}_1, \bar{a}_1, \bar{b}_1) \equiv_q^{\text{GSO}} (\mathfrak{A}_2 \uplus \mathfrak{B}_2, \bar{a}_2, \bar{b}_2).$$

 Proof. Our proof is by induction on q. Every quantifier-free formula is a Boolean combination of atomic formulas, so for q=0 it suffices to consider atomic formulas ϕ . By symmetry, it suffices to show that if $(\mathfrak{A}_1 \uplus \mathfrak{B}_1, \bar{a}_1, \bar{b}_1) \models \phi$ then $(\mathfrak{A}_2 \uplus \mathfrak{B}_2, \bar{a}_2, \bar{b}_2) \models \phi$. Then ϕ is built using a relation symbol $R \in \tau$, and the tuple that witnesses the truth of ϕ in $\mathfrak{A}_1 \uplus \mathfrak{B}_1$ must be from $R^{\mathfrak{A}_1}$ or from $R^{\mathfrak{B}_1}$, by the definition of $\mathfrak{A}_1 \uplus \mathfrak{B}_1$. We first consider the former case; the latter case can be treated similarly. If a constant that appears in ϕ is from $A_1 \cap B_1$, then by the definition of \mathcal{D}_n this element is denoted by a constant symbol $c \in \rho$, and therefore we may assume without loss of generality that ϕ is a formula over the signature of $(\mathfrak{A}_1, \bar{a}_1)$. Hence, $(\mathfrak{A}_1, \bar{a}_1) \models \phi$ and by assumption $(\mathfrak{A}_2, \bar{a}_2) \models \phi$. This in turn implies that $(\mathfrak{A}_2 \uplus \mathfrak{B}_2, \bar{a}_2, \bar{b}_2) \models \phi$. For the inductive step, suppose that the claim holds for q, and that $(\mathfrak{A}_1, \bar{a}_1) \equiv_{q+1}^{\text{GSO}} (\mathfrak{A}_2, \bar{a}_2)$ and $(\mathfrak{B}_1, \bar{b}_1) \equiv_{q+1}^{\text{GSO}} (\mathfrak{B}_2, \bar{b}_2)$. By symmetry and Lemma 7 it suffices to verify the properties (first-order forth) and (second-order forth). Let $c_1 \in A_1 \cup B_1$. We may assume that $c_1 \in A_1$; the case that $c_1 \in B_1$ can be shown similarly. By Lemma 7, there exists $c_2 \in A_2$ such that $(\mathfrak{A}_1, \bar{a}_1, c_1) \equiv_{q}^{\text{GSO}} (\mathfrak{A}_2, \bar{a}_2, c_2)$. By the inductive assumption, this implies that

$$(\mathfrak{A}_1 \uplus \mathfrak{B}_1, \bar{a}_1, c_1, \bar{b}_1) \equiv_q^{\mathrm{GSO}} (\mathfrak{A}_2 \uplus \mathfrak{B}_2, \bar{a}_2, c_2, \bar{b}_2)$$

and concludes the proof of (first-order forth).

Now let R be a guarded relation of $\mathfrak{A}_1 \uplus \mathfrak{B}_1$ of arity k. Let \mathfrak{A}'_1 be the expansion of \mathfrak{A}_1 by the guarded relation $R \cap A_1^k$, and \mathfrak{B}'_1 be the expansion of \mathfrak{B}_1 by the guarded relation $R \cap B_1^k$. By Lemma 7 there are expansions \mathfrak{A}'_2 of \mathfrak{A} and \mathfrak{B}'_2 of \mathfrak{B}_2 by guarded relations such that $(\mathfrak{A}'_1, \bar{a}_1) \equiv_q^{\text{GSO}} (\mathfrak{A}'_2, \bar{a}_2)$ and $(\mathfrak{B}'_1, \bar{b}_1) \equiv_q^{\text{GSO}} (\mathfrak{B}'_2, \bar{b}_2)$. By the inductive assumption, this implies that $(\mathfrak{A}'_1 \uplus \mathfrak{B}'_1, \bar{a}_1, \bar{b}_1) \equiv_q^{\text{GSO}} (\mathfrak{A}'_2 \uplus \mathfrak{B}'_2, \bar{a}_2, \bar{b}_2)$, which completes the proof of (second-order forth).

▶ Corollary 10. Let C be a CSP that can be expressed in GSO. Then there exists a countable ω -categorical structure \mathfrak{B} such that $C = \mathrm{CSP}(\mathfrak{B})$.

Proof. Let τ be the signature of \mathcal{C} , and let Φ be a GSO τ -formula with quantifierrank q such that $\mathcal{C} = \llbracket \Phi \rrbracket$. By Theorem 4 it suffices to show that the equivalence relation $\sim_n^{\mathcal{C}}$ has finite index for every $n \in \mathbb{N}$. Let $\rho \coloneqq \{c_1, \ldots, c_n\}$ be a set of new constant symbols. By Lemma 6, there exists an $m \in \mathbb{N}$ such that \equiv_q^{GSO} has m equivalence classes on $(\tau \cup \rho)$ -structures. If $\phi(x_1, \ldots, x_n)$ is a primitive positive τ -formula, then define \mathfrak{S}_{ϕ} to be the $(\tau \cup \rho)$ -structure whose elements are the equivalence classes of the smallest equivalence relation on the variables of ϕ that contains all pairs x, y such that ϕ contains the conjunct x = y, and such that $(C_1, \ldots, C_n) \in R^{\mathfrak{S}}$ for $R \in \tau$ if and only if there are $y_1 \in C_1, \ldots, y_n \in C_2$ such that $R(y_1, \ldots, y_n)$ is a conjunct of ϕ ; finally, we set $c_i^{\mathfrak{S}_{\phi}} \coloneqq [x_i]$ for all $i \in \{1, \ldots, n\}$.

We claim that if $\mathfrak{S}_{\phi} \equiv_{q}^{\mathrm{GSO}} \mathfrak{S}_{\psi}$, then $\phi \sim_{n}^{\mathcal{C}} \psi$. Let $\theta(x_{1}, \ldots, x_{n})$ be a primitive positive τ -formula; we may assume that the existentially quantified variables of θ are disjoint from the existentially quantified variables of ϕ and of ψ , so that $(\mathfrak{S}_{\phi}, \mathfrak{S}_{\theta}), (\mathfrak{S}_{\psi}, \mathfrak{S}_{\theta}) \in \mathcal{D}_{n}$. Since $\mathfrak{S}_{\phi} \equiv_{q}^{\mathrm{GSO}} \mathfrak{S}_{\psi}$ and $\mathfrak{S}_{\theta} \equiv_{q}^{\mathrm{GSO}} \mathfrak{S}_{\theta}$, we have $\mathfrak{S}_{\phi} \uplus \mathfrak{S}_{\theta} \equiv_{q}^{\mathrm{GSO}} \mathfrak{S}_{\psi} \uplus \mathfrak{S}_{\theta}$ by Theorem 9. Now suppose that $\phi \wedge \theta$ is satisfiable in a model of Φ . This is the case if and only if $\mathfrak{S}_{\phi} \uplus \mathfrak{S}_{\theta}$ satisfies Φ , which in turn implies that $\mathfrak{S}_{\psi} \uplus \mathfrak{S}_{\theta}$ satisfies Φ since Φ has quantifierrank q. This in turn is the case if and only if $\psi \wedge \theta$ is satisfiable in a model of Φ , which proves the claim.

The claim implies that $\sim_n^{\mathcal{C}}$ has at most m equivalence classes, concluding the proof.

Example 11. Let Φ be the following MSO sentence.

$$\forall X (\exists x : X(x) \Rightarrow \exists x, y \in X \ \forall z \in X (\neg E(x, z) \lor \neg E(y, z)))$$

It is easy to see that $\llbracket \Phi \rrbracket$ is closed under disjoint unions and that its complement is closed under homomorphisms. Corollary 10 implies that there exists a countable ω -categorical structure with $CSP(\mathfrak{B}) = \llbracket \Phi \rrbracket$.

3.3 Finite Unions of CSPs

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In this section we prove that every class in GSO whose complement is closed under homomorphisms is a finite union of CSPs (Lemma 16); the statement announced at the beginning of Section 3 then follows (Corollary 17). Throughout this section, let \mathcal{C} be a non-empty class of finite τ -structures whose complement is closed under homomorphisms. In particular, \mathcal{C} contains the structure \mathfrak{I} with only one element where all relations are empty.

Let \sim be the equivalence relation defined on \mathcal{C} by letting $\mathfrak{A} \sim \mathfrak{B}$ if for every $\mathfrak{C} \in \mathcal{C}$ we have $\mathfrak{A} \uplus \mathfrak{C} \in \mathcal{C}$ if and only if $\mathfrak{B} \uplus \mathfrak{C} \in \mathcal{C}$; here \uplus denotes the usual disjoint union of structures, which is a special case of Definition 8 for n=0. Note that the equivalence classes of \sim are in one-to-one correspondence to the equivalence classes of $\sim_0^{\mathcal{C}}$. Also note that \mathcal{C} is closed under disjoint unions if and only if \sim has only one equivalence class.

If $\mathfrak{A} \in \mathcal{C}$, then we write $[\mathfrak{A}]$ for the equivalence class of \mathfrak{A} with respect to \sim . The following observations are immediate consequences from the definitions:

- 1. each \sim -equivalence class is closed under homomorphic equivalence.
- 2. each \sim -equivalence class is closed under disjoint unions.
- 394 3. $\mathfrak{A} \in [\mathfrak{I}]$ if and only if $\mathfrak{A} \uplus \mathfrak{B} \in \mathcal{C}$ for all $\mathfrak{B} \in \mathcal{C}$.
- Lemma 12. Let $\mathfrak{A} \in \mathcal{C}$ and let \mathcal{D} be the smallest subclass of \mathcal{C} that contains $[\mathfrak{A}]$ and whose complement is closed under homomorphisms. Then
- 397 1. \mathcal{D} is a union of equivalence classes of \sim , and
 - **2.** if \sim has more than one equivalence class, then $\mathcal{C} \setminus \mathcal{D}$ is non-empty.

Proof. Let $\mathfrak{C} \in [\mathfrak{A}]$, let \mathfrak{B} be a finite structure with a homomorphism to \mathfrak{C} , and let $\mathfrak{B}' \in [\mathfrak{B}]$.

Since $\mathfrak{B} \uplus \mathfrak{C}$ and \mathfrak{C} are homomorphically equivalent, we have that $\mathfrak{B} \uplus \mathfrak{C} \sim \mathfrak{C}$. We claim that $\mathfrak{B}' \uplus \mathfrak{C} \sim \mathfrak{C}$. To see this, let $\mathfrak{D} \in \mathcal{C}$. Then

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\begin{array}{lll} \text{402} & \mathfrak{C} \uplus \mathfrak{D} \in \mathcal{C} \Leftrightarrow (\mathfrak{B} \uplus \mathfrak{C}) \uplus \mathfrak{D} \in \mathcal{C} & \text{(since } \mathfrak{B} \uplus \mathfrak{C} \sim \mathfrak{C}) \\ \text{403} & \Leftrightarrow \mathfrak{B} \uplus (\mathfrak{C} \uplus \mathfrak{D}) \in \mathcal{C} \\ \text{404} & \Leftrightarrow \mathfrak{B}' \uplus (\mathfrak{C} \uplus \mathfrak{D}) \in \mathcal{C} & \text{(since } \mathfrak{B} \sim \mathfrak{B}') \\ & \Leftrightarrow (\mathfrak{B}' \uplus \mathfrak{C}) \uplus \mathfrak{D} \in \mathcal{C} \end{array}
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which shows the claim. So $\mathfrak{B}' \uplus \mathfrak{C} \in [\mathfrak{C}] = [\mathfrak{A}]$. Since \mathfrak{B}' has a homomorphism to $\mathfrak{B}' \uplus \mathfrak{C}$ we obtain that $\mathfrak{B}' \in \mathcal{D}$; this proves the first statement.

To prove the second statement, first observe that the statement is clear if $\mathfrak{A} \in [\mathfrak{I}]$, since the complement of $[\mathfrak{I}]$ is closed under homomorphisms. The statement therefore follows from the assumption that \sim has more than one equivalence class. Otherwise, if $\mathfrak{A} \notin [\mathfrak{I}]$, then there exists a structure $\mathfrak{B} \in \mathcal{C}$ such that $\mathfrak{A} \uplus \mathfrak{B} \notin \mathcal{C}$. Then $\mathfrak{B} \in \mathcal{C} \setminus \mathcal{D}$ can be shown indirectly as follows: otherwise \mathfrak{B} would have a homomorphism to a structure $\mathfrak{A}' \in [\mathfrak{A}]$. Since $\mathfrak{B} \uplus \mathfrak{A}'$ is homomorphically equivalent to \mathfrak{A}' , we have $\mathfrak{B} \uplus \mathfrak{A}' \sim \mathfrak{A}' \sim \mathfrak{A}$ and in particular $\mathfrak{B} \uplus \mathfrak{A}' \in \mathcal{C}$. But $\mathfrak{B} \uplus \mathfrak{A}' \in \mathcal{C}$ if and only if $\mathfrak{B} \uplus \mathfrak{A} \in \mathcal{C}$ since $\mathfrak{A} \sim \mathfrak{A}'$. This is in contradiction to our assumption on \mathfrak{B} .

▶ **Example 13.** We consider a signature $\tau := \{R_1, R_2, R_3\}$ of unary relation symbols. Define for every $i \in \{1, 2, 3\}$ the τ -structure \mathfrak{S}_i to be a one-element structure where R_i is non-empty

and R_i , for $i \neq i$, is empty. Let

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$$\mathcal{C} \coloneqq \mathrm{CSP}(\mathfrak{S}_1 \uplus \mathfrak{S}_2) \cup \mathrm{CSP}(\mathfrak{S}_2 \uplus \mathfrak{S}_3) \cup \mathrm{CSP}(\mathfrak{S}_3 \uplus \mathfrak{S}_1).$$

Clearly, the complement of \mathcal{C} is closed under homomorphisms. The equivalence classes of \sim can be described as follows. For distinct $i, j \in \{1, 2, 3\}$,

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[\mathfrak{S}_{i} \uplus \mathfrak{S}_{j}] = \operatorname{CSP}(\mathfrak{S}_{i} \uplus \mathfrak{S}_{j}) \setminus (\operatorname{CSP}(\mathfrak{S}_{i}) \cup \operatorname{CSP}(\mathfrak{S}_{j}))
[\mathfrak{S}_{i}] = \operatorname{CSP}(\mathfrak{S}_{i}) \setminus [\mathfrak{I}]
[\mathfrak{I}] = \operatorname{CSP}(\mathfrak{I}).
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For the remainder of the section we fix a GSO τ -sentence Φ of quantifier rank q. Recall that Lemma 6 asserts that the equivalence relation \equiv_q^{GSO} on the class of finite τ -structures has finitely many equivalence classes $\mathcal{C}_1, \ldots, \mathcal{C}_m$, and that each of the equivalence classes \mathcal{C}_i can be defined by a single GSO τ -sentence Ψ_i with quantifier rank q; we write $T_q^{\tau} \coloneqq \{\Psi_1, \ldots, \Psi_m\}$ for this set of GSO sentences. Let $J \subseteq \{1, \ldots, m\}$ be such that $\{\Psi_j \in T_q^{\tau} \mid j \in J\}$ is exactly the set of all sentences in T_q^{τ} that imply Φ . Then |J| is called the degree of Φ . It is easy to see that the degree of Φ is exactly the index of \equiv_q^{GSO} restricted to $\llbracket \Phi \rrbracket$. Let \sim be the equivalence relation defined in the beginning of this section for the class $\mathcal{C} \coloneqq \llbracket \Phi \rrbracket$.

▶ **Lemma 14.** For every \sim -class \mathcal{D} there exists $I \subseteq \{1, ..., m\}$ such that $\mathcal{D} = \bigcup_{i \in I} \llbracket \Psi_i \rrbracket$.

Proof. As in the proof of Corollary 10 one can use Theorem 9 to show for all finite τ -structures $\mathfrak{A},\mathfrak{B}$ that if $\mathfrak{A} \equiv_q^{\mathrm{GSO}} \mathfrak{B}$, then $\mathfrak{A} \sim \mathfrak{B}$. This means that \mathcal{D} is a union of \equiv_q^{GSO} -classes and therefore there exists $I \subseteq J \subseteq \{1,\ldots,m\}$ such that $\mathcal{D} = \bigcup_{i \in I} \llbracket \Psi_i \rrbracket$.

▶ Corollary 15. The index of \sim is smaller than or equal to the degree of Φ .

▶ **Lemma 16.** If the complement of $\llbracket \Phi \rrbracket$ is closed under homomorphisms, then there are GSO τ -sentences Φ_1, \ldots, Φ_t each of which describes a CSP such that Φ is equivalent to $\Phi_1 \vee \cdots \vee \Phi_t$. If Φ is an MSO sentence, then Φ_1, \ldots, Φ_t can be be chosen to be MSO sentences as well.

Proof. We prove the statement by induction on the degree n of Φ . By Lemma 15 the equivalence relation \sim has at most n equivalence classes on τ -structures. Hence, if n=1, then $\llbracket \Phi \rrbracket$ is closed under disjoint unions, and we are done.

Let $\mathfrak{A}_1,\ldots,\mathfrak{A}_s$ be τ -structures such that $\{[\mathfrak{A}_1],\ldots,[\mathfrak{A}_s]\}$ is the set of all equivalence classes of \sim that are distinct from $[\mathfrak{I}]$. Let \mathcal{D}_i be the smallest subclass of $[\![\Phi]\!]$ that contains $[\mathfrak{A}_i]$ and whose complement is closed under homomorphisms. Note that $[\![\Phi]\!] = \bigcup_{i \leq s} \mathcal{D}_i$ since $[\![\mathfrak{I}]\!]$ is contained in \mathcal{D}_i for all $i \leq s$. By Lemma 12 (1), each \mathcal{D}_i is a union of \sim -classes which are themselves a union of \equiv_q^{GSO} -classes by Lemma 14. It follows that there exists $I_i \subseteq \{1,\ldots,m\}$ such that $\mathcal{D}_i = \bigcup_{j \in I_i} [\![\Psi_j]\!]$. We define $\Phi_i := \bigvee_{j \in I_i} \Psi_j$. Note that the GSO sentence Φ_i is of quantifier rank q such that $\mathcal{D}_i = [\![\Phi_i]\!]$. Hence, Φ is equivalent to $\bigvee_{i \leq s} \Phi_i$. Lemma 12 (2) asserts that $[\![\Phi]\!] \setminus \mathcal{D}_i$ is non-empty, and hence the degree of Φ_i must be strictly smaller than n for all $i \in \{1,\ldots,s\}$. The statement now follows from the inductive assumption. The same argument applies to MSO as well.

Lemma 16 together with Corollary 10 implies the following.

▶ Corollary 17. Every GSO sentence which is closed under homomorphisms is equivalent to a finite conjunction of GSO sentences each of which describes the complement of a CSP of a countable ω -categorical structure. The analogous statement holds for MSO.

Not every homomorphism-closed class of structures that can be expressed in Second-order Logic is a finite intersection of complements of CSPs. We even have an example of a class of finite τ -structures that can be expressed in Datalog but cannot be written in this form.

Example 18. Let S and T be unary, and let R be a binary relation symbol. Let C be the class of all finite $\{S, T, R\}$ -structures $\mathfrak A$ such that the following Datalog program Π with the binary IDB E derives goal on $\mathfrak A$.

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\begin{array}{ll} {}_{463} & E(x,y):=S(x),S(y) \\ {}_{464} & E(x,y):=E(x',y'),R(x',x),R(y',y) \\ {}_{465} & \text{goal}:=T(x),E(x,x'),R(x',y) \end{array}
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For $n \in \mathbb{N}$, let \mathfrak{P}_n be the $\{S, T, R\}$ -structure on the domain $\{1, \ldots, n\}$ with

$$S^{\mathfrak{P}_n} \coloneqq \{1\} \qquad \qquad T^{\mathfrak{P}_n} \coloneqq \{n\} \qquad \qquad R^{\mathfrak{P}_n} \coloneqq \{(i,i+1) \mid i \in \{1,\ldots,n-1\}\}.$$

It is easy to see that each of the structures in $\{\mathfrak{P}_n \mid n \geq 1\}$ is not contained in \mathcal{C} , and that the disjoint union of \mathfrak{P}_i and \mathfrak{P}_j , for $i \neq j$, is contained in \mathcal{C} . It follows that \mathcal{C} is not a finite intersection of complements of CSPs (and, by Corollary 17, cannot be expressed in GSO).

4 Canonical Datalog Programs

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A remarkable fact about the expressive power of Datalog for constraint satisfaction problems over finite domains is the existence of *canonical Datalog programs* [19]; this has been generalised to CSPs for ω-categorical structures.

Theorem 19 (Bodirsky and Dalmau [7]). Let \mathfrak{B} be a countable ω -categorical τ -structure.

Then for all $\ell, k \in \mathbb{N}$ there exists a canonical Datalog program Π of width (ℓ, k) for the complement of $CSP(\mathfrak{B})$. Moreover, for every finite τ -structure \mathfrak{A} the following are equivalent: Π derives goal on \mathfrak{A} ;

 $\qquad \qquad \textit{Spoiler has a winning strategy for the existential (ℓ,k)-pebble game on $(\mathfrak{A},\mathfrak{B})$.}$

We later need the following well-known fact.

Lemma 20. If C_1 and C_2 are in Datalog, then so are $C_1 \cup C_2$ and $C_1 \cap C_2$. If Π_1 and Π_2 are Datalog programs of width (ℓ, k) , then there is a Datalog program Π of width (ℓ, k) for $\Pi_1 \cup \Pi_2$ and for $\Pi_1 \cap \Pi_2$.

Proof. For union, let Π be obtained by taking the union of the rules of Π_1 and of Π_2 , possibly after renaming IDB predicate names to make them disjoint except for goal. For intersection, we proceed similarly, but we first rename the symbol goal in Π_1 to goal₁ and the symbol goal in Π_2 to goal₂. Finally we add the new rule goal: - goal₁, goal₂ to the union of Π_1 and Π_2 .

It is clear that these constructions preserve the width.

▶ **Theorem 21.** Let Φ be a GSO sentence such that $\llbracket \Phi \rrbracket$ is closed under homomorphisms. Let $\ell, k \in \mathbb{N}$. Then there exists a canonical Datalog program Π of width (ℓ, k) for $\llbracket \Phi \rrbracket$.

Proof. By Corollary 17 there are GSO sentences Φ_1, \ldots, Φ_m and ω -categorical structures $\mathfrak{B}_1, \ldots, \mathfrak{B}_m$ such that Φ is equivalent to $\Phi_1 \wedge \cdots \wedge \Phi_m$ and $\llbracket \neg \Phi_i \rrbracket = \operatorname{CSP}(\mathfrak{B}_i)$. Let Π_i be the canonical Datalog program for $\operatorname{CSP}(\mathfrak{B}_i)$ which exists by Theorem 19. Then Lemma 20 implies that there exists a Datalog program Π such that $\llbracket \Pi \rrbracket = \llbracket \Pi_1 \rrbracket \cap \cdots \cap \llbracket \Pi_m \rrbracket$. It is clear that Π is sound for $\llbracket \Phi \rrbracket$. To see that Π is a canonical Datalog program for $\llbracket \Phi \rrbracket$, suppose

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that \mathfrak{A} is such that some Datalog program Π' of width (ℓ, k) which is sound for $\llbracket \Phi \rrbracket$ derives goal on \mathfrak{A} . Since, for every $i \in \{1, \ldots, m\}$, the program Π' is also sound for $\llbracket \Phi_i \rrbracket$, and Π_i is a canonical Datalog program for $\llbracket \Phi_i \rrbracket$, the program Π_i derives goal on \mathfrak{A} . Hence, $\mathfrak{A} \in \llbracket \Pi \rrbracket = \llbracket \Pi_1 \rrbracket \cap \cdots \cap \llbracket \Pi_m \rrbracket$.

Theorem 22. Let Φ be a GSO sentence. Then $\llbracket \Phi \rrbracket$ can be defined in Datalog if and only if 1. $\llbracket \Phi \rrbracket$ is closed under homomorphisms, and

2. there exist $\ell, k \in \mathbb{N}$ such that for all finite structures \mathfrak{A} , Spoiler wins the (ℓ, k) -game for $\llbracket \Phi \rrbracket$ on \mathfrak{A} if and only if $\mathfrak{A} \models \Phi$.

Proof. First suppose that $\llbracket \Phi \rrbracket$ is in Datalog. That is, there exists $\ell, k \in \mathbb{N}$ and a Datalog 506 program Π of width (ℓ, k) such that $\llbracket \Phi \rrbracket = \llbracket \Pi \rrbracket$. Then clearly $\llbracket \Phi \rrbracket$ is closed under homomor-507 phisms, and by Lemma 16, there are GSO sentences Φ_1, \ldots, Φ_m such that Φ is equivalent 508 to $\Phi_1 \wedge \cdots \wedge \Phi_m$ and $\llbracket \Phi_i \rrbracket$ is the complement of a CSP, for each $i \in \{1, \ldots, m\}$. Corollary 10 implies that there exists an ω -categorical structure \mathfrak{B}_i such that $CSP(\mathfrak{B}_i) = \llbracket \neg \Phi_i \rrbracket$. 510 Now suppose that $\mathfrak A$ is a finite τ -structure such that $\mathfrak A \models \Phi$. Then Spoiler wins the (ℓ,k) -game as follows. Suppose that Duplicator plays the countable structure $\mathfrak B$ such that 512 $CSP(\mathfrak{B}) \cap \llbracket \Phi \rrbracket = \emptyset$. Then $CSP(\mathfrak{B}) \cap \llbracket \Phi_i \rrbracket = \emptyset$ for some $i \in \{1, \ldots, m\}$; otherwise, if there 513 is a structure $\mathfrak{A}_i \in \mathrm{CSP}(\mathfrak{B}) \cap \llbracket \Phi_i \rrbracket$ for every $i \in \{1,\ldots,m\}$, then the disjoint union of $\mathfrak{A}_1,\ldots,\mathfrak{A}_m$ satisfies Φ_i since Φ_i is closed under homomorphisms, and is in CSP(\mathfrak{B}) since 515 $CSP(\mathfrak{B})$ is closed under disjoint unions; but this is in contradiction to our assumption that 516 $CSP(\mathfrak{B}) \cap \llbracket \Phi \rrbracket = \emptyset$. Hence, $CSP(\mathfrak{B}) \subseteq CSP(\mathfrak{B}_i)$ and hence there is a homomorphism h from \mathfrak{B} to \mathfrak{B}_i (see [7]). Note that Π is sound for $\mathrm{CSP}(\mathfrak{B}_i)$, and Π derives goal on \mathfrak{A} , and hence 518 Theorem 19 implies that Spoiler wins the existential (ℓ, k) -pebble game on $(\mathfrak{A}, \mathfrak{B}_i)$. But since \mathfrak{B} homomorphically maps to \mathfrak{B}_i , this implies that Spoiler wins the existential (ℓ, k) -pebble 520 game on $(\mathfrak{A},\mathfrak{B}_i)$. Now suppose that $\mathfrak{A} \models \neg \Phi$. Hence, there exists $i \in \{1,\ldots,m\}$ such that 521 $\mathfrak{A} \models \neg \Phi_i$. Then Duplicator wins the (ℓ, k) -game as follows. She starts by playing \mathfrak{B}_i . Then \mathfrak{A} homomorphically maps to \mathfrak{B}_i , and Duplicator can win the existential (ℓ, k) pebble game 523 on $(\mathfrak{A},\mathfrak{B}_i)$ by always playing along the homomorphism. 524

For the converse implication, suppose that 1. and 2. hold. Since $\llbracket \Phi \rrbracket$ is closed under homomorphisms, Corollary 17 implies that there are GSO sentences Φ_1, \ldots, Φ_m and ω -categorical structures $\mathfrak{B}_1, \ldots, \mathfrak{B}_m$ such that Φ is equivalent to $\Phi_1 \wedge \cdots \wedge \Phi_m$ and $\llbracket \neg \Phi_i \rrbracket = \operatorname{CSP}(\mathfrak{B}_i)$. By Theorem 19, for every $i \in \{1, \ldots, m\}$ there exists a canonical Datalog program Π_i of width (ℓ, k) for $\llbracket \Phi_i \rrbracket$. Then Lemma 20 implies that there exists a Datalog program Π such that $\llbracket \Pi \rrbracket = \llbracket \Pi_1 \rrbracket \cap \cdots \cap \llbracket \Pi_m \rrbracket$. Since each Π_i is sound for $\llbracket \Phi_i \rrbracket$, it follows that Π is sound for $\llbracket \Phi \rrbracket$. Hence, it suffices to show that if \mathfrak{A} is a finite τ -structure such that $\mathfrak{A} \models \Phi$, then Π derives goal on \mathfrak{A} . Since $\mathfrak{A} \models \Phi_i$ for all $i \in \{1, \ldots, m\}$, the assumption implies that Spoiler wins the existential (ℓ, k) pebble game on $(\mathfrak{A}, \mathfrak{B}_i)$. By Theorem 19, it follows that Π_i derives goal on \mathfrak{A} . Hence, Π derives goal on \mathfrak{A} .

5 A coNP-complete CSP in MSO

The class \mathcal{C} of all finite loopless digraphs that do not embed any of the digraphs from \mathcal{T} is an amalgamation class, and hence there exists a homogenous structure \mathfrak{H} with age \mathcal{C} . It has been shown in [9] that $\mathrm{CSP}(\mathfrak{H})$ is coNP-complete.

▶ Proposition 23. $CSP(\mathfrak{H})$ can be expressed in MSO.

Proof. We have to find an MSO sentence that holds on a given digraph (V; E) if and only if (V; E) does not embed any of the tournaments from \mathcal{T} . We specify an MSO $\{X, E\}$ -sentence Φ , for a unary relation symbol X, that is true on a finite $\{X, E\}$ -structure \mathfrak{S} if and only if $(X^{\mathfrak{S}}; E^{\mathfrak{S}})$ is isomorphic to \mathfrak{T}_n , for some $n \geq 2$. In ϕ we existentially quantify over

two vertices $s, t \in X$ (that stand for the vertex 0 and the vertex n+1 in \mathfrak{T}_n).

a partition of $X \setminus \{s\}$ into two sets A and B (they stand for the set of even and the set of odd numbers in $\{1, \ldots, n+1\}$).

The formula Φ has the following conjuncts:

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- 1. a first-order formula that states that E defines a tournament on X;
- 2. a first-order formula that expresses that E is a linear order on A with maximal element a;
- 3. a first-order formula that expresses that E is a linear order on B with maximal element b;
- **4.** E(s,t), E(s,a), E(a,b), and E(x,s) for all $x \in X \setminus \{a,t\}$;
 - **5.** a first-order formula that states that if there is an edge from an element $x \in A$ to an element $y \in B$ then there is precisely one element $z \in A$ such that $(y, z), (z, x) \in E$, unless y = t;
 - **6.** a first-order formula that states that if there is an edge from an element $x \in B$ to an element $y \in A$ then there is precisely one element $z \in B$ such that $(y, z), (z, x) \in E$, unless y = t.

We claim that the MSO sentence $\forall x \colon \neg E(x,x) \land \forall X \colon \neg \Phi$ holds on a finite digraph if and only if the digraph is loopless and does not embed \mathfrak{T}_n , for all $n \geq 3$. The forwards implication easily follows from the observation that if (X;T) is isomorphic to \mathfrak{T}_n , for some $n \geq 2$, then ϕ holds; this is straightforward from the construction of Φ (and the explanations above given in brackets). Conversely, suppose that Φ holds. Then (X;T) is a tournament. We construct an isomorphism f from (X;T) to $\mathfrak{T}_{|X|-1}$ as follows. Define $f(s) \coloneqq 0$, $f(a) \coloneqq 1$, and f(b) = 2. Since E(a,b), by item 5 there exists exactly one $a' \in A$ such that E(b,a') and E(a',a). Define $f(a') \coloneqq 3$. If a' = t then we have found an isomorphism with \mathfrak{T}_2 . Otherwise, the partial map f defined so far is an embedding into \mathfrak{T}_n for some $n \geq 3$. Item 6 and E(b,a') imply that there exists exactly one $b' \in B$ such that E(a',b') and E(b',b), and we define $f(b') \coloneqq 4$. Continuing in this manner, we eventually define f on all of f and find an isomorphism with $\mathfrak{T}_{|X|-1}$.

This shows that $CSP(\mathfrak{H})$ cannot be expressed, unless NP = coNP, as $CSP(\mathfrak{B})$ for some reduct of a finitely bounded structure and such CSPs are in NP. We do not know how to show this statement without complexity-theoretic assumptions, even if we just want to rule out that $CSP(\mathfrak{H})$ can be expressed as $CSP(\mathfrak{B})$ for some reduct of a finitely bounded *homogeneous* structure.

6 Conclusion and Open Problems

We provided a game-theoretic characterisation of those problems in Guarded Second-order Logic that are equivalent to a Datalog program. We also proved the existence of canonical Datalog programs for GSO sentences whose models are closed under homomorphisms. To prove these results, we showed that every class of finite τ -structures in GSO whose complement is closed under homomorphisms is a finite union of CSPs. We also showed that every CSP in

GSO can be formulated as a CSP of an ω -categorical structure. These results also imply that the so-called universal-algebraic approach, which has eventually led to the classification of finite-domain CSPs in Datalog [3], can be applied to study problems that are simultaneously in Datalog and in GSO (also see [11]). Our results might also pave the way towards a syntactic characterisation of Datalog \cap GSO. We close with two open problems.

- 1. Nested monadically defined queries (Nemodeq) have been introduced by Rudolph and Krötzsch [25]; they prove that Nemodeq is contained both in MSO and in Datalog. We ask wether conversely, every problem in MSO ∩ Datalog is expressible as a Nemodeq.
- 2. Is every CSP of a reduct of a finitely bounded homogeneous structure in GSO?

We are also confident that our results will advance the understanding of CSPs (the complements of) which are obtained as the homomorphism-closure of the set of some theory's finite models. For example, the homomorphism-closures of the model sets of guarded- and guarded-negation-theories have recently been found to be GSO-expressible [8] so, by virtue of our results, we immediately know they must be (complements of) ω -categorical CSPs.

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