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 \( \Pi \) of width \( (\ell, k) \) in the sense of Feder and Vardi. 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 \( \omega \)-categorical structures. The intersection of MSO and Datalog is known to contain the class of nested monadically defined queries (Nemodeq); likewise, we show that the intersection of GSO and Datalog contains all problems that can be expressed by the more expressive language of nested guarded queries (GQ\( ^+ \)). Yet, by exploiting our results, we can show that neither of the two query languages can serve as a characterization, as we exhibit a query in the intersection of MSO and Datalog that is not expressible in GQ\( ^+ \).

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1 Introduction

Monadic Second-order Logic (MSO) is a logic of great importance in theoretical computer science. While it significantly exceeds the expressive capabilities of First-order Logic (allowing for expressing crucial structural properties like reachability or connectedness), it is still computationally reasonably well-behaved: By Büchi’s theorem (see, e.g., [38]), the formal languages definable in MSO are precisely the regular ones; by Courcelle’s theorem [24], MSO sentences can be evaluated in polynomial time on classes of structures whose treewidth is bounded by a constant. The latter result even holds for the more expressive logic of Guarded Second-order Logic (GSO) [33, 28], which extends First-order Logic by second-order quantifiers over guarded relations.

Another fundamental formalism in theoretical computer science, which is particularly heavily studied in database theory and logic-based knowledge representation, is Datalog (see, e.g., [26, 38]). Every fixed Datalog program can be evaluated on given finite structures in polynomial time. If a linear order is present and if the available relations are closed under complement, Datalog can even express all polytime-computable queries [1]. That is, like MSO, Datalog strikes a good balance between expressivity and good mathematical and computational properties.

Neither of the two formalisms subsumes the other in terms of what can be expressed. Yet, in various scenarios, we are interested in simultaneously having the good computational properties of expressibility in Datalog and having the good computational properties of expressibility in MSO or GSO. A wide variety of popular query formalisms (among them (unions of) conjunctive queries, (2-way conjunctive) regular path queries, monadic Datalog, the recently introduced almost monadic Datalog [43], guarded Datalog, monadically defined queries, or nested monadically defined queries) are known to be both in Datalog and GSO [42]. Query languages expressible both in Datalog and MSO have been shown to warrant decidable query entailment over logical theories exhibiting universal models of finite treewidth and cliquewidth [32, 31]. Also, all these formalisms have favourable properties when it comes to static analysis, most notably decidable query containment [42]. Note that on the contrary, query containment in unrestricted Datalog is undecidable, as is query containment in unrestricted MSO / GSO. The same holds for query entailment under logical theories, even if the latter are extremely simple. So it is really the interplay of the restrictions imposed by both formalisms that is required to ensure decidability of central tasks in databases and
knowledge representation. This makes the semantic intersection of Datalog and MSO / GSO so interesting and worthwhile investigating.

In this article, we investigate two questions that turn out to be closely related:
1. Which classes of finite structures are expressible both in MSO/GSO and in Datalog?
2. Which constraint satisfaction problems (CSPs) can be expressed in MSO/GSO?
Indeed, as our investigation reveals, the versatile and vibrant discipline of constraint satisfaction problems offers many suitable notions and tools for our endeavour to understand “MSO/GSO ∩ Datalog”. While this might come as a surprise at the first glance, interesting correspondences connecting CSPs with expressivity characterizations of logical formalisms from database theory and knowledge representation have been observed before [5, 30].

We recall that, for a structure $\mathfrak{B}$ with a finite relational signature $\tau$, the constraint satisfaction problem for $\mathfrak{B}$ is the class of all finite $\tau$-structures that homomorphically map to $\mathfrak{B}$. It is well known that, whenever $\mathfrak{B}$ is finite, its constraint satisfaction problem can already be expressed in a small fragment of MSO, called monotone monadic SNP (MMSNP, [29]). Yet, this correspondence does not hold for infinite $\mathfrak{B}$.

Example 1. The constraint satisfaction problem for the structure $(\mathbb{Q}; <)$, which is the class of all finite acyclic digraphs $(V; E)$, cannot be expressed in MMSNP [8]. It can, however, be expressed in MSO by the sentence
$$\forall X \neq \emptyset \exists x \in X \forall y \in X : \neg E(x, y).$$
To see this, note that if $(V; E)$ is a digraph such that there exists a non-empty $X \subseteq V$ such that for every $x \in X$ there is $y \in Z$ with $E(x, y)$, then $X$ contains a directed cycle, and hence has no homomorphism to $(\mathbb{Q}; <)$. Conversely, if $(V; E)$ is a finite digraph and contains no directed cycle, then every non-empty subset of $V$ must contain a sink, i.e., a vertex $x$ with no outgoing $E$-edges, and hence satisfies the given sentence.

The class of CSPs of arbitrary infinite structures $\mathfrak{B}$ is quite large; it is easy to see that, given any finite relational signature $\tau$, a class $\mathcal{D}$ of finite $\tau$-structures is a CSP of some countably infinite structure if and only if
- it is closed under disjoint unions, and
- it contains any $\mathfrak{A}$ that maps homomorphically to some $\mathfrak{A}' \in \mathcal{D}$.

The second condition, which is sometimes also referred to as closure under inverse homomorphisms, can be equivalently rephrased by requiring that the complement\(^1\) of $\mathcal{D}$ is closed under homomorphisms, where a class $\mathcal{C}$ is closed under homomorphisms if for any structure $\mathfrak{A} \in \mathcal{C}$ that maps homomorphically to some $\mathfrak{C} \in \mathcal{C}$ 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 $\tau$-structures is definable in Datalog\(^2\) if there exists a Datalog program $\Pi$ with a distinguished nullary predicate $\text{goal}$ such that $\Pi$ derives $\text{goal}$ on a finite $\tau$-structure if and only if the structure is in $\mathcal{C}$; in this case, we may denote $\mathcal{C}$ by $[\Pi]$. Every class of $\tau$-structures in Datalog is closed under homomorphisms, but the converse does not hold: there are classes of finite structures in Datalog not corresponding to the complement of any CSP.

\(^1\) Whenever in this paper we refer to the complement of some class $\mathcal{D}$ of finite $\tau$-structures, we mean the class of all finite $\tau$-structures not contained in $\mathcal{D}$ – we will make $\tau$ explicit or it will be clear from the context.

\(^2\) Warning: Feder and Vardi [29] say that a CSP is in Datalog if its complement in the class of all finite $\tau$-structures is in Datalog.
Example 2. Consider, for unary predicates $R$ and $B$, the class $C_{R,B}$ of finite $\{R, B\}$-structures $\mathfrak{A}$ such that $R^\mathfrak{A}$ is empty or $B^\mathfrak{A}$ is empty. Clearly, $C_{R,B}$ is not closed under disjoint unions, so it cannot correspond to the CSP of any structure. Yet, it is easy to see that a finite structure is in $C_{R,B}$ if and only if the Datalog program consisting of just the one rule

$$\text{goal} := R(x), B(y)$$

does not derive $\text{goal}$ on that structure.

A noteworthy subclass of all CSPs are the CSPs of structures $\mathcal{B}$ that are countably infinite and $\omega$-categorical. A structure $\mathfrak{B}$ is $\omega$-categorical if all countable models of $\mathfrak{B}$’s first-order theory are isomorphic to $\mathfrak{B}$. A well-known example of an $\omega$-categorical structure is $(\mathbb{Q}; <)$, a result going back to Cantor [20]. Constraint satisfaction problems of $\omega$-categorical structures can be evaluated in polynomial time on any class of structures whose treewidth is bounded by some constant $k \in \mathbb{N}$, by a result of Bodirsky and Dalmau [12], using Datalog programs.

Two important parameters of a Datalog program $\Pi$ are the maximal arity $\ell$ of its auxiliary predicates (IDBs), and the maximal number $k$ of variables per rule in $\Pi$ – we then say that $\Pi$ has width $(\ell, k)$, following the terminology of Feder and Vardi [29]. The special case of $\ell = 1$ is typically referred to as monadic Datalog. The parameters $\ell$ and $k$ are important in theory, but they also bear some practical relevance: When evaluating $\Pi$ on a given structure $\mathfrak{A}$ with domain $A$, the memory needed is bounded by $O(|A|^\ell)$ and the number of computation steps by $O(|A|^k)$. The polynomial-time algorithm for instances of an $\omega$-categorical CSP of treewidth at most $k$ presented by Bodirsky and Dalmau is in fact a Datalog program of width $(k - 1, k)$. A Datalog program $\Pi$ is called sound for a class of $\tau$-structures $\mathcal{C}$ if $[\Pi] \subseteq \mathcal{C}$. Bodirsky and Dalmau showed that if $\mathcal{C}$ is the complement of the CSP of an $\omega$-categorical $\tau$-structure $\mathcal{B}$ then there exists, for any $\ell, k \in \mathbb{N}$, a Datalog program $\Pi$ of width $(\ell, k)$ such that

1. $\Pi$ is sound for $\mathcal{C}$, and
2. $[\Pi'] \subseteq [\Pi]$ for every Datalog program $\Pi'$ of width $(\ell, k)$ which is sound for $\mathcal{C}$.

This $\Pi$ (which is unique up to immaterial syntactic variations) is then referred to as the canonical Datalog program of width $(\ell, k)$ for $\mathcal{C}$.

Interestingly and conveniently, there is a game-theoretic characterisation capturing whether the canonical Datalog program of width $(\ell, k)$ for $\mathcal{C}$ derives $\text{goal}$ on a given $\tau$-structure $\mathfrak{A}$ [12]. This characterisation is based on the existential pebble game from finite model theory, which is played on a pair $(\mathfrak{A}, \mathcal{B})$ of structures. In more detail, the existential $(\ell, k)$-pebble game is played by two players, called Spoiler and Duplicator (see, e.g., [25, 29, 35]). Spoiler starts by placing $k$ pebbles on elements $a_1, \ldots, a_k$ of $\mathfrak{A}$, and Duplicator responds by placing $k$ pebbles $b_1, \ldots, b_k$ on $\mathcal{B}$. If the map that sends $a_1, \ldots, a_k$ to $b_1, \ldots, b_k$ is not a partial homomorphism from $\mathfrak{A}$ to $\mathcal{B}$, then the game is over and Spoiler wins. Otherwise, Spoiler removes all but at most $\ell$ pebbles from $\mathfrak{A}$, and Duplicator has to respond by removing the corresponding pebbles from $\mathcal{B}$. Then Spoiler can again place all his pebbles on $\mathfrak{A}$, and Duplicator must again respond by placing her pebbles on $\mathcal{B}$. If the game continues forever, then Duplicator wins. If $\mathcal{B}$ is a finite, or more generally a countable $\omega$-categorical structure then Spoiler has a winning strategy for the existential $(\ell, k)$-pebble game on $(\mathfrak{A}, \mathcal{B})$ if and only if the canonical Datalog program for CSP($\mathcal{B}$) derives $\text{goal}$ on $\mathfrak{A}$ (Theorem 24). This connection played an essential role in proving Datalog inexpressibility results, for example for the class of finite-domain CSPs [3] (leading to a complete classification of those finite structures $\mathcal{B}$ such that the complement of CSP($\mathcal{B}$) can be expressed in Datalog [4]).
Results and Consequences

In this article, we present a characterisation of those GSO sentences \( \Phi \) 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 \((\ell, k)\)-game. This game is defined for a homomorphism-closed class \( C \) of finite \( \tau \)-structures, and it is played by the two players Spoiler and Duplicator on a finite \( \tau \)-structure \( \mathfrak{A} \) as follows.

- Duplicator picks a countable \( \tau \)-structure \( \mathfrak{B} \) such that \( \text{CSP}(\mathfrak{B}) \cap C = \emptyset \).
- The game then continues as the existential \((\ell, k)\)-pebble game played by Spoiler and Duplicator on \((\mathfrak{A}, \mathfrak{B})\), as described above.

In Section 4 we show that a GSO sentence \( \Phi \) is over finite structures equivalent to a Datalog program of width \((\ell, k)\) if and only if \( J^\Phi \subseteq K \) is closed under homomorphisms, and Spoiler wins the existential \((\ell, k)\)-game for \( J^\Phi \) on \( \mathfrak{A} \) if and only if \( \mathfrak{A} \models \Phi \).

We also show that for every GSO sentence \( \Phi \) whose class of finite models \( C \) is closed under homomorphisms and for all \( \ell, k \in \mathbb{N} \) there exists a canonical Datalog program \( \Pi \) of width \((\ell, k)\) for \( C \) (Theorem 30). 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 CSPs that can also be expressed in GSO (Lemma 20; an analogous statement holds for MSO). Moreover, every CSP in GSO is the CSP of a countable \( \omega \)-categorical structure (Corollary 14); this allows us to use results from [12] to make the link to existential pebble games. We highlight that this result elegantly generalises known results:

- our result generalises the fact that every CSP in FO is the CSP of a countable \( \omega \)-categorical structure, which can be seen from combining Rossman’s theorem [41] with a generalisation of the theorem of Cherlin, Shelah, and Shi [23] from graphs to general relational structures.
- Our result also generalises the fact that every CSP in the logic MMSNP (for monotone monadic strict NP [29]) is the CSP of a countable \( \omega \)-categorical structure [12].

Note that our results imply that every class of finite structures that can be expressed both in GSO and in Datalog is an intersection of \textit{finitely many} complemented CSPs of \( \omega \)-categorical structures. In contrast, it is \textit{not} generally true that a Datalog program describes a finite intersection of complements of CSPs (we present a counterexample in Example 22). We also present an example of a CSP which is expressible in MSO and coNP-complete, and hence not the CSP of a reduct of a finitely bounded homogeneous structure, unless NP=coNP (Proposition 31).

Our final results concern the most expressive syntactically defined formalism known from the literature that is contained in both Datalog and MSO, namely \textit{nested monadically defined queries} [42], and the most expressive syntactically defined formalism known from the literature that is contained in both Datalog and GSO, namely \textit{nested guarded queries} [18].

We prove that there are problems in the intersection of Datalog and GSO that cannot be expressed as a nested guarded query. To prove this result, we introduce a modified version of the existential pebble game, which we call the \textit{nested guarded pebble game}, and which captures precisely the expressiveness of nested guarded queries (Theorem 51). We also present an example of a problem which lies in the intersection of Datalog and MSO that cannot be expressed by nested monadically defined queries (and not even by nested guarded queries; Corollary 64).

Some of the results of this article until Section 5 have been announced in a conference paper with the title “Datalog-Expressibility for Monadic and Guarded Second-Order Logic”
in the proceedings of ICALP’21 [16]; the results in Section 6 about nested monadic and nested guarded queries were not yet present in the conference version.

2 Preliminaries

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

A primitive positive $\tau$-formula (in database theory also referred to as conjunctive query) is a first-order $\tau$-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 $\psi_1, \ldots, \psi_m$ are atomic $\tau$-formulas, i.e., formulas built from relation symbols in $\tau$ or equality. An existential positive $\tau$-formula is a first-order $\tau$-formula without negation and universal quantification. We write $\psi(x_1, \ldots, x_n)$ if the free variables of $\psi$ are from $x_1, \ldots, x_n$. If $\mathfrak{A}$ is a $\tau$-structure and $\psi(x_1, \ldots, x_n)$ is a $\tau$-formula, then the relation

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

is called the relation defined by $\psi$ over $\mathfrak{A}$; if $\psi$ 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 $\tau$ 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) $\tau$-structures $\mathfrak{A}$ and all $a_1, \ldots, a_n \in A$ we have

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

It is easy to see that every existential positive $\tau$-formula is a disjunction of primitive positive $\tau$-formulas (and hence referred to as a union of conjunctive queries in database theory). If $\Phi$ is a primitive positive $\tau$-formula without equality for a relational signature $\tau$, then the canonical database is the $\tau$-structure $\mathfrak{A}$ whose domain consists of all the variables of $\Phi$, and where $R^\mathfrak{A}$, for $R \in \tau$ of arity $k$, consists of all tuples $(x_1, \ldots, x_k)$ such that $\Phi$ contains the conjunct $R(x_1, \ldots, x_k)$.

Formulas without free variables are called sentences; in database theory, formulas are often called queries and sentences are often called Boolean queries. If $\Phi$ is a sentence, we write $[\Phi]$ for the class of all finite models of $\Phi$.

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 consider a finite set $\tau$ of constant and relation symbols, the latter being referred to as EDBs (for extensional database predicates). Let $\rho$ 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

$$\psi_0 := \psi_1, \ldots, \psi_n$$
where ψ0 is an atomic ρ-formula and ψ1, . . . , ψn are atomic (ρ ∪ τ)-formulas; we also assume that all rules are safe, i.e., that every variable that appears in the head also appears in the body. If A is a τ-structure, and Π is a Datalog program with EDBs from τ and IDBs ρ, then a (τ ∪ ρ)-expansion A′ of A is called a fixed point of Π on A if A′ satisfies the sentence

\[ \forall x (\psi_0 \lor \psi_1 \lor \ldots \lor \psi_n) \]

for each rule ψ0 := ψ1, . . . , ψn. If A1 and A2 are two (ρ ∪ τ)-structures with the same domain A, then A1 ∩ A2 denotes the (ρ ∪ τ)-structure with domain A such that

- \[ R^{A_1 \cap A_2} := R^{A_1} \cap R^{A_2}, \]
- \[ c^{A_1 \cap A_2} = c^{A_1} \cap c^{A_2}. \]

Note that if A1 and A2 are two fixed points of Π on A, then A1 ∩ A2 is a fixed point of Π on A, too. Hence, there exists a unique smallest (with respect to inclusion) fixed point of Π on A, which we denote by Π(A).

Remark 3. There is an equivalent ‘operational’ definition of the semantics of Datalog, and in particular of Π(A); roughly speaking, we compute RΠ(A) for R ∈ ρ ‘bottom up’, starting from the empty relation, and adding tuples that must be contained in all fixed points, until we reach a (the) smallest fixed point (for details see, e.g., Libkin’s book [38, Section 10.5]; an explicit treatment of the equivalence can e.g. be found in [8, Theorem 8.1.6]). From this equivalent description of Π(A) it is apparent that if A is a finite structure then Π(A) can be computed in polynomial time in the size of A.

If R ∈ ρ, we also say that Π defines RΠ(A) on A. A Datalog program together with a distinguished predicate R ∈ ρ may also be viewed as a formula, which we also call a Datalog query, and which over a given τ-structure A denotes the relation RΠ(A). If the distinguished predicate has arity 0, we often call it the goal predicate; we say that Π derives goal on A if goalΠ(A) = \{ \} . The class C of finite τ-structures A such that Π derives goal on A is called the class of finite τ-structures defined by Π, and denoted by \[[Π]\]. Note that this class C is definable in universal second-order logic (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).

2.2 Second-Order Logic

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 τ ∪ {R}-formula, then 3R.ϕ and ∀R.ϕ are second-order τ-formulas. If A is a τ-structure and Φ is a second-order τ-sentence, we write A ⊨ Φ (and say that A is a model of Φ) if A satisfies Φ, which is defined in the usual Tarskian style. We write [Φ] 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 ∀x ∈ X: ψ instead of ∀x(X(x) ⇒ ψ) and ∃x ∈ X: ψ instead of ∃x(X(x) ∧ ψ).

Monadic second-order logic (MSO) is surprisingly powerful for expressing CSPs, which we illustrate with the following example.

Example 4. Let E := \{(x, x) | x ∈ \mathbb{N}\} be the binary equality relation on \mathbb{N} and let D := \{(x, y) ∈ \mathbb{N}^2 | x \neq y\} be the binary disequality relation on \mathbb{N}. The problem CSP(\mathbb{N}; E, D) is expressible in MSO. To see this, let ϕX, for a unary relation symbol X, be the following \{E, D, X\}-sentence.

\[ \exists x. X(x) \land \forall x, y (X(x) \land E(x, y) \Rightarrow X(y)) \land (X(x) \land E(y, x) \Rightarrow X(y)) \]
For IDBs $X$ and $Y$ we write $Y \subseteq X$ as a shortcut for
\[
\forall x(Y(x) \Rightarrow X(x)) \land \exists x(X(x) \land \neg Y(x)).
\]

Let $\psi_X$ be the sentence that states that $X$ is a smallest set which satisfies $\phi_X$:
\[
\phi_X \land \forall Y(Y \subseteq X \Rightarrow \neg \phi_Y).
\]

Note that if $\mathfrak{A}$ is a $(E, D)$-structure and $X \subseteq A$ satisfies $\psi_X$, then any homomorphism from $\mathfrak{A}$ to $\mathfrak{B}$ must be constant on $X$. Also note that if $X, Y \subseteq A$ satisfy $\psi_X$ and $\psi_Y$ and $X \cap Y \neq \emptyset$, then $Z := X \cap Y$ satisfies $\psi_Z$. Hence, for every element $a \in A$ there exists a unique smallest set $X = X_a$ that satisfies $\psi_X$ and contains $a$.

We claim that the CSP above can be expressed by
\[
\forall X(\psi_X \Rightarrow \forall x, y(D(x, y) \Rightarrow (\neg X(x) \lor \neg X(y)))).
\]

Indeed, suppose that $\mathfrak{A}$ is an $(E, D)$-structure and let $X \subseteq A$ be smallest with the property that it satisfies $\phi_X$. If there are $x, y \in X$ such that $(x, y) \in D^\mathfrak{A}$ then clearly there is no homomorphism from $\mathfrak{A}$ to $(\N; E, D)$. On the other hand, if $\mathfrak{A}$ satisfies (1), then any map $h: A \rightarrow \N$ such that $h^{-1}(h(n)) = X_a$ for all $x \in A$ is a homomorphism from $\mathfrak{A}$ to $(\N; E, D)$. Clearly, there exists such a map $h$, which proves the claim.

### 2.3 Guarded Second-Order Logic

Guarded Second-order Logic (GSO), introduced by Grädel, Hirsch, and Otto [33], is the extension of guarded first-order logic by second-order quantifiers. Guarded (first-order) $\tau$-formulas are defined inductively by the following rules [2]:

1. all atomic $\tau$-formulas are guarded $\tau$-formulas;
2. if $\phi$ and $\psi$ are guarded $\tau$-formulas, then so are $\phi \land \psi$, $\phi \lor \psi$, and $\neg \phi$.
3. if $\psi(\vec{x}, \vec{y})$ is a guarded $\tau$-formula and $\alpha(\vec{x}, \vec{y})$ is an atomic $\tau$-formula such that all free variables of $\psi$ occur in $\alpha$ then $\exists \vec{y} (\alpha(\vec{x}, \vec{y}) \land \psi(\vec{x}, \vec{y}))$ and $\forall \vec{y} (\alpha(\vec{x}, \vec{y}) \Rightarrow \psi(\vec{x}, \vec{y}))$ are guarded $\tau$-formulas.

Guarded second-order formulas are defined similarly, but we additionally allow (unrestricted) second-order quantification; GSO generalises Courcelle’s logic MSO$_2$ from graphs to general relational structures.

**Definition 5.** A second-order $\tau$-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 [33]. Let $\mathfrak{B}$ be a $\tau$-structure. Then $(t_1, \ldots, t_n) \in B^n$ is called guarded in $\mathfrak{B}$ if there exists an atomic $\tau$-formula $\phi$ 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 $\Psi$ is an arbitrary second-order sentence, we say that a structure $\mathfrak{B}$ satisfies $\Psi$ with guarded semantics, in symbols $\mathfrak{B} \models_{g} \Psi$, if all second-order quantifiers in $\Psi$ are evaluated over guarded relations only. Note that for MSO sentences, the usual semantics and the guarded semantics coincide.

**Proposition 6** (see Proposition 3.9 in [33]). 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 many Datalog programs that are equivalent to a GSO sentence, but not to an MSO sentence. However, since MSO is surprisingly expressive (see Example 4) it can be quite challenging to prove that a specific problem is inexpressible in MSO. E.g., it is an open problem whether CSP(Q; B) is expressible in MSO, where

\[ B = \{(x, y, z) \in \mathbb{Q}^3 \mid x < y < z \lor z < y < x\} \]

is the so-called betweenness relation [24]. The proof of the following proposition is based on a variant of an example of a Datalog query in GSO given in [18] (Example 2).

**Proposition 7.** There is a Datalog query that can be expressed in GSO but not in MSO.

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

\[
U(x, y) :- S(x, y) \\
U(x', y') :- U(x, y), N(x, x'), N(y, y'), R(x', y')
\]

\[
goal :- U(x, y), T(x, y)
\]

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 \textit{goal}. To show that \( \mathcal{C} \) is not MSO definable, suppose for contradiction that there exists an MSO sentence \( \Phi \) such that \( \models \Phi = \mathcal{C} \). We use \( \Phi \) to construct an MSO sentence \( \Phi' \) which holds on a finite word \( w \in \{a, b\}^* \) (represented as a structure with signature \( P_a, P_b, < \)) 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., [38]). Let \( \Phi' \) be the MSO sentence obtained from \( \Phi \) by replacing all subformulas of \( \Phi \) of the form

1. \( S(x, y) \) by a formula \( \phi_S(x, y) \) that states that \( x \) is the smallest element with respect to \( < \), that \( P_b(y) \), and that there is no \( z < y \) in \( P_b \);
2. \( T(x, y) \) by a formula \( \phi_T(x, y) \) that states that \( P_a(x) \), that there is no \( z > x \) in \( P_a \), and that \( y \) is the largest element with respect to \( < \);
3. \( R(x, y) \) by the formula \( \phi_R(x, y) \) given by \( x < y \);
4. \( N(x, y) \) by a formula \( \phi_N(x, y) \) stating that \( y \) is the next element after \( x \) w.r.t. \( < \).

The resulting MSO sentence \( \Psi_1 \) has the signature \( \{P_a, P_b, <\} \); let \( \Psi \) be the conjunction of \( \Psi_1 \) with the sentence \( \Psi_2 \) which states that for all \( x, y \in A \), if \( x < y \) and \( P_a(y) \) then \( P_a(x) \).

**Claim.** 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 \( a^n b^n \) 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 $\Psi_2$. To show that it also satisfies $\Psi_1$, let $v_1, \ldots, v_n, w_1, \ldots, w_n \in A$ be such that $\{v_1, \ldots, v_n\} = P^a_A$ and $\{w_1, \ldots, w_n\} = P^a_B$ such that for all $i, j \in \{1, \ldots, n\}$, if $i < j$ then $v_i \prec^a v_j$ and $w_i \prec^a w_j$. Then

$$
(v_1, w_1) \in S^a_B, \quad (v_n, w_n) \in T^a_B,
(v_i, w_i) \in R^a_B \text{ for all } i \in \{2, \ldots, n-1\},
(v_i, v_{i+1}), (w_i, w_{i+1}) \in N^a_B \text{ for all } i \in \{1, \ldots, n-1\}.
$$

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

For the converse direction, suppose that $\mathfrak{A} \models \Psi$. Clearly, $w_\mathfrak{A} \models a^*b^*$ because $\mathfrak{A} \models \Psi_2$. Moreover, since $\mathfrak{A} \models \Phi$, 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 (2). We first prove that $P^a_A = \{v_1, \ldots, v_n\}$ and $|P^a_A| = n$. Since $(v_n, w_n) \in T^a_B$ we have $\phi_T(v_n, w_n)$ and hence $v_n \in P^a_A$. 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 $|P^a_A| = n$. Then for every $i \in n$ we have that $v_i \in P^a_A$ because $v_i \leq v_n$, $v_n \in P^a_A$, and $w_\mathfrak{A} \models a^*b^*$. Now suppose for contradiction that there exists $x \in P^a_A \setminus \{v_1, \ldots, v_n\}$; choose $x$ largest with respect to $<_A$. Since $(v_n, w_n) \in T^a_B$ and $x \in P^a_A$ we must have $x \leq v_n$, and hence $x < v_n$ since $x \notin \{v_1, \ldots, v_n\}$. Then there exists $y \in A$ such that $\phi_N(x, y)$ holds in $\mathfrak{A}$. Since $y \leq v_n$, $v_n \in P^a_A$, and $w_\mathfrak{A} \models a^*b^*$, we must have $P^a_A$. By the maximal choice of $x$ we get that $y = v_i$ for some $i \in \{1, \ldots, n\}$. But then $\phi_N(x, v_i)$ implies that $x \in \{v_1, \ldots, v_{n-1}\}$, a contradiction. Similarly, one can prove that $P^a_B = \{w_1, \ldots, w_n\}$ and that $|P^a_B| = n$. This implies that $w_\mathfrak{A} \models a^*b^*$.

We finally have to prove that $C$ is in GSO. Let $\Phi$ 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

1. 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;
2. for every $x \in V \setminus \{v_1\}$ there is a unique element $y \in V \setminus \{v_n\}$ such that $N'(y, x)$ holds;
3. for every $x \in V \setminus \{v_n\}$ there is a unique element $y \in V \setminus \{v_1\}$ such that $N'(x, y)$ holds;
4. for every $x \in W \setminus \{w_1\}$ there is a unique element $y \in W \setminus \{w_n\}$ such that $N'(x, y)$ holds;
5. for every $x \in W \setminus \{w_n\}$ there is a unique element $y \in W \setminus \{w_1\}$ such that $N'(x, y)$ holds;
6. for all $v \in V$ and $w \in W$ we have that $N'(v, w) \wedge N'(v, w_n)$ implies $R'(v, w)$;
7. 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 $w \in W$ 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 (2), which is the case if and only if $\mathfrak{B} \in \mathfrak{C}$.

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 (the complement of) a certain CSP is \emph{in} GSO (MSO, Datalog).

## 3 Homomorphism-Closed GSO

In this section, we prove that the class of finite models of a GSO sentence is a finite union of CSPs of $\omega$-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 $\omega$-categorical structure. CSPs that can be formulated as the CSP of an $\omega$-categorical structure have been characterised [15]; this characterisation will be recalled next.
3.1 CSPs for Countably Categorical Structures

By the theorem of Ryll-Nardzewski, a countable structure $\mathcal{B}$ is $\omega$-categorical if and only if for every $n \in \mathbb{N}$ there are finitely many orbits of the componentwise action of the automorphism group $\text{Aut}(\mathcal{B})$ of $\mathcal{B}$ on $B^n$ (see, e.g., [34]). There is a known condition that characterises classes of structures that are CSPs of $\omega$-categorical structures. Let $\tau$ be a relational signature and let $C$ be a class of finite $\tau$-structures. Let $\Lambda_n$ be the class of primitive positive $\tau$-formulas with free variables $x_1, \ldots, x_n$ whose canonical database is in $C$. We define $\sim_n^C$ to be the equivalence relation on $\Lambda_n$ such that $\phi_1 \sim_n^C \phi_2$ holds if for all primitive positive $\tau$-formulas $\psi(x_1, \ldots, x_n)$ we have that $\phi_1(x_1, \ldots, x_n) \land \psi(x_1, \ldots, x_n)$ is satisfiable in a structure from $C$ if and only if $\phi_2(x_1, \ldots, x_n) \land \psi(x_1, \ldots, x_n)$ is satisfiable in a structure from $C$. The index of an equivalence relation is the number of its equivalence classes. If $\sim$ is an equivalence relation on a set $A$, and $a \in A$, then $[a]_\sim$ denotes the equivalence class of $\sim$; if the reference to $\sim$ is clear, we omit $\sim$ in this notation.

- **Theorem 8** (Bodirsky, Hils, Martin [15], Theorem 4.27). Let $\mathcal{C}$ be a constraint satisfaction problem. Then there is an $\omega$-categorical structure $\mathcal{B}$ such that $\mathcal{C} = \text{CSP}(\mathcal{B})$ iff $\sim_n^\text{CSP}(\mathcal{B})$ has finite index for all $n$. Moreover, the structure $\mathcal{B}$ can be chosen so that for all $n \in \mathbb{N}$ the orbits of the componentwise action of $\text{Aut}(\mathcal{B})$ on $B^n$ are positively definable in $\mathcal{B}$.

- **Example 9.** The structure $\mathcal{B}_1 := (\mathbb{Z}; <)$ is not $\omega$-categorical. However, $\sim_n^{\text{CSP}(\mathcal{B}_1)}$ has finite index for all $n$, and indeed $\text{CSP}(\mathbb{Z}; <) = \text{CSP}(\mathbb{Q}; <)$ and $(\mathbb{Q}; <)$ is $\omega$-categorical. On the other hand, for $\mathcal{B}_2 := (\mathbb{Z}; \text{Succ})$ we have that the index $\sim_2^{\text{CSP}(\mathcal{B}_2)}$ is infinite, and it follows that there is no $\omega$-categorical structure $\mathcal{B}$ such that $\text{CSP}(\mathcal{B}_2) = \text{CSP}(\mathcal{B})$; see [8].

A rich source of examples of $\omega$-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. The age of a structure $\mathcal{B}$ is the class of all finite structures that embed into $\mathcal{B}$. A structure $\mathcal{B}$ is called finitely bounded if there exists a finite set $\mathcal{F}$ of finite structures such that a finite structure $\mathcal{A}$ belongs to the age of $\mathcal{B}$ if and only if no structure in $\mathcal{F}$ embeds into $\mathcal{A}$.

It is well-known that if a structure is $\omega$-categorical, then all of its reducts are $\omega$-categorical as well [34]. 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 [17]. This conjecture generalises the finite-domain complexity dichotomy that was conjectured by Feder and Vardi [29] and proved by Bulatov [19] and by Zhuk [45]. However, the generalisation of this result to finitely bounded homogeneous structures is wide open [40].

3.2 Quantifier Rank

In order to construct $\omega$-categorical structures for a given CSP in GSO, we need to verify the condition given in Theorem 8. In this context, it will be convenient to work with signatures that also contain constant symbols. The quantifier rank of a second-order $\tau$-formula $\Phi$ is the maximal number of nested (first-order or second-order) quantifiers in $\Phi$; for this definition,
we view $\Phi$ as a second-order sentence with guarded semantics, just as in [6]. If $\mathfrak{A}$ and $\mathfrak{B}$ are $\tau$-structures and $q \in \mathbb{N}$ we write $\mathfrak{A} \equiv^q_{\text{GSO}} \mathfrak{B}$ if $\mathfrak{A}$ and $\mathfrak{B}$ satisfy the same GSO $\tau$-sentences of quantifier rank at most $q$.

**Lemma 10** (Proposition 3.3 in [6]). Let $q \in \mathbb{N}$ and $\tau$ be a finite signature with relation and constant symbols. Then $\equiv^q_{\text{GSO}}$ is an equivalence relation with finite index on the class of all finite $\tau$-structures. Moreover, every class of $\equiv^q_{\text{GSO}}$ 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 $\tau$-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 $\tau$-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 11** (Proposition 3.4 in [6]). Let $q \in \mathbb{N}$ and let $\mathfrak{A}$ and $\mathfrak{B}$ be $\tau$-structures. Then $\mathfrak{A} \equiv^{q+1}_{\text{GSO}} \mathfrak{B}$ if and only if the following properties hold:

1. (first-order forth) For every $a \in A$, there exists $b \in B$ such that $(\mathfrak{A}, a) \equiv^{\text{GSO}} (\mathfrak{B}, b)$.
2. (first-order back) For every $b \in B$, there exists $a \in A$ such that $(\mathfrak{A}, a) \equiv^{\text{GSO}} (\mathfrak{B}, b)$.
3. (second-order forth) For every expansion $\mathfrak{A}'$ of $\mathfrak{A}$ by a guarded relation, there exists an expansion $\mathfrak{B}'$ of $\mathfrak{B}$ by a guarded relation such that $\mathfrak{A}' \equiv^q_{\text{GSO}} \mathfrak{B}'$.
4. (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 $\mathfrak{A}' \equiv^q_{\text{GSO}} \mathfrak{B}'$.

In the following, $\tau$ denotes a finite relational signature.

**Definition 12.** Let $\rho := \{c_1, \ldots, c_n\}$ be a finite set of constant symbols. Then $D_n$ is defined to be the set of all pairs $(\mathfrak{A}, \mathfrak{B})$ of finite $(\tau \cup \rho)$-structures such that

1. $c^\mathfrak{A} = c^\mathfrak{B}$ for all constant symbols $c \in \rho$;
2. $\{c_1^{\mathfrak{A}}, \ldots, c_n^{\mathfrak{A}}\} = A \cap B = \{c_1^{\mathfrak{B}}, \ldots, c_n^{\mathfrak{B}}\}$.

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

The following theorem in the special case of $n = 0$ is Proposition 4.1 in [6].

**Theorem 13.** Let $q, n, r, s \in \mathbb{N}$, let $(\mathfrak{A}_1, \mathfrak{B}_1), (\mathfrak{A}_2, \mathfrak{B}_2) \in D_n$, 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 $(\mathfrak{A}_1, \bar{a}_1) \equiv^q_{\text{GSO}} (\mathfrak{A}_2, \bar{a}_2)$ and $(\mathfrak{B}_1, \bar{b}_1) \equiv^q_{\text{GSO}} (\mathfrak{B}_2, \bar{b}_2)$. 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 $\phi$. 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 $\phi$ is built using a relation symbol $R \in \tau$, and the tuple that witnesses the truth of $\phi$ 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 $D_n$. We first consider the former case; the latter case can be treated similarly. If a constant that appears in $\phi$ is from $A_1 \cup B_1$, then by the definition of $D_n$ this element is denoted by a constant symbol $c \in \rho$, and therefore we may assume without loss of generality that $\phi$ 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 $(\mathfrak{A}_1, \bar{a}_1) \equiv^q_{\text{GSO}} (\mathfrak{A}_2, \bar{a}_2)$ and $(\mathfrak{B}_1, \bar{b}_1) \equiv^q_{\text{GSO}} (\mathfrak{B}_2, \bar{b}_2)$. By symmetry and Lemma 11 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 11, there exists $c_2 \in A_2$ such that $(\mathfrak{A}_1, \mathfrak{a}_1, c_1) \equiv^GSO_q (\mathfrak{A}_2, \mathfrak{a}_2, c_2)$. By the inductive assumption, this implies that

$$(\mathfrak{A}_1 \uplus \mathfrak{B}_1, \mathfrak{a}_1, c_1, b_1) \equiv^GSO_q (\mathfrak{A}_2 \uplus \mathfrak{B}_2, \mathfrak{a}_2, c_2, b_2)$$

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 $R \cap \mathfrak{A}_1^k$, and $\mathfrak{B}_1'$ be the expansion of $\mathfrak{B}_1$ by the guarded relation $R \cap B_1^k$. By Lemma 11 there are expansions $\mathfrak{A}_2'$ of $\mathfrak{A}$ and $\mathfrak{B}_2'$ of $\mathfrak{B}_2$ by guarded relations such that $(\mathfrak{A}_1', \mathfrak{a}_1) \equiv^GSO_q (\mathfrak{A}_2', \mathfrak{a}_2)$ and $(\mathfrak{B}_1', b_1) \equiv^GSO_q (\mathfrak{B}_2', b_2)$. By the inductive assumption, this implies that $(\mathfrak{A}_1' \uplus \mathfrak{B}_1', \mathfrak{a}_1, b_1) \equiv^GSO_q (\mathfrak{A}_2' \uplus \mathfrak{B}_2', \mathfrak{a}_2, b_2)$, which completes the proof of (second-order forth).

\begin{corollary}
Let $C$ be a CSP that can be expressed in GSO. Then there exists a countable \(\omega\)-categorical structure $\mathfrak{B}$ such that $C = \text{CSP}(\mathfrak{B})$.
\end{corollary}

\begin{proof}
Let $\tau$ be the signature of $C$, and let $\Phi$ be a GSO $\tau$-formula with quantifier-rank $q$ such that $C = [\Phi]$. By Theorem 8 it suffices to show that the equivalence relation $\sim_n^C$ has finite index for every $n \in \mathbb{N}$. Let $\rho := \{c_1, \ldots, c_n\}$ be a set of new constant symbols. By Lemma 10, there exists an $m \in \mathbb{N}$ such that $\equiv^GSO_q$ has $m$ equivalence classes on $(\tau \cup \rho)$-structures. If $\phi(x_1, \ldots, x_n)$ is a primitive positive $\tau$-formula, then define $\mathfrak{S}_\phi$ to be the $(\tau \cup \rho)$-structure whose elements are the equivalence classes of the smallest equivalence relation on the variables of $\phi$ that contains all pairs $x, y$ such that $\phi$ contains the conjunct $x = y$, and such that $(C_1, \ldots, C_n) \in R^\rho$ for $R \in \tau$ if and only if there are $y_1 \in C_1, \ldots, y_n \in C_2$ such that $\phi(y_1, \ldots, y_n)$ is a conjunct of $\phi$; finally, we set $\mathfrak{S}_\phi^i := [x_i]$ for all $i \in \{1, \ldots, n\}$.

We claim that if $\mathfrak{S}_\phi \equiv^GSO_q \mathfrak{S}_\psi$, then $\phi \sim_n^C \psi$. Let $\theta(x_1, \ldots, x_n)$ be a primitive positive $\tau$-formula; we may assume that the existentially quantified variables of $\theta$ are disjoint from the existentially quantified variables of $\phi$ and of $\psi$, so that $(\mathfrak{S}_\phi, \mathfrak{S}_\theta), (\mathfrak{S}_\psi, \mathfrak{S}_\theta) \in P_n$. Since $\mathfrak{S}_\phi \equiv^GSO_q \mathfrak{S}_\psi$ and $\mathfrak{S}_\theta \equiv^GSO_q \mathfrak{S}_\theta$, we have $\mathfrak{S}_\phi \uplus \mathfrak{S}_\theta \equiv^GSO_q \mathfrak{S}_\phi \uplus \mathfrak{S}_\theta$ by Theorem 13. Now suppose that $\phi \land \theta$ is satisfiable in a model of $\Phi$. This is the case if and only if $\mathfrak{S}_\phi \uplus \mathfrak{S}_\theta$ satisfies $\Phi$, which in turn implies that $\mathfrak{S}_\phi \uplus \mathfrak{S}_\theta$ satisfies $\Phi$ since $\Phi$ has quantifier-rank $q$. This in turn is the case if and only if $\psi \land \theta$ is satisfiable in a model of $\Phi$, which proves the claim.

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

\begin{example}
Let $\Phi$ be the following MSO sentence $\Phi$.

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

Note that a finite digraph does not satisfy $\Phi$ if it has a non-empty subgraph with the following extension property: for any $x, y \in X$ there exists $z \in X$ such that $E(x, z)$ and $E(y, z)$.

It is easy to see that $[\Phi]$ is closed under disjoint unions and that its complement is closed under homomorphisms. Corollary 14 implies that there exists a countable $\omega$-categorical structure with CSP$(\mathfrak{B}) = [\Phi]$. We claim that this statement cannot be deduced from the
theorem of Cherlin, Shelah, and Shi [23]. To see this, first note that the following graphs \( W_i \), for \( i \geq 2 \), satisfy the mentioned extension property: the vertex set of \( W_i \) is \( \{0, 1, \ldots, i\} \), there is an edge from \( p \) to \( q \), for \( p, q \in \{0, \ldots, i - 1\} \), if \( p - q = 1 \mod i \), and additionally we have the edges \( (p, i) \) and \( (i, p) \) for every \( p \in \{0, \ldots, i - 1\} \). See Figure 2 for an illustration of \( W_i \). Note that for every \( i \geq 2 \) the graph \( W_i \) is a core, and that they are pairwise homomorphically incomparable. Moreover, every subgraph of \( W_i \) does not satisfy the extension property.

### 3.3 Finite Unions of CSPs

In this section we prove that every class in GSO whose complement is closed under homomorphisms is a finite union of CSPs (Lemma 20); the statement announced at the beginning of Section 3 then follows (Corollary 21). Throughout this section, let \( \tau \) be a relational signature and let \( \mathcal{C} \) be a non-empty class of finite \( \tau \)-structures whose complement is closed under homomorphisms. In particular, \( \mathcal{C} \) contains the structure \( \mathcal{I} \) with only one element where all relations are empty.

Let \( \sim \) be the equivalence relation defined on \( \mathcal{C} \) by letting \( \mathcal{A} \sim \mathcal{B} \) if for every \( \mathcal{C} \in \mathcal{C} \) we have \( \mathcal{A} \uplus \mathcal{C} \in \mathcal{C} \) if and only if \( \mathcal{B} \uplus \mathcal{C} \in \mathcal{C} \); here \( \uplus \) denotes the usual disjoint union of structures, which is a special case of Definition 12 for \( n = 0 \). Note that the equivalence classes of \( \sim \) are in one-to-one correspondence to the equivalence classes of \( \sim_0^\mathcal{I} \). Also note that \( \mathcal{C} \) is closed under disjoint unions if and only if \( \sim \) has only one equivalence class.

If \( \mathcal{A} \in \mathcal{C} \), then we write \([\mathcal{A}]\) for the equivalence class of \( \mathcal{A} \) 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.
3. \( \mathcal{A} \in [\mathcal{I}] \) if and only if \( \mathcal{A} \uplus \mathcal{B} \in \mathcal{C} \) for all \( \mathcal{B} \in \mathcal{C} \).

\[ \triangleright \textbf{Lemma 16}. \] Let \( \mathcal{A} \in \mathcal{C} \) and let \( \mathcal{D} \) be the smallest subclass of \( \mathcal{C} \) that contains \([\mathcal{A}]\) and whose complement is closed under homomorphisms. Then

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 \( \mathcal{C} \in [\mathcal{A}] \), let \( \mathcal{B} \) be a finite structure with a homomorphism to \( \mathcal{C} \), and let \( \mathcal{B'} \in [\mathcal{B}] \). Since \( \mathcal{B} \uplus \mathcal{C} \) and \( \mathcal{C} \) are homomorphically equivalent, we have that \( \mathcal{B} \uplus \mathcal{C} \sim \mathcal{C} \). We claim that \( \mathcal{B'} \uplus \mathcal{C} \sim \mathcal{C} \). To see this, let \( \mathcal{D} \in \mathcal{C} \). Then

\[
\begin{align*}
\mathcal{C} \uplus \mathcal{D} \in \mathcal{C} & \iff (\mathcal{B} \uplus \mathcal{C}) \uplus \mathcal{D} \in \mathcal{C} \\
& \iff \mathcal{B} \uplus (\mathcal{C} \uplus \mathcal{D}) \in \mathcal{C} \\
& \iff \mathcal{B'} \uplus (\mathcal{C} \uplus \mathcal{D}) \in \mathcal{C} \\
& \iff (\mathcal{B'} \uplus \mathcal{C}) \uplus \mathcal{D} \in \mathcal{C}
\end{align*}
\]

which shows the claim. So \( \mathcal{B'} \uplus \mathcal{C} \in [\mathcal{C}] = [\mathcal{A}] \). Since \( \mathcal{B'} \) has a homomorphism to \( \mathcal{B'} \uplus \mathcal{C} \) we obtain that \( \mathcal{B'} \in \mathcal{D} \); this proves the first statement.

To prove the second statement, first observe that the statement is clear if \( \mathcal{A} \in [\mathcal{I}] \), since the complement of \([\mathcal{I}]\) is closed under homomorphisms. The statement therefore follows from the assumption that \( \sim \) has more than one equivalence class. Otherwise, if \( \mathcal{A} \notin [\mathcal{I}] \), then there exists a structure \( \mathcal{B} \in \mathcal{C} \) such that \( \mathcal{A} \uplus \mathcal{B} \notin \mathcal{C} \). Then \( \mathcal{B} \in \mathcal{C} \setminus \mathcal{D} \) can be shown indirectly as follows: otherwise \( \mathcal{B} \) would have a homomorphism to a structure \( \mathcal{A'} \in [\mathcal{A}] \). Since \( \mathcal{B} \uplus \mathcal{A'} \) is homomorphically equivalent to \( \mathcal{A'} \), we have \( \mathcal{B} \uplus \mathcal{A'} \sim \mathcal{A'} \sim \mathcal{A} \) and in particular \( \mathcal{B} \uplus \mathcal{A'} \in \mathcal{C} \). But \( \mathcal{B} \uplus \mathcal{A'} \in \mathcal{C} \) if and only if \( \mathcal{B} \uplus \mathcal{A} \in \mathcal{C} \) since \( \mathcal{A} \sim \mathcal{A'} \). This is in contradiction to our assumption on \( \mathcal{B} \). \( \triangleright \)
Example 17. We consider a signature $\tau := \{ R_1, R_2, R_3 \}$ of unary relation symbols. Define for every $i \in \{ 1, 2, 3 \}$ the $\tau$-structure $\mathfrak{S}_i$ to be a one-element structure where $R_i$ is non-empty and $R_j$, for $j \neq i$, is empty. Let

$$C := \text{CSP}(\mathfrak{S}_1 \uplus \mathfrak{S}_2) \cup \text{CSP}(\mathfrak{S}_2 \uplus \mathfrak{S}_3) \cup \text{CSP}(\mathfrak{S}_3 \uplus \mathfrak{S}_1).$$

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

$$[\mathfrak{S}_i \uplus \mathfrak{S}_j] = \text{CSP}(\mathfrak{S}_i \uplus \mathfrak{S}_j) \setminus (\text{CSP}(\mathfrak{S}_i) \cup \text{CSP}(\mathfrak{S}_j)),$$

$$[\mathfrak{S}_i] = \text{CSP}(\mathfrak{S}_i) \setminus [3],$$

$$[3] = \text{CSP}(3).$$

For the remainder of the section we fix a GSO $\tau$-sentence $\Phi$ of quantifier rank $q$. Recall that Lemma 10 asserts that the equivalence relation $\equiv^\text{GSO}_q$ on the class of finite $\tau$-structures has finitely many equivalence classes $C_1, \ldots, C_m$, and that each of the equivalence classes $C_i$ can be defined by a single GSO $\tau$-sentence $\Psi_i$ with quantifier rank $q$; we write $T^\tau_q := \{ \Psi_1, \ldots, \Psi_m \}$ for this set of GSO sentences. Let $J \subseteq \{ 1, \ldots, m \}$ be such that $\{ \Psi_j \in T^\tau_q \mid j \in J \}$ is exactly the set of all sentences in $T^\tau_q$ that imply $\Phi$. Then $|J|$ is called the degree of $\Phi$. It is easy to see that the degree of $\Phi$ is exactly the index of $\equiv^\text{GSO}_q$ restricted to $[\Phi]$. Let $\sim$ be the equivalence relation defined in the beginning of this section for the class $C := [\Phi]$.

Lemma 18. For every $\sim$-class $\mathcal{D}$ there exists $I \subseteq \{ 1, \ldots, m \}$ such that $\mathcal{D} = \bigcup_{i \in I} [\Psi_i]$.

Proof. As in the proof of Corollary 14 one can use Theorem 13 to show for all finite $\tau$-structures $\mathfrak{A}, \mathfrak{B}$ that if $\mathfrak{A} \equiv^\text{GSO}_q \mathfrak{B}$, then $\mathfrak{A} \sim \mathfrak{B}$. This means that $\mathcal{D}$ is a union of $\equiv^\text{GSO}_q$-classes and therefore there exists $I \subseteq J \subseteq \{ 1, \ldots, m \}$ such that $\mathcal{D} = \bigcup_{i \in I} [\Psi_i]$.

Corollary 19. The index of $\sim$ is smaller than or equal to the degree of $\Phi$.

Lemma 20. If the complement of $[\Phi]$ is closed under homomorphisms, then there are finitely many GSO $\tau$-sentences $\Phi_1, \ldots, \Phi_t$ each of which describes a CSP such that $\Phi$ is equivalent to $\Phi_1 \lor \cdots \lor \Phi_t$. If $\Phi$ is an MSO sentence, then $\Phi_1, \ldots, \Phi_t$ can be chosen to be MSO sentences as well.

Proof. We prove the statement by induction on the degree $n$ of $\Phi$. By Lemma 19 the equivalence relation $\sim$ has at most $n$ equivalence classes on $\tau$-structures. Hence, if $n = 1$, then $[\Phi]$ is closed under disjoint unions, and we are done.

Let $\mathfrak{A}_1, \ldots, \mathfrak{A}_s$ be $\tau$-structures such that $\{ [\mathfrak{A}_1], \ldots, [\mathfrak{A}_s] \}$ is the set of all equivalence classes of $\sim$ that are distinct from $[3]$. 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 $[3]$ is contained in $\mathcal{D}_i$ for all $i \leq s$. By Lemma 16 (1), each $\mathcal{D}_i$ is a union of $\sim$-classes which are themselves a union of $\equiv^\text{GSO}_q$-classes. By Lemma 18. It follows that there exists $I_i \subseteq \{ 1, \ldots, m \}$ such that $\mathcal{D}_i = \bigcup_{j \in I_i} [\Psi_{j_i}]$. We define $\Phi_i := \bigvee_{j \in I_i} \Psi_j$. Note that the GSO sentence $\Phi_i$ is of quantifier rank $q$ such that $\mathcal{D}_i = [\Phi_i]$. Hence, $\Phi$ is equivalent to $\bigvee_{i \leq s} \Phi_i$. Lemma 16 (2) asserts that $[\Phi] \setminus \mathcal{D}_i$ is non-empty, and hence the degree of $\Phi_i$ 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.
Corollary 21. 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 22. 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 \(\Pi\) with the binary IDB \(E\) derives goal on \(\mathfrak{A}\).

\[\begin{align*}
E(x, y) &:= S(x), S(y) \\
E(x, y) &:= E(x', y'), R(x', x), R(y', y) \\
\text{goal} &:= T(x), E(x, x'), R(x', y)
\end{align*}\]

For \(n \in \mathbb{N}\), let \(\mathfrak{P}_n\) be the \{S, T, R\}-structure on the domain \(\{1, \ldots, n\}\) with

\[S^{\mathfrak{P}_n} := \{1\} \quad T^{\mathfrak{P}_n} := \{n\} \quad R^{\mathfrak{P}_n} := \{(i, i + 1) \mid i \in \{1, \ldots, n - 1\}\}.
\]

It is easy to see that each of the structures in \(\{\mathfrak{P}_n \mid n \geq 1\}\) is not contained in \(C\), and that the disjoint union of \(\mathfrak{P}_i\) and \(\mathfrak{P}_j\), for \(i \neq j\), is contained in \(C\). It follows that \(C\) is not a finite intersection of complements of CSPs (and, by Corollary 21, cannot be expressed in GSO).

4 Canonical Datalog Programs

A remarkable fact about the expressive power of Datalog for constraint satisfaction problems over finite domains is the existence of canonical Datalog programs and the characterisation of Datalog expressivity in terms of an existential pebble game [29]; this has been generalised to CSPs for ω-categorical structures.

4.1 The Canonical Program of Width \((\ell, k)\)

The following concept is due to Feder and Vardi [29] for complements of finite-domain CSPs and has been generalised to complements of ω-categorical CSPs by Bodirsky and Dalmau [12].

Definition 23. Let \(\mathcal{B}\) be an \(\omega\)-categorical structure with a finite relational signature \(\tau\). Let \(\mathcal{B}'\) be the expansion of \(\mathcal{B}\) by all primitively positively definable relations of arity at most \(\ell\) and let \(\tau'\) be the (finite) signature of \(\mathcal{B}'\). Then the canonical \((\ell, k)\)-Datalog program for \(\mathcal{B}\) has IDBs \(\tau' \setminus \tau\) and EDBs \(\tau\). The empty 0-ary relation serves as goal. There is a finite number of inequivalent formulas \(\psi(x, y)\) of the form

\[(\psi_1(x, y) \land \cdots \land \psi_j(x, y)) \Rightarrow R(\bar{x})\]

having at most \(k\) variables and where \(\psi_1, \ldots, \psi_j\) are atomic \((\tau \cup \tau')\)-formulas and \(R \in \tau\). For each of the inequivalent formulas \(\psi(x, y)\) such that \(\mathcal{B}' \models \forall \bar{x} \exists \bar{y} . \psi(\bar{x}, \bar{y})\) we introduce a rule

\[R(\bar{x}) := \neg \psi_1(\bar{x}, \bar{y}), \ldots, \neg \psi_j(\bar{x}, \bar{y}).\]

Theorem 24 (Bodirsky and Dalmau [12], Theorem 4). Let \(\mathcal{B}\) be a countable \(\omega\)-categorical \(\tau\)-structure. Let \(\ell, k \in \mathbb{N}\) and let \(\Pi\) be the canonical Datalog program of width \((\ell, k)\) for the complement of CSP(\(\mathcal{B}\)). Then for every finite \(\tau\)-structure \(\mathfrak{A}\) the following are equivalent:
π derives goal on A;

Spoiler has a winning strategy for the existential (ℓ, k)-pebble game on (A, B).

Moreover, π is also a canonical Datalog program of width (ℓ, k) in the sense defined in the introduction.

These results can be applied to finite unions of complements of CSPs for ω-categorical structures because of the following well-known fact.

Lemma 25. If C_1 and C_2 are in Datalog, then so are C_1 ∪ C_2 and C_1 ∩ 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 [π_1] ∪ [π_2] and for [π_1] ∩ [π_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 goal_1 and the symbol goal in π_2 to goal_2. Finally we add the new rule goal := goal_1, goal_2 to the union of π_1 and π_2. It is clear that these constructions preserve the width.

Theorem 26. Let Φ be a GSO sentence such that [Φ] is closed under homomorphisms. Let ℓ, k ∈ N. Then there exists a canonical Datalog program π of width (ℓ, k) for [Φ].

Proof. By Corollary 21 there are GSO sentences Φ_1, . . . , Φ_m and ω-categorical structures B_1, . . . , B_m such that Φ is equivalent to Φ_1 ∧ · · · ∧ Φ_m and [−Φ] = CSP(B_i). Let π_i be a canonical Datalog program for CSP(B_i) which exists by Theorem 24. Then Lemma 25 implies that there exists a Datalog program π_i such that [π] = [π_1] ∩ · · · ∩ [π_m]. It is clear that π is sound for [Φ]. To see that π is a canonical Datalog program for [Φ], suppose that A is such that some Datalog program π’ of width (ℓ, k) which is sound for [Φ] derives goal on A. Since, for every i ∈ {1, . . . , m}, the program π_i is also sound for [Φ_i], and π_i is a canonical Datalog program for [Φ_i], the program π_i derives goal on A. Hence, A ∈ [π] = [π_1] ∩ · · · ∩ [π_m].

We say that a Datalog rule ψ_0;−ψ_1, . . . , ψ_m is connected if {ψ_1, . . . , ψ_m} cannot be partitioned into two non-empty subsets with disjoint sets of variables.

Proposition 27. Let π be a connected Datalog program. Then [π] equals the complement of a CSP.

Proof. As we have mentioned in the introduction, it suffices to show that the complement of [π] is closed under disjoint unions. So let A and B be structures where π does not derive the goal predicate. Let A’ and B’ be the structure computed by π on A and on B, respectively. If the body of a rule of π holds on A’ ⊔ B’, then all variables must take values from A’, or all variables must take values from B’, because the rule is connected. Hence, π does not derive new facts on A’ ⊔ B’, and in particular does not derive the goal predicate. Hence A ⊔ B belongs to the complement of [π] we well.

Proposition 28. Let B be a countable ω-categorical structure such that there exists a Datalog program π for the complement of CSP(B). Then there also exists a connected Datalog program for the complement of CSP(B). In fact, if π has width (ℓ, k), then such a program can be obtained from the canonical Datalog program of width (ℓ, k) by removing all rules that are not connected.
Proof. Let $\Pi$ be the canonical Datalog program for CSP($\mathcal{B}$) (Theorem 24). Suppose that $\Pi$ contains a rule which is not connected, e.g., a rule of the form $\psi_0 : \neg \psi_1, \psi_2$ where $\psi_1$ and $\psi_2$ are conjunctions of atomic formulas with disjoint sets of variables. We claim that then $\psi_0 : \neg \psi_1$ or $\psi_0 : \neg \psi_2$ must be a rule of $\Pi$ as well. Otherwise, for each $i \in \{1, 2\}$ there would be a substructure of $\mathfrak{A}_i$ of $\mathcal{B}$ that satisfies $\psi_i \land \neg \psi_0$. Then the disjoint union of $\mathfrak{A}_1$ and $\mathfrak{A}_2$ satisfies $\psi_1 \land \psi_2 \land \neg \psi_0$, a contradiction to the definition of the canonical Datalog program. ▷

4.2 The Existential Pebble Game

An informal definition of the existential pebble game was given in the introduction; we now present a formal definition of the concept of a (positional) winning strategies for Duplicator in this game.

Definition 29 ([12]). A winning strategy for Duplicator for the existential $(\ell, k)$-pebble game on two relational $\tau$-structures $\mathfrak{A}$, $\mathcal{B}$ is a non-empty set $\mathcal{H}$ of partial homomorphisms from $\mathfrak{A}$ to $\mathcal{B}$ such that
1. $\mathcal{H}$ is closed under restrictions;
2. for all $h \in \mathcal{H}$ with $|\text{dom}(h)| = d \leq \ell$ and for all $a_1, \ldots, a_{k-d} \in A$ there is an extension $h' \in \mathcal{H}$ of $h$ such that $h'$ is also defined on $a_1, \ldots, a_{k-d}$.

In all our arguments about the existential pebble game, we only need this definition; in particular, we do not need the presentation of the existential pebble game as we have presented it in the introduction.

Theorem 30. Let $\Phi$ be a GSO sentence. Then $[\Phi]$ can be defined in Datalog if and only if
1. $[\Phi]$ is closed under homomorphisms, and
2. there exist $\ell, k \in \mathbb{N}$ such that for all finite structures $\mathfrak{A}$, Spoiler wins the $(\ell, k)$-game for $[\Phi]$ on $\mathfrak{A}$ if and only if $\mathfrak{A} \models \Phi$.

Proof. First suppose that $[\Phi]$ is in Datalog. That is, there exists $\ell, k \in \mathbb{N}$ and a Datalog program $\Pi$ of width $(\ell, k)$ such that $[\Phi] = [\Pi]$. Then clearly $[\Phi]$ is closed under homomorphisms, and by Lemma 20, there are GSO sentences $\Phi_1, \ldots, \Phi_m$ such that $\Phi$ is equivalent to $\Phi_1 \land \cdots \land \Phi_m$ and $[\Phi_i]$ is the complement of a CSP, for each $i \in \{1, \ldots, m\}$. Corollary 14 implies that there exists an $\omega$-categorical structure $\mathcal{B}_i$ such that CSP($\mathcal{B}_i$) = $[\neg \Phi_i]$.

Suppose that $\mathfrak{A}$ is a finite $\tau$-structure such that $\mathfrak{A} \models \Phi$. Then Spoiler wins the $(\ell, k)$-game as follows. Suppose that Duplicator plays the countable structure $\mathcal{B}$ such that CSP($\mathcal{B}$) $\cap [\Phi] = \emptyset$. Then CSP($\mathcal{B}$) $\cap [\Phi_i] = \emptyset$ for some $i \in \{1, \ldots, m\}$; otherwise, if there is a structure $\mathfrak{A}_i \in$ CSP($\mathcal{B}$) $\cap [\Phi_i]$ for every $i \in \{1, \ldots, m\}$, then the disjoint union of $\mathfrak{A}_1, \ldots, \mathfrak{A}_m$ satisfies $\Phi$ since $\Phi_i$ is closed under homomorphisms, and is in CSP($\mathcal{B}$) since CSP($\mathcal{B}$) is closed under disjoint unions; but this is in contradiction to our assumption that CSP($\mathcal{B}$) $\cap [\Phi] = \emptyset$. Hence, CSP($\mathcal{B}$) $\subseteq$ CSP($\mathcal{B}_i$) and there is a homomorphism $h$ from $\mathcal{B}$ to $\mathcal{B}_i$ (see [12]). Note that $\Pi$ is sound for the complement of CSP($\mathcal{B}_i$), and $\Pi$ derives $\text{goal}$ on $\mathfrak{A}$, and thus Theorem 24 implies that Spoiler wins the existential $(\ell, k)$-pebble game on $(\mathfrak{A}, \mathcal{B}_i)$. But since $\mathcal{B}$ homomorphically maps to $\mathcal{B}_i$, this implies that Spoiler wins the existential $(\ell, k)$-pebble game on $(\mathfrak{A}, \mathcal{B})$.

Now suppose that $\mathfrak{A} \models \neg \Phi$. Hence, there exists $i \in \{1, \ldots, m\}$ such that $\mathfrak{A} \models \neg \Phi_i$. Then Duplicator wins the $(\ell, k)$-game as follows. She starts by playing $\mathcal{B}_i$. Then $\mathfrak{A}$ homomorphically maps to $\mathcal{B}_i$, and Duplicator can win the existential $(\ell, k)$-pebble game on $(\mathfrak{A}, \mathcal{B}_i)$ by always playing along the homomorphism.
For the converse implication, suppose that 1. and 2. hold. Since \([\Phi]\) is closed under homomorphisms, Corollary 21 implies that there are GSO sentences \(\Phi_1, \ldots, \Phi_m\) and \(\omega\)-categorical structures \(\mathfrak{B}_1, \ldots, \mathfrak{B}_m\) such that \(\Phi\) is equivalent to \(\Phi_1 \land \cdots \land \Phi_m\) and \(|\Phi| = \text{CSP}(\mathfrak{B}_1)\). By Theorem 24, for every \(i \in \{1, \ldots, m\}\) there exists a canonical Datalog program \(\Pi_i\) of width \((\ell, k)\) for \([\Phi_i]\). Then Lemma 25 implies that there exists a Datalog program \(\Pi\) such that \(|\Pi| = |\Pi_1| \cap \cdots \cap |\Pi_m|\). Since each \(\Pi_i\) is sound for \([\Phi_i]\), it follows that \(\Pi\) is sound for \([\Phi]\). Hence, it suffices to show that if \(\mathfrak{A}\) is a finite \(\tau\)-structure such that \(\mathfrak{A} \models \Phi\), then \(\text{Spoiler}\) wins the existential \((\ell, k)\)-pebble game on \((\mathfrak{A}, \mathfrak{B}_i)\). By Theorem 24, it follows that \(\Pi\) derives \text{goal} on \(\mathfrak{A}\). Hence, \(\Pi\) derives \text{goal} on \(\mathfrak{A}\).

\section{A coNP-complete CSP in MSO}

In this section we show that the class of CSPs in MSO is (under complexity-theoretic assumptions) larger than the class of CSPs for reducts of finitely bounded structures (see Section 3.1). Let \(\mathcal{T} = \{\mathfrak{T}_2, \mathfrak{T}_3, \ldots\}\) be the set of Henson tournaments: the tournament \(\mathfrak{T}_n\), for \(n \geq 2\), has vertices \(0, 1, \ldots, n + 1\) and the following edges:

- \((i, i + 1)\) for \(i \in \{0, \ldots, n\}\);
- \((0, n + 1)\);
- \((j, i)\) for \(i + 1 < j\) and \((i, j) \neq (0, n + 1)\).

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 [14] that \(\text{CSP(}\mathfrak{H}\))\) is coNP-complete.

\begin{proposition}
\text{CSP(}\mathfrak{H}\))\) can be expressed in MSO.
\end{proposition}

\begin{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 \(\Phi\), for a unary relation symbol \(X\), that is true on a finite \(\{X, E\}\)-structure \(\mathfrak{G}\) if and only if \((X^G; E^G)\) is isomorphic to \(\mathfrak{T}_n\), for some \(n \geq 2\). In \(\phi\) 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 \(\Phi\) has the following conjuncts:

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 \(\forall x: \neg E(x, x) \land \forall X: \neg \Phi\) 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 \(\phi\) holds; this is straightforward from the construction of \(\Phi\) (and the explanations above given in brackets). Conversely, suppose that \(\Phi\) holds. Then \((X; T)\) is a tournament. We
construct an isomorphism $f$ from $(X; T)$ to $T_{|X|−1}$ as follows. Define $f(s) := 0$, $f(a) := 1$, 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 $f(a') := 3$. If $a' = t$ then we have found an isomorphism with $T_2$.

Otherwise, the partial map $f$ defined so far is an embedding into $T_n$ for some $n \geq 3$. Item 6 implies that there exists exactly one $b' \in B$ such that $E(a', b')$ and $E(b', b)$, and we define $f(b') := 4$. Continuing in this manner, we eventually define $f$ on all of $X$ and find an isomorphism with $T_{|X|−1}$.

This shows that CSP($\mathcal{H}$) cannot be expressed, unless NP = coNP, as CSP($\mathcal{B}$) 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($\mathcal{H}$) can be expressed as CSP($\mathcal{B}$) for some reduct of a finitely bounded homogeneous structure.

6 Nested Guarded Queries

Frontier-guarded Datalog is a fragment of Datalog that is contained in GSO. Guarded queries (GQ) and the more expressive Nested guarded queries (GQ$^+$) are extensions of frontier-guarded Datalog that have been introduced by Bourhis, Krötzsch, and Rudolph [18]; the definitions will be recalled below. GQ is also strictly more expressive than Nested Monadically Defined Queries (Nemodeq), Monadically defined queries (Modeq) [42], and the recently introduced almost monadic queries [43]. Both GQ and GQ$^+$ are contained in the intersection of Datalog and GSO. We show that GQ$^+$ does not contain all queries from the intersection of Datalog and MSO (and hence, neither does GQ, frontier-guarded Datalog, Nemodeq, Modeq, and almost monadic Datalog): there are CSPs that are both in MSO and in Datalog, but not in GQ$^+$ (Corollary 64).

6.1 Frontier-Guarded Datalog

A rule of a Datalog program is called frontier-guarded if all variables of the head appear in a single EDB atom in the rule body. A Datalog program is called frontier-guarded if all its rules are frontier-guarded. Note that every monadic Datalog program is frontier-guarded. Also the Datalog program from the proof of Proposition 7 is guarded.

$\blacktriangleright$ Proposition 32. Every problem in frontier-guarded Datalog is in GSO.

$\triangleright$ Proof. Let $\Pi$ be a Datalog program. Let $\Phi_{\Pi}$ be the SO sentence obtained by

existentially quantifying over the IDBs of $\Pi$,

replacing each rule $\psi := \phi_1, \ldots, \phi_m$ of $\Pi$ by the conjunct $\forall \bar{x}(\psi \lor \neg \phi_1 \lor \cdots \lor \neg \phi_m)$ of $\Phi$,

additionally adding the conjunct $\neg \text{goal}$ to $\Phi$.

Clearly, $\Pi$ derives $\text{goal}$ on a finite structure $\mathfrak{A}$ if and only if $\mathfrak{A}$ satisfies $\neg \Phi_{\Pi}$.

We will now show that, if $\Pi$ is frontier-guarded, then $\Phi_{\Pi}$ can be expressed by a GSO sentence. To this end, we establish that $\Phi_{\Pi}$ has the same meaning under standard and under guarded semantics, from which the desired result follows via Proposition 6. Toward a

4 The term frontier-guarded was originally introduced for existential rules (also referred to as tuple-generating dependencies or Datalog$^+$), an expressive extension of Datalog. Frontier-guarded Datalog is then simply the syntactic intersection of frontier-guarded existential rules and Datalog. The name guarded is reserved for rules where all variables of the rule appear in a single EDB atom in the rule body.
contradiction, assume some structure $\mathfrak{A}$ satisfies $\Phi_{\Pi}$ under standard but not under guarded semantics (as $\Phi_{\Pi}$ is preceded only by existentially quantified relation symbols, this is the only possibility). Assume that instantiating the IDBs with the relations $R_1, \ldots, R_k$ over $A$ witnesses that $\mathfrak{A}$ satisfies $\Phi_{\Pi}$ under standard semantics. Obtain now the guarded relations $R'_1, \ldots, R'_k$ by removing all unguarded tuples from $R_1, \ldots, R_k$, respectively. The desired contradiction is now obtained by arguing that instantiating the IDBs with the relations $R'_1, \ldots, R'_k$ witnesses that $\mathfrak{A}$ satisfies $\Phi_{\Pi}$ under guarded semantics: First, we note that $\neg \text{goal}$ is still satisfied. Second, for any rule $\psi ::= \phi_1, \ldots, \phi_m$ of $\Pi$, fixing any variable assignment of $\bar{x}$ with elements of $A$, we obtain that the truth of $\psi \lor \neg \phi_1 \lor \cdots \lor \neg \phi_m$ under the instantiation with $R_1, \ldots, R_k$ implies its truth under the instantiation with $R'_1, \ldots, R'_k$: On the one hand, should any $\neg \phi_i$ be true, this is immediate (both for EDB and IDB atoms). On the other hand, in case all $\neg \phi_i$ are false, then so is the one $\neg \phi_j$ where $\phi_j = \phi_j(\bar{y})$ is the rule’s “frontier guard”, i.e., it consists of an EDB atom where $\bar{y}$ contains at least all the variables of $\bar{z}$ from $\psi(\bar{z}) = \psi$. Truth of $\phi_j(\bar{y})$ under the chosen assignment implies that the tuple assigned to $\bar{y}$ is guarded and therefore also the tuple assigned to $\bar{z}$ must be guarded. Yet, then, truth of $\psi(\bar{z})$ under the two IDB instantiations coincides, hence $\psi(z)$ must hold.

However, not every problem in GSO which is in Datalog can be expressed by a frontier-guarded Datalog program. To prove this we need the following definition.

**Definition 33.** Let $\mathfrak{B}$ be an $\omega$-categorical structure with finite relational signature $\tau$ and $k \in \mathbb{N}$. Let $s$ be the maximal arity of $\tau$. Then the guarded canonical Datalog program of width $k$ for the complement of $\text{CSP}(\mathfrak{B})$ is the subset of the canonical Datalog program of width $(s,k)$ for the complement of $\text{CSP}(\mathfrak{B})$ which contains all rules that are guarded.

If $\Pi$ the guarded canonical Datalog program of width $k$ for the complement of $\text{CSP}(\mathfrak{B})$, then it follows from Proposition 35 below that $[\Pi'] \subseteq [\Pi]$ for every frontier-guarded Datalog program $\Pi'$ of width $(k,k)$ which is sound for the complement of $\text{CSP}(\mathfrak{B})$. We need to adapt the existential pebble game on $\mathfrak{A}$ and $\mathfrak{B}$ to the guarded setting as well. In our informal definition of the existential pebble game, we only change the rules for Spoiler: we additionally require that when Spoiler removes pebbles from $\mathfrak{A}$, then all the pebbles that remain on $\mathfrak{A}$ must be guarded, i.e., there must exist a tuple in a relation of $\mathfrak{A}$ such that these pebbles must be from the entries of this tuple. The resulting game will be called the existential guarded $k$ pebble game. Formally, we again work exclusively with the concept of a winning strategy $\mathcal{H}$ for Duplicator (similarly as in Definition 29). A partial homomorphism from $\mathfrak{A}$ to $\mathfrak{B}$ is called guarded if there exists a tuple in a relation of $\mathfrak{A}$ whose entries contain $\text{dom}(h)$.

**Definition 34.** Let $k \in \mathbb{N}$ and let $\tau$ be a finite relational signature. A winning strategy for Duplicator for the existential guarded $k$-pebble game on two relational $\tau$-structures $\mathfrak{A}, \mathfrak{B}$ is a set $\mathcal{H}$ of partial homomorphisms from $\mathfrak{A}$ to $\mathfrak{B}$ such that $\mathcal{H}$ is closed under restrictions, and for every $S \subseteq A$ with $|S| \leq k$ and every guarded $h \in \mathcal{H}$ with $\text{dom}(h) \subseteq S$, there is an extension $h' \in \mathcal{H}$ of $h$ with domain $S$.

The following can be shown analogously to the proof of Theorem 4 in [12]. We omit the proof because all the ideas are already present in the proof of a more interesting theorem that we present in full detail in Section 6.4 (Theorem 51).

**Proposition 35.** Let $\mathfrak{B}$ be $\omega$-categorical with finite relational signature $\tau$ and let $\mathfrak{A}$ be a finite $\tau$-structure. Then for all $k \in \mathbb{N}$ the following statements are equivalent.

- Every sound frontier-guarded Datalog program of width $k$ for the complement of $\text{CSP}(\mathfrak{B})$ does not derive $\text{goal}$ on $\mathfrak{A}$. 

The canonical frontier-guarded Datalog program of width $k$ for the complement of CSP($\mathcal{B}$) does not derive goal on $\mathfrak{A}$.

Duplicator has a winning strategy for the existential guarded $k$ pebble game on $\mathfrak{A}$, $\mathcal{B}$.

**Proposition 36.** The complement of CSP($\mathcal{Q}$; $<$) cannot be defined by a frontier-guarded Datalog program.

**Proof.** Let $k \in \mathbb{N}$. By Proposition 35, it suffices to show that there exists a structure $\mathfrak{A}$ which has no homomorphism to ($\mathcal{Q}$; $<$) but Duplicator has a winning strategy for the existential guarded $k$ pebble game on $\mathfrak{A}$, ($\mathcal{Q}$; $<$). Let $\mathfrak{A}$ be a directed cycle of length at least $k + 1$. Let $\mathcal{H}$ be the set of all partial homomorphisms $h$ from $\mathfrak{A}$ to ($\mathcal{Q}$; $<$) with a domain of size at most $k$. We claim that $\mathcal{H}$ is a winning strategy for the existential guarded $(\ell, k)$-pebble game. Clearly, $\mathcal{H}$ is closed under restrictions. Now, let $h$ be a partial homomorphism whose domain is contained in a tuple from a relation of $\mathfrak{A}$, that is, contained in $\{a_1, a_2\}$ for two subsequent elements of $A$ on the cycle. Let $a_3, \ldots, a_k$ be elements of $A$. Since $|A| \geq k + 1$ there must be some $b \in A \setminus \{a_1, \ldots, a_k\}$. Let $<$ be the order on $a_1, \ldots, a_k$ in which these elements are traversed on the cycle, starting with $b$. Note that $<$ is a linear extension of $<^\mathfrak{A}$. We may then extend $h$ to a partial homomorphism $h'$ from $\mathfrak{A}$ to ($\mathcal{Q}$; $<$) such that $h(a_i) < h(a_j)$ if $a_i < a_j$, for all $i, j \in \{1, \ldots, k\}$. Note that $h' \in \mathcal{H}$; this finishes the proof. ▶

### 6.2 Flag and Check

A general mechanism, called flag and check, to turn a query language into a potentially more powerful query language has been introduced by Bourhis, Krötzsch, and Rudolph [18], generalising earlier work of Rudolph and Krötzsch [42]. The idea is best described for some fundamental constraint satisfaction problems. It is easy to see that there is no $k$ such that CSP($\{0, 1\}; \neq$) (i.e., graph 2-colorability) is solved by a Datalog program of width $(1, k)$. However, to decide whether a graph is 2-colorable, it suffices to show that there is no vertex $v$ which can reach $v$ via a path of odd length. Note that such a 'check' can be performed by a Datalog program of width $(1, 2)$ once a 'flag' has been put on $v$. Similarly, there is no $k \in \mathbb{N}$ such that CSP($\mathcal{Q}$; $<$) (i.e., digraph acyclicity) can be solved by a Datalog program of width $(1, k)$ [7]. However, to decide whether a graph contains a directed cycle, it suffices to find a vertex $v$ which can reach $v$ by a directed path with at least one edge. Again, after $v$ has been found and 'flagged' such a computation can be performed by a Datalog program of width $(1, 2)$.

We now present the formal definition of flag-and-check programs of Bourhis, Krötzsch, and Rudolph [18].

**Definition 37.** Let $\tau$ be a finite set of relation and constant symbols. A flag-and-check $\tau$-program ($\tau$-FCP) of arity $m$ is a set of Datalog rules $\Pi$ with EDBs $\tau \cup \{\lambda_1, \ldots, \lambda_m\}$, where $\lambda_1, \ldots, \lambda_m$ are new constant symbols, and the IDBs $\{\text{goal}, P_1, \ldots, P_k\}$ where goal is a distinguished predicate of arity 0. If $\mathfrak{A}$ is a $\tau$-structure, then $\mathfrak{A}^\mathfrak{A}$ is the set of all tuples $(a_1, \ldots, a_m) \in A^m$ such that $\Pi$ derives goal on the $\tau \cup \{\lambda_1, \ldots, \lambda_m\}$-expansion $\mathfrak{A}'$ of $\mathfrak{A}$ where $\lambda_i^{\mathfrak{A}'} = a_i$ for all $i \in \{1, \ldots, m\}$.

Several formalisms in the literature are based on flag-and-check programs:

- A guarded $\tau$-query ($GQ$) is a query with free variables $y_1, \ldots, y_k$, for some $k \in \mathbb{N}$, of the form $\exists x_1, \ldots, x_\ell. \Pi(\vec{x}, \vec{y})$ where $\Pi$ is a frontier-guarded $\tau$-FCP of arity $m = k + \ell$, with the obvious semantics [18].
A monadically defined query (Modeq) is a query with free variables $y_1, \ldots, y_k$, for some $k \in \mathbb{N}$, of the form $\exists x_1, \ldots, x_\ell. \Pi(\bar{x}, \bar{y})$ where $\Pi$ is a monadic $\tau$-FCP of arity $m = k + \ell$, i.e., all IDBs of $\Pi$ have arity at most one [42] (we follow the presentation in [18]).

We omit the reference to $\tau$ in the notation if the reference is clear from the context. It has been shown that every problem in Modeq can be expressed in MSO [42]; similarly, we obtain the following.

\begin{proposition}
Every problem in GQ is in GSO.
\end{proposition}

\begin{proof}
Let $k, \ell \in \mathbb{N}$ and let $\Pi$ be a guarded flag-and-check program of arity $k + \ell$. We have to find a GSO sentence which is equivalent to $\exists x_1, \ldots, x_\ell. \Pi(\bar{x}, \bar{y})$. Let $\Phi_\Pi$ be the GSO sentence that is equivalent to $\Pi$ (Proposition 32). Then we define $\Psi$ to be the GSO sentence obtained from $\Phi_\Pi$ as follows.

- Replace each occurrence of $\lambda_i$, for $i \in \{1, \ldots, m\}$, by a fresh variable $x_i$.
- Existentially quantify $x_1, \ldots, x_\ell$.

An example of a query that can be expressed in GQ, but not in Modeq can be found in [18] (Example 2). Certain flag-and-check programs have been studied in the context of the complexity of constraint satisfaction under the name peek arc consistency, extending the famous (hyper-) arc consistency procedure [9]. In the following, $\tau$ denotes a finite relational signature.

\begin{definition}
Let $\mathfrak{B}$ be a countable $\omega$-categorical $\tau$-structure with the orbits $O_1, \ldots, O_n$ and let $b_1, \ldots, b_n$ be representatives from these orbits. Then the PAC procedure for $\text{CSP}(\mathfrak{B})$ derives $\text{goal}$ on a $\tau$-structure $\mathfrak{A}$ if there exists an $a \in A$ such that for all $i \leq n$ the hyperarc consistency procedure for $\text{CSP}(\mathfrak{B}, \{b_i\})$ derives $\text{goal}$ on $(\mathfrak{A}, \{a\})$.
\end{definition}

For example, the PAC procedure for $\text{CSP}(\{0, 1\}; \neq)$ derives $\text{goal}$ on a finite structure $\mathfrak{A}$ if and only if $\mathfrak{A}$ has no homomorphism to $(\{0, 1\}; \neq)$; similarly, the PAC procedure solves $\text{CSP}(\mathbb{Q}; \prec)$. We prove that the PAC procedure can be expressed as a Modeq.

\begin{lemma}
Let $\mathfrak{B}$ be a countable $\omega$-categorical $\tau$-structure with maximal arity $p$. Then there exists a Boolean Modeq $\Theta$ of width $(1, p)$ such that $[\Theta]$ equals the class of all finite $\tau$-structures where the PAC procedure for $\text{CSP}(\mathfrak{B})$ derives $\text{goal}$.
\end{lemma}

\begin{proof}
Theorem 8 implies that we may assume without loss of generality that the automorphism group of $\mathfrak{B}$ has finitely many orbits $O_1, \ldots, O_n$; choose representatives $b_1, \ldots, b_n$ from these orbits. For every $i \leq n$, let $\Pi_i$ be the Datalog program for the hyperarc consistency procedure for $\text{CSP}(\mathfrak{B}, \{b_i\})$ (which has width $(1, p)$; see Section 8.4 in [8]). Let $C_i$ be the unary IDB of $\Pi_i$ for the relation $\{b_i\}$, and let $\Pi'_i$ be the Datalog program obtained from $\Pi_i$ by adding the rule $C_i(\lambda_1) :- \cdots$ (without precondition). Since expressibility by Datalog programs of width $(1, p)$ is closed under intersection (Lemma 25), there is a Datalog program $\Pi$ of width $(1, p)$ expressing $\Pi_1' \land \cdots \land \Pi_n'$. Also note that $\Theta := \exists x . \Pi$ holds on a $\tau$-structure $\mathfrak{A}$ if and only if there exists an element $a \in A$ such that for every $i \leq n$ the program $\Pi'_i$ derives $\text{goal}$ on $(\mathfrak{A}, \{a\})$, which by definition is the case if and only if the PAC procedure derives $\text{goal}$ on $\mathfrak{A}$. This shows the statement.
\end{proof}

\begin{example}
The following is based on an example from [22] of a structure such that the complement of the CSP of this structure cannot be solved by PAC, but can be solved by
singleton arc consistency (SAC), and hence is in Datalog. We will show below that it is even in Modeq. Let $\mathfrak{B}$ be the structure with domain $\{-1,0,1,2\}$ and relations

$$R^\mathfrak{B} := \{-1,0,1,2\}^2 \setminus \{(-1,-1)\}$$

$$S^\mathfrak{B} := \{(0,1),(1,2),(2,0),(-1,-1)\}$$

and let $\mathfrak{A}$ be the structure with the domain $\{a,b,c,a',b',c'\}$ and the relations

$$R^\mathfrak{A} := \{(a,a')\}$$

$$S^\mathfrak{A} := \{(a,b),(b,c),(a,c),(a',b'),(b',c'),(a',c')\}$$

Then there is no homomorphism from $\mathfrak{A}$ to $\mathfrak{B}$, but the PAC procedure for CSP($\mathfrak{B}$) does not derive goal on $\mathfrak{A}$ [22]. However, the problem can be solved by the Modeq $\exists x_1,x_2. \Pi$ where $\Pi$ is the following monadic flag-and-check program of arity two.

$$U_0(\lambda_1) := \quad U_0(\lambda_2) := \quad \neg \text{goal}$$

$$U_1(z) := U_0(y), S(y,z) \quad U_1(y) := U_0(z), S(y,z)$$

$$U_2(z) := U_1(y), S(y,z) \quad U_0(y) := U_1(z), S(y,z)$$

$$U_0(z) := U_2(y), S(y,z) \quad U_1(y) := U_2(z), S(y,z)$$

$$\text{goal} := U_0(y), U_1(y), R(y,z), U_0(z), U_1(z)$$

Claim. $\exists x_1,x_2. \Pi$ evaluates to true on a finite $\{R,S\}$-structure $\mathfrak{A}$ if and only if there is no homomorphism from $\mathfrak{A}$ to $\mathfrak{B}$. First suppose that there are $a_1,a_2 \in A$ such that $\Pi$ derives goal on the $\{\lambda_1,\lambda_2\}$-expansion $\mathfrak{A}'$ of $\mathfrak{A}$ where $\lambda_i^{\mathfrak{A}'} = a_i$ for $i \in \{1,2\}$. This means that there are $b_1,b_2 \in A$ such that $(b_1,b_2) \in R^\mathfrak{A}$, and there are paths of net length 0 and 1 from $a_1$ to $b_1$, and paths of net length 0 and 1 from $a_2$ to $b_2$. In general, the existence of paths of net length 0 and 1 between two vertices implies that both have to be mapped to $-1$. Therefore, any homomorphism from $\mathfrak{A}$ to $\mathfrak{B}$ must map both $b_1$ and $b_2$ to $-1$, which is impossible since $(b_1,b_2) \in R^\mathfrak{A}$.

Now suppose that for any $a_1,a_2 \in A$ the program $\Pi$ does not derive goal on the structure $\mathfrak{A}'$ defined above. That is, for every $(b_1,b_2) \in R^\mathfrak{A}$ there exists $i \in \{1,2\}$ such that the for all $u \in A$ that are connected to $b_i$ in the graph defined by $S^\mathfrak{A}$ there is no path of net length 0 and no path of net length 1 to $b_i$. Hence, there must exist a path of net length 2 from $u$ to $b_i$. We then define $h(u) := b_i + 2 \mod 3$. For all other $u \in A$, we define $h(u) := -1$. It is straightforward to verify that $h$ is a homomorphism from $\mathfrak{A}$ to $\mathfrak{B}$. \hfill \triangle$

An example of a Datalog query in MSO which cannot be expressed in Modeq has been presented in [42] (Example 6); in fact, the same query is not even expressible in GQ, as we will show in Section 6.4 (Example 53), so we present it in more detail in the following.

Example 42. Let $\tau$ be the EDB signature consisting of the binary relation symbols $C$, $L$, and $D$. Let $\Phi_1(x,y)$ be the MSO $\tau$-formula

$$\exists U_2, U_3 \exists \forall u,v \left((C(u,z) \Rightarrow U_3(u)) \right. \left. \wedge \quad (U_2(v) \wedge C(u,v) \Rightarrow U_3(u)) \right.$$

$$\wedge \quad (L(x,u) \Rightarrow U_2(u)) \left. \right. \wedge \left. \quad (U_2(u) \wedge U_3(u) \wedge L(u,v) \Rightarrow U_2(v)) \wedge \neg U_2(y) \right);$$

Figure 3 depicts a $\tau$-structure that satisfies $\neg \Phi_1(x,y)$ for the elements of the structure labelled with $x$ and $y$. Let $\Phi_2(u,v)$ be the MSO formula
Figure 3 An illustration of a structure that satisfies the sentence $\Psi$ in Example 42.

$\exists U_1 \forall x, y (U_1(u) \land (U_1(x) \land \neg \Phi_1(x, y) \Rightarrow U_1(y)) \land \neg (U_1(x) \land \neg \Phi_1(x, v)))$.

Finally, let $\Psi$ be the MSO sentence $\exists u, v (D(u, v) \land \neg \Phi_2(u, v))$. See Figure 3 for an illustration of a $\tau$-structure that satisfies $\Psi$. It follows from the results of Rudolph and Krötzsch [42] (Example 46) that $\Psi$ can be expressed by a Datalog program.

### 6.3 Nested Queries

The expressive power of Datalog fragments can sometimes be increased by considering nesting, which is a concept introduced in [42] and further studied in [18]. The idea is that in nested queries we allow the use of other nested queries as if they were atomic formulas. Depending on the query language we start with, nesting may or may not increase the expressive power. Nested Datalog programs, for example, can be rewritten into equivalent Datalog programs without nesting. Similarly, MSO and GSO are closed under nesting. On the other hand, nested monadic queries (Nemodeq) are strictly more expressive than monadic queries [42], and similarly nested guarded queries ($GQ^+$) are strictly more expressive than guarded queries, as we will see below (Proposition 53). We mention that the layered tree programs studied in [21] are in fact the queries obtained from linear monadic Datalog programs with at most one EDB per rule via nesting.

\begin{definition}[$\tau$-FCP]
Let $q, m \in \mathbb{N}$ and let $\tau$ be a finite relational signature. A $q$-nested (monadic, guarded) flag-and-check $\tau$-program of arity $m$ is defined inductively as follows. A 1-nested (monadic, guarded) $\tau$-FCP of arity $m$ is the same as a (monadic, guarded) $\tau$-FCP of arity $m$ as defined in Definition 37. A $q + 1$-nested (monadic, guarded) $\tau$-FCP of arity $m$ is a (monadic, guarded) $\tau$-FCP $\Pi$ of arity $m$ that may use in rule bodies $q$-nested (monadic, guarded) $\tau$-FCPs of arity $\ell$ in addition to $\ell$-ary relation symbols. These queries are called the subqueries of $\Pi$ at nesting level $q$; the subqueries of $\Pi$ at nesting level $j$ are inductively defined as the subqueries of the subqueries at nesting level $j - 1$. In the case of guarded $q + 1$-nested FCPs, the $q$-nested FCPs may not serve as guards. An FCP has width $m$ if all its subqueries have arity at most $m$.

A $(q$-nested, monadic, guarded, width $m)$ $\tau$-query is a query of the form $\exists \bar{x}. \Pi$ where $\Pi$ is a $(q$-nested, monadic, guarded, width $m)$ $\tau$-FCP.
\end{definition}

\begin{remark}
Note that all the classes of queries defined in Definition 43 are closed under disjunction by appropriately taking the union of the rule sets, just as in the proof of Lemma 25 for Datalog.

The class of nested guarded queries is denoted by $GQ^+$, and the class of nested monadic queries by Nemodeq. It is known that every nested monadic query is equivalent to a Datalog program [42]; the same is even true for every nested guarded query [18, Figure 1]. The following fact is implicit in [18].
Theorem 45. Let $\tau$ be a finite relational signature with maximal arity $s$. Let $\Pi$ be a $q$-nested guarded FCP of arity $m$ and EDBs $\tau$ such that all rules have at most $k$ variables. Then there exists a Datalog program $\Pi'$ of width $(m + s, m + k)$ with a distinguished IDB $P_\Pi$ of arity $m$ such that for every $\tau$-structure $\mathfrak{A}$, a tuple $\bar{a} \in \mathcal{A}^m$ satisfies $\Pi(\bar{a})$ if and only if $\bar{a} \in P_\Pi^\Pi(\mathfrak{A})$. The program $\Pi'$ can be computed in polynomial time from $\Pi$.

Proof. The proof follows closely the corresponding statement for Nemodeq [42]. For $q = 1$, the Datalog program $\Pi'$ contains for each rule in $\Pi$ a new rule obtained by

- replacing each constant $\lambda_i$ by a new variable $x_i$,
- replacing each occurrence of $\text{goal}$ by $P_\Pi(x_1, \ldots, x_m)$ where $P_\Pi$ is a new IDB of arity $m$;
- replacing each atomic formula $R(\bar{y})$ by a new atomic formula $R'(\bar{x}_1, \ldots, x_m, \bar{y})$ where $R'$ is a new IDB.

For $q > 1$, the translation is defined recursively: let $\Pi_1, \ldots, \Pi_s$ be the subqueries of $\Pi$ at nesting level $q - 1$. Let $\Pi'_1, \ldots, \Pi'_s$ be the Datalog programs that can be associated to these FCPs by the inductive assumption; we may assume that the IDBs for all these programs are pairwise disjoint. Then $\Pi'$ is defined to be the union over the rules of $\Pi_1, \ldots, \Pi_s$ together with the rules of $\Pi$ where we replace each subquery $\Pi_i$ at nesting level $q$ by $P_\Pi$.

To verify that the Datalog program $\Pi'$ defined in this way satisfies the required properties, let $\mathfrak{A}$ a $\tau$-structure and suppose that $\bar{a} \in \mathcal{A}^m$ satisfies $\Pi(\bar{a})$. This means that $\Pi$ derives $\text{goal}$ on the $\tau \cup \{\lambda_1, \ldots, \lambda_m\}$-expansion $\mathfrak{A}'$ of $\mathfrak{A}$ where $\lambda_i^{\mathfrak{A}'} = a_i$ for all $i \in \{1, \ldots, m\}$, that is, $\text{goal}^{\Pi(\mathfrak{A}')}$ = $\{()\}$. It can be shown by induction over the evaluation of Datalog programs (see Remark 3) that this is the case if and only if $\bar{a} \in P_\Pi^\Pi(\mathfrak{A})$.

We therefore use some of the terminology that we introduced for Datalog also for Nemodeq and for GQ+. It is also known that Nemodeq is contained in MSO [42].

Example 46. Example 42 can be expressed in Nemodeq [42], and hence is in Datalog and in MSO.

Proposition 47. Every problem in GQ+ is contained in GSO.

Proof. This is an immediate consequence of Proposition 38, because GSO is closed under nesting.

6.4 The Nested Guarded Game

In this section we present a modification of the existential guarded $k$ pebble game that allows to capture the expressive power of GQ and GQ+. In particular, we will prove that the query in Example 42 is not in GQ. We call this game the nested guarded game; it will also be used in the next section to prove that there are problems in the intersection of Datalog and GSO that cannot be expressed in GQ+.

Again we start with an informal description of the game. Let $\tau$ be a finite relational signature. The game has three parameters, $q$, $m$, and $k$. There are two players, Spoiler and Duplicator, that play on a pair of $\tau$-structures $(\mathfrak{A}, \mathfrak{B})$. Each player has $k$ labelled pebbles, out of which $m$ pebbles are blue, the others are red. Spoiler places the blue pebbles on $\mathfrak{A}$, Duplicator answers by placing her blue pebbles on elements of $\mathfrak{B}$. Then the two players play the existential guarded $k - m$ pebble game with the red vertices, with the difference that Duplicator looses if the map between all the pebbled vertices (blue and red alike) is not a partial homomorphism. At most $q$ times, Spoiler can relocate the red pebbles (without the guard restriction). We present a formal definition of winning strategies for Duplicator in the
nested guarded game; all statements about the game only involve such winning strategies for Duplicator.

**Definition 48.** Let $k, q, m \in \mathbb{N}$. A winning strategy for Duplicator for the $q$ nested width $m$ guarded $k$ pebble game on two $\tau$-structures $(\mathfrak{A}, \mathfrak{B})$ is a sequence $H_0, H_1, \ldots, H_q$ of non-empty sets of partial homomorphisms from $\mathfrak{A}$ to $\mathfrak{B}$ such that
1. each of $H_0, H_1, \ldots, H_q$ is closed under restriction;
2. if $h \in H_i$, for $i \in \{1, \ldots, q\}$, is such that there exists a tuple in a relation of $\mathfrak{A}$ whose entries contain $\text{dom}(h)$, then $H_i$ contains for every $S \subseteq A$ with $|S| \leq k$ and $\text{dom}(h) \subseteq S$ an extension of $h$ with domain $S$;
3. if $h \in H_i$, for $i \in \{1, \ldots, q\}$ and $S \subseteq A$ with $|S| \leq k$ is such that $\text{dom}(h) \subseteq S$ and $|\text{dom}(h)| \leq m$, then $H_{i+1}$ contains an extension of $h$ with domain $S$.

To prove the connection between GQ$^+$ and the $q$ nested guarded $k$ pebble game we need an appropriate notion of canonical Boolean $q$ nested guarded queries. In analogy to Section 4, it suffices to present this connection for complements of CSPs of $\omega$-categorical structures $\mathfrak{B}$, by Corollary 21.

**Definition 49 (Canonical nested guarded queries).** Let $\mathfrak{B}$ be an $\omega$-categorical structure with a finite relational signature $\tau$ and let $R \subseteq B^m$ be a relation with a primitive positive definition over $\mathfrak{B}$. The canonical $q$ nested guarded query $\Pi_R$ of width $\langle m, k \rangle$ for $(\mathfrak{B}, R)$ is defined by induction over $q$ as follows. For $q = 1$, let $o^1 = (o^1_1, \ldots, o^1_m), \ldots, o^s = (o^s_1, \ldots, o^s_m) \in B^m$ be representatives of all orbits of $m$-tuples of Aut($\mathfrak{B}$) that are not contained in $R$. For $i \in \{1, \ldots, s\}$ let $\Pi_{\omega^i}$ be the canonical frontier-guarded Datalog program of the $\omega$-categorical structure $(\mathfrak{B}; o^1_1, \ldots, o^1_m)$. We transform $\Pi_{\omega^i}$ into an $m$-ary FCP by replacing literals of the form $o^i_j = x$ by $\lambda_j = x$. Let $\Pi$ be obtained by taking the conjunction of all the resulting FCPs for each $i \in \{1, \ldots, s\}$ (which is again an FCP by Lemma 25).

For $q > 1$, we suppose inductively that for all $m \geq 0$ and relations $S$ with a primitive positive definition over $\mathfrak{B}$ the canonical $q - 1$ nested guarded query $\Xi_S$ of width $\langle m, k \rangle$ for $(\mathfrak{B}, S)$ is already defined. Replace in the canonical $1$ nested guarded query of width $\langle m, k \rangle$ for $(\mathfrak{B}, R)$ every occurrence of an EDB $S$ by $\Xi_S$. We define $\Pi_R$ to be the resulting $q$-nested query. The canonical $q$ nested guarded query $\Pi$ of width $\langle m, k \rangle$ for $\mathfrak{B}$ is obtained from the canonical $q$ nested guarded query $\Pi$ of width $\langle m, k \rangle$ for $(\mathfrak{B}, \emptyset)$ by existentially quantifying all free variables.

**Definition 50 ($q$ nested $m$ bounded $k$ variable logic).** Let $\tau$ be a relational signature and let $q, m, k \in \mathbb{N}$. Then $\tau$-sentences in $q$ nested $m$ bounded $k$ variable logic $L^{m,k}_q$ are built inductively from atomic $\tau$-formulas and the following operation: if $\phi_1, \ldots, \phi_s$ are formulas from $L^{m,k}_q$, then
\[
\exists y (\phi_1 \land \cdots \land \phi_s)
\]
is in $L^{m,k}_q$ if
- there exists an $i \in \{1, \ldots, s\}$ and an atomic formula $\psi$ in $\phi_i$ whose variables contain all the variables that are not existentially quantified in $y$,
- each of the formulas $\phi_1, \ldots, \phi_s$ is from $L^{m,k}_{q-1}$.

**Theorem 51.** Let $\mathfrak{B}$ be an $\omega$-categorical structure with finite relational signature $\tau$ and let $\mathfrak{A}$ be a finite $\tau$-structure. Then for all $q, m, k \in \mathbb{N}$ the following statements are equivalent.
1. Every $q$ nested guarded query of width $\langle m, k \rangle$ which is sound for the complement of CSP($\mathfrak{B}$) is false on $\mathfrak{A}$.
2. The canonical $q$-nested guarded query of width $\langle m, k \rangle$ for the complement of CSP($\mathfrak{B}$) is false on $\mathfrak{A}$. 


3. Duplicator has a winning strategy for the \( q \) nested width \( m \) guarded \( k \) pebble game on \((\mathfrak{A}, \mathfrak{B})\).

4. Every sentence from \( F_{q}^{m,k} \) which holds in \( \mathfrak{A} \) also holds in \( \mathfrak{B} \).

**Proof.** For the implication from 1. to 2., it suffices to prove that the canonical \( q \)-nested guarded query \( \Pi \) of width \((m, k)\) is sound for the complement of \( \text{CSP}(\mathfrak{B}) \). Let \( \mathfrak{A} \) be a finite \( \tau \)-structure. Let \( R \subseteq B^{m} \) be primitively positively definable over \( \mathfrak{B} \). First observe that if \( (s_{1}, \ldots, s_{m}) \) and \( (s'_{1}, \ldots, s'_{m}) \) have the same orbit in \( \text{Aut}(\mathfrak{B}) \), then \((\mathfrak{B}, s_{1}, \ldots, s_{m}) \) and \((\mathfrak{B}, s'_{1}, \ldots, s'_{m}) \) have the same canonical frontier-guarded Datalog program. Hence, if \( q = 1 \) then \( \Pi(t_{1}, \ldots, t_{m}) \) holds in \( \mathfrak{A} \) if and only if for every tuple \((s_{1}, \ldots, s_{m}) \in B^{m} \setminus R \) the canonical frontier-guarded Datalog program for \((\mathfrak{B}, s_{1}, \ldots, s_{m}) \) derives goal. This in turn means that there exists no homomorphism from \( \mathfrak{A} \) to \( \mathfrak{B} \) which maps \((t_{1}, \ldots, t_{m}) \) to \((s_{1}, \ldots, s_{m}) \).

By induction on the nesting depth \( q \) it follows that if \( \mathfrak{A} \) satisfies the canonical \( q \) nested guarded query of with \((m, k)\) for \( \mathfrak{B} \) then there is no homomorphism from \( \mathfrak{A} \) to \( \mathfrak{B} \), and hence \( \Pi \) is sound for \( \text{CSP}(\mathfrak{B}) \).

For the implication from 2. to 3., let \( \mathfrak{B}' \) be the expansion of \( \mathfrak{B} \) by all primitive positive definable relations of arity at most \( m \); since \( \mathfrak{B} \) is \( \omega \)-categorical, the structure \( \mathfrak{B}' \) still has a finite relational signature \( \tau' \). We compute a winning strategy \( H_{0}, H_{1}, \ldots, H_{q} \) for Duplicator for the \( q \) nested width \( m \) guarded \( k \) pebble game on \((\mathfrak{A}, \mathfrak{B})\) using the canonical \( q \)-nested guarded query of width \((m, k)\) for \((\mathfrak{B}', R)\) for every relation \( R \) of arity \( m \) which has a primitive positive definition in \( \mathfrak{B} \). Define \( \mathfrak{A}'_{0} \) be the expansion of \( \mathfrak{A} \) with the same signature as \( \mathfrak{B}' \) that contains for every \( m \)-ary relation symbol \( R \in \tau' \setminus \tau \) the empty relation, i.e., \( R^{\mathfrak{A}'_{0}} = \emptyset \). For \( i \in \{0, \ldots, q-1\} \), suppose that \( \mathfrak{A}'_{i}, \ldots, \mathfrak{A}'_{i} \) have already been defined. Let \( \mathfrak{A}'_{i+1} \) be the expansion of \( \mathfrak{A} \) with the same signature as \( \mathfrak{B}' \) that contains for every \( m \)-ary relation symbol \( R \in \tau' \setminus \tau \) the relation computed by the canonical \( i \)-nested guarded query of width \((m, k)\) for \((\mathfrak{B}', R)\) on \( \mathfrak{A}'_{i} \). For \( i \in \{0, \ldots, q\} \), let \( H_{i} \) be the set of all partial homomorphisms \( f \) from \( \mathfrak{A}'_{i} \) to \( \mathfrak{B}' \) with domain of size at most \( k \). Note that since the canonical \( q \) nested guarded query of width \((m, k)\) for \( \mathfrak{B} \) is false on \( \mathfrak{A} \), the relation symbol \( F \) of arity \( 0 \) which denotes the empty relation over \( \mathfrak{B} \) (which is primitively positively definable) denotes the empty relation over \( \mathfrak{A}'_{i} \) as well, and hence \( H_{0}, H_{1}, \ldots, H_{q} \) are non-empty. Clearly, these sets are closed under restriction.

We claim that the sequence \( H_{0}, H_{1}, \ldots, H_{q} \) also satisfies items 2. and 3. in the definition of winning strategies (Definition 48). Indeed, for item 2., let \( h \in H_{i} \), for \( i \in \{1, \ldots, q\} \), be such that there exists a tuple in a relation of \( \mathfrak{A} \) whose entries contain \( \text{dom}(h) = \{a_{1}, \ldots, a_{j}\} \), and let \( S \subseteq A \) be a superset of \( \text{dom}(h) \) of size at most \( k \). Consider the following frontier-guarded rule in the canonical Datalog program for \((\mathfrak{B}, h(a_{1}), \ldots, h(a_{j}))\): the body of the rule is the canonical query \( \phi \) of the substructure of \( \mathfrak{A}'_{q} \) induced on \( S \). The head of the rule is \( R(a_{1}, \ldots, a_{j}) \) where \( R \in \tau' \) is such that \( R^{\mathfrak{A}'} \) is the projection of the relation defined by \( \phi \) in \( \mathfrak{B}' \) to \( a_{1}, \ldots, a_{j} \). By the assumption that there exists a tuple in a relation of \( \mathfrak{A} \) whose entries contain \( \{a_{1}, \ldots, a_{j}\} \), this rule is indeed frontier guarded. Since the rule applies to \( \mathfrak{B}' \) we obtain that \( (a_{1}, \ldots, a_{j}) \in R^{\mathfrak{A}'} \). By the definition of \( H_{i} \), we have that \( (h(a_{1}), \ldots, h(a_{j})) \in R^{\mathfrak{B}'} \). By the definition of \( R^{\mathfrak{B}'} \) we can find elements in \( B' \) for the other variables of \( \phi \) so that \( \phi \) is satisfied, and this shows that \( h \) can be extended to a partial homomorphism from \( \mathfrak{A}'_{q} \) to \( \mathfrak{B}' \) defined on all of \( S \).

We show item 3. by induction over \( i \in \{1, \ldots, q\} \). Let \( h \in H_{i} \) be such that \( \text{dom}(h) \) has size at most \( m \) and let \( S \subseteq A \) be a superset of \( \text{dom}(h) = \{a_{1}, \ldots, a_{j}\} \) of size \( j \leq k \). We have to show that \( H_{i-1} \) contains an extension of \( h \) with domain \( S \). Let \( \phi \) be the primitive positive formula obtained from the canonical query of the substructure \( \mathfrak{A}_{S} \) of \( \mathfrak{A}'_{i} \) induced on \( S \) by existentially quantifying all variables except the ones in the domain of \( h \). Then \( \phi \)
is equivalent to a primitive positive formula over the signature of $\mathcal{B}$; let $R$ be the relation symbol of $\mathcal{B}'$ for the relation defined by $\phi$ in $\mathcal{B}$. For any $t \in B' \setminus R^{B'}$ the canonical $q$-nested query derives goal since the canonical query of $\mathcal{A}_S$ together with $a_1 = t_1, \ldots, a_j = t_j$ is unsatisfiable in $\langle \mathcal{B}, t_1, \ldots, t_j \rangle$. Hence, $a \in R^{B'}$. In this case, $h(a) \in R^\mathcal{B}$ since $h$ is a partial homomorphism on the entries of $a$. Therefore, $h(a)$ satisfies $\phi$ and the witnesses for the existentially quantified variables of $\phi$ provide an extension of $h$ to a partial homomorphism from $\mathcal{A}_{i+1}$ to $\mathcal{B}$ which is defined on all of $S$.

3. implies 4: We show by induction over the syntactic structure of $L_{q}^{m,k}$ formulas that if $\phi(v_1, \ldots, v_m)$ is an $L_{q}^{k}$ formula, then for all $h \in H_q$ and all elements $a_1, \ldots, a_m$ from the domain of $h$, if $\mathcal{A}$ satisfies $\phi(a_1, \ldots, a_m)$, then $\mathcal{A}$ satisfies $\phi(h(a_1), \ldots, h(a_m))$. For $m = 0$ this implies 4. The base case of the induction is obvious because atomic formulas are preserved by homomorphisms. Now suppose that $\phi$ is of the form $\exists \bar{y}(\phi_1 \land \cdots \land \phi_s)$ where $\phi_1, \ldots, \phi_s$ are formulas from $L_{q}^{m,k}$. Let $\bar{c}$ be a tuple providing witnesses for the variables $\bar{y}$ that shows that $\phi(a_1, \ldots, a_m)$ holds in $\mathcal{A}$.

If there exists an $i \in \{1, \ldots, s\}$ and an atomic formula $\psi(\bar{z})$ in $\phi_i$ whose variables contain all the variables that are not existentially quantified in $\bar{y}$, then $h(\bar{z})$ is a tuple in a relation of $\mathcal{A}$ that contains the domain of $h$. Hence, $h$ has an extension $h'$ whose domain contains the entries of $\bar{c}$, because $h \in H_q$. Then $h'(\bar{c})$ provides the witnesses for $\bar{y}$ that show that $\phi(h(a_1), \ldots, h(a_m))$ holds in $\mathcal{A}$, because $\phi_i(h(a_1), \ldots, h(a_m), h'(\bar{c}))$ holds by inductive assumption for every $i \leq s$. If each of the formulas $\phi_1, \ldots, \phi_s$ is even from $L_{q-1}^{m,k}$, then we consider the extension $h'$ of $h$ from $H_{q-1}$ whose domain also contains the entries of $\bar{c}$; such an extension exists because $h \in H_q$. By the inductive assumption, $\mathcal{A}$ satisfies $\phi_i(h'(a_1), \ldots, h'(a_m), h'(\bar{c}))$ for every $i \leq s$. This concludes the induction.

Finally, 4. implies 1: suppose that there is a $q$-nested guarded query $\phi$ of width $(m, k)$ which is sound for the complement of CSP($\mathcal{B}$) and true on $\mathcal{A}$. We translate the evaluation of $\phi$ on $\mathcal{A}$ into a sentence from $L_{q}^{m,k}$ which is true on $\mathcal{B}$ but false on $\mathcal{B}$. Suppose that $\phi$ is of the form $\exists \bar{x}. \Pi$ where $\Pi$ is a $q$-nested guarded FCP, and let $\bar{a}$ be elements of $A$ for the variables in $\bar{x}$ that show that $\phi$ is true in $\mathcal{A}$.

For each IDB $R$ of $\Pi$ of arity $k$ and every $k$-tuple $\bar{a}$ such that $\Pi$ derives $R(\bar{a})$ on $\mathcal{A}$ we define an $L_{q}^{m,k}$-formula $\psi(x_1, \ldots, x_k)$ which holds on $\bar{a}$ in $\mathcal{A}$ and such that $\Pi$ derives $R(\bar{x})$ on the canonical database of $\psi(\bar{x})$ (after transforming it into prenex normal form) by induction over the evaluation of $\Pi$ on $\mathcal{A}$. Let $\theta(x_1, \ldots, x_k, \bar{y})$ be the body of the rule of $\Pi$ that derived $R(\bar{a})$ on $(\bar{a}, \bar{b})$. For every atomic formula $S(\bar{z})$ of $\theta$ we may assume by inductive assumption that there exists an $L_{q}^{m,k}$-formula $\chi(\bar{z})$ which holds on the respective entries $\bar{c}$ of $(\bar{a}, \bar{b})$ in $\mathcal{A}$ and such that $\Pi$ derives $S(\bar{c})$ on the canonical database of $\chi(\bar{z})$. Then we define $\psi$ to be the conjunction of all these formulas where all variables $\bar{y}$ are existentially quantified. This formula clearly holds on $\bar{a}$ in $\mathcal{A}$, and $\Pi$ derives $R(\bar{x})$ on the canonical database of $\psi$. By the guard assumption, the rule of $\Pi$ that derives $R(\bar{a})$ must contain an atomic formula whose variables contain $x_1, \ldots, x_k$, so the formula $\psi$ is indeed an $L_{q}^{m,k}$-formula. Then the formula that we obtain for the IDB $R$ of $\Pi$ that denotes $B_k$ in $\mathcal{B}$ by existentially quantifying all variables is true on $\mathcal{A}$ but false on $\mathcal{B}$.

\textbf{Corollary 52.} Let $\mathcal{B}$ be an $\omega$-categorical structure with a finite relational signature $\tau$ and let $q, m \geq 1$. Then the complement of CSP($\mathcal{B}$) cannot be expressed by a $q$-nested width $m$ guarded query if and only if for all $k \geq 1$ there exists an unsatisfiable instance $\mathcal{A}$ of CSP($\mathcal{B}$) such that Duplicator has a winning strategy for the $q$ nested width $m$ guarded $k$ pebble game on $(\mathcal{A}, \mathcal{B})$.

\textbf{Proof.} For the backwards direction, let $\Pi$ be a $q$-nested guarded query of width $(m, k)$
which is sound for the complement of CSP($\mathfrak{B}$). By assumption, there exists an unsatisfiable instance $\mathfrak{A}$ of CSP($\mathfrak{B}$) such that Duplicator has a winning strategy for the $q$ nested width $m$ guarded $k$ pebble game on ($\mathfrak{A}$, $\mathfrak{B}$). By the implication from 3. to 1. in Theorem 51, the query $\Pi$ is false on $\mathfrak{A}$. But then $\Pi$ does not express the complement of CSP($\mathfrak{B}$).

For the forwards direction, we show the contraposition. We assume that there exists a $k \geq 1$ such that for every unsatisfiable instance $\mathfrak{A}$ of CSP($\mathfrak{B}$) Duplicator has no winning strategy for the $q$ nested width $m$ guarded $k$ pebble game on ($\mathfrak{A}$, $\mathfrak{B}$). It suffices to prove that the canonical $q$ nested guarded query $\Pi$ of width $(m, k)$ for the complement of CSP($\mathfrak{B}$) expresses the complement of CSP($\mathfrak{B}$). Let $\mathfrak{A}$ be an instance of CSP($\mathfrak{B}$). If $\mathfrak{A}$ is satisfiable then $\Pi$ is false on $\mathfrak{A}$, because $\Pi$ is sound for the complement of CSP($\mathfrak{B}$) as shown in the proof of the implication 1. implies 2. in Theorem 51. If $\mathfrak{A}$ is unsatisfiable then the contraposition of the implication from 2. to 3. in Theorem 51 implies that $\Pi$ is true on $\mathfrak{A}$. Hence, $\Pi$ expresses the complement of CSP($\mathfrak{B}$).

\begin{proposition}
The class of finite structures described by the MSO sentence $\Psi$ from Example 42 is (in Datalog, but) not expressible in GQ.
\end{proposition}

\begin{proof}
It is easy to see that $\Psi$ describes a class $C$ of finite structures whose complement is closed under disjoint unions, and hence is the complement of a CSP. By Corollary 21 there exists an $\omega$-categorical structure $\mathfrak{B}$ such that the complement of CSP($\mathfrak{B}$) equals $C$.

To prove the statement we use Corollary 52 for the special case $q = 1$. Let $m, k \geq 1$. Let $\phi_1(x_0, x_k)$ be the formula

$$\exists x_1, \ldots, x_{k-1} \bigwedge_{i \in \{0, \ldots, k-1\}} C(x_1, x_{i+1}).$$

Let $\phi_2(y_0, y_k)$ be formula $\exists z, y_1, \ldots, y_{k-1} \bigwedge_{i \in \{1, \ldots, k-1\}} \{(\phi_1(y, z) \land L(y_i, y_{i+1}))\}$. Let $\phi$ be the formula $\bigwedge_{i \in \{0, \ldots, m\}} \phi_2(z_i, z_{i+1}) \land D(z_0, z_{m+1})$, rewritten in prenex normal form, and let $\mathfrak{A}$ be the canonical database of $\phi$.

\begin{claim}
$\mathfrak{A}$ satisfies $\Psi$, and hence is an unsatisfiable instance of CSP($\mathfrak{B}$). First note that $(z_0, z_1), (z_1, z_2), \ldots, (z_m, z_{m+1})$ are precisely the pairs in $A^2$ that do not satisfy $\Phi_1$. Then the vertices $z_0, z_{m+1}$ play the role of $u$ and $v$: to see that $\Phi_2(u, v)$ does not hold in $A$, let $U_1 \subseteq A$ be such that it satisfies the first two conjuncts of $\Phi_2$ for all $x, y \in A$. Then $U_1$ must contain $z_0$ by the first conjunct, and $z_1$ by the second conjunct, and inductively by the second conjunct it must contain all of $z_0, z_1, \ldots, z_{m+1}$, and hence $v$. But then the last disjunct $\neg(U_1(x) \land \neg\Phi_1(x, v))$ is not satisfied for $x = z_m$.

\begin{claim}
Duplicator has a winning strategy $H_0, H_1$ for the $1$-nested width $m$ guarded $k$ pebble game on $\mathfrak{A}$ and $\mathfrak{B}$: we set $H_0$ to be the set of all partial homomorphisms $h$ from $\mathfrak{A}$ to $\mathfrak{B}$ such that $\text{dom}(h) \subseteq m$. Set $H_1$ to be the set of all partial homomorphisms $h$ from $\mathfrak{A}$ to $\mathfrak{B}$ such that if $\text{dom}(h)$ contains the variable $z$ from a conjunct $\phi_2(y_0, y_k)$ of $\phi$, and $\phi_2(\bar{u})$ is the formula obtained from the rewriting of $\phi_2$ into prenex normal form and existentially quantifying all variables except for the ones that are in the domain of $h$, then $h(\bar{u})$ satisfies $\phi_2$ in $\mathfrak{B}$. Note that $\text{dom}(h)$ cannot contain the variable $z$ for all of the conjuncts of $\phi$ of the from $\phi_2(y_0, y_k)$, and hence $H_1$ is non-empty. It is straightforward to verify that $H_0, H_1$ satisfies the three items from Definition 48.

The statement is an immediate consequence of Corollary 52 for $q = 1$ and the two claims.
\end{claim}
\end{proof}
6.5 Separation in GSO

In this section we present an example of a GSO sentence which is in Datalog, but cannot be expressed in GQ'. The GSO sentence describes the complement of the CSP of the following structure \( \mathcal{B} \), which is fixed throughout this section. Define \( \mathcal{B} := (\mathbb{N}; D, R) \) where

\[
D := \{(x, y) \in \mathbb{N}^2 \mid x \neq y\}
\]
\[
R := \{(x, y, z) \in \mathbb{N}^3 \mid x = y \Rightarrow y = z\}.
\]

Clearly, the structure \( \mathcal{B} \) is \( \omega \)-categorical; it is even finitely bounded homogeneous. The structure \( \mathcal{B} \) plays a prominent role in the classification of structures preserved by all permutations [11] and the complexity of quantified constraint satisfaction problems for equality constraints [10, 44]. The proof of the following proposition uses ideas from Example 4.

**Proposition 54.** There is a GSO sentence that expresses \( \text{CSP}(\mathcal{B}) \).

**Proof.** Let \( \tau = \{D, R\} \) be the signature of \( \mathcal{B} \). Let \( S \) be a new ternary and \( X \) a new unary relation symbol. Let \( \chi_X \) be the formula which specifies that

- \( X \) is non-empty,
- if \( x, y, z \) are such that \( S(x, y, z) \), then \( y \in X \) if and only if \( z \in X \), and
- \( X \) is minimal with respect to the properties above (the details are similar as in Example 4).

Let \( \phi \) be the \( \tau \cup \{S, X\} \)-sentence which expresses that there exists \( S \subseteq R \) such that for all \( X \) that satisfy \( \chi_X \) we have

1. for all \( x, y, \) if \( D(x, y) \) then \( x \notin X \) or \( y \notin X \), and
2. for all \( x, y, z \), if \( R(x, y, z) \) but not \( S(x, y, z) \), then \( x \notin X \) or \( y \notin X \).

We claim that a finite structure \( \mathfrak{A} \) satisfies \( \phi \) if and only if \( \mathfrak{A} \) has a homomorphism to \( \mathcal{B} \). If \( h \) is a homomorphism from \( \mathfrak{A} \) to \( \mathcal{B} \), then we define \( S \subseteq R \) to be the relation that contains \((x, y, z) \in R \) if and only if \( h(x) = h(y) \). Let \( X \subseteq A \) be such that \( \chi_X \) is satisfied. We have to show that 1. and 2. above are satisfied. Let \( \mathfrak{A}' \) be the \( \{E, D\} \)-structure with domain \( A \) and the relations

\[
E^{\mathfrak{A}'} := \bigcup \{(x, y) \mid (x, y, z) \in S\}
\]
\[
D^{\mathfrak{A}'} := D^\mathfrak{A} \cup \{(x, y) \mid \exists z (R(x, y, z) \land \neg S(x, y, z))\}
\]

Note that \( h \) is a homomorphism from \( \mathfrak{A}' \) to structure \( (\mathbb{N}; E, D) \) from Example 4. Recall from Example 4 that any homomorphism from \( \mathfrak{A}' \) to \( (\mathbb{N}; E, D) \) must be constant on \( X \). Hence, if \( (x, y) \in D \) then \( h(x) \neq h(y) \) and hence we must have \( x \notin X \) or \( y \notin X \). To see that 2. is satisfied as well, note that if \( (x, y, z) \in R \setminus S \), then \( (x, y) \in D^{\mathfrak{A}'} \), and hence \( h(x) \neq h(y) \) by the definition of \( S \), which again implies that \( x \notin X \) or \( y \notin X \).

Now suppose that \( \mathfrak{A} \) satisfies \( \phi \). Let \( S \subseteq R \) be the ternary relation witnessing this. Define the structure \( \mathfrak{A}' \) as above. As in Example 4 we may argue that there exists a homomorphism from \( \mathfrak{A}' \) to \( (\mathbb{N}; E, D) \), which is a homomorphism from \( \mathfrak{A} \) to \( \mathcal{B} \) as well. \( \blacklozenge \)

**Proposition 55.** The complement of \( \text{CSP}(\mathcal{B}) \) cannot be expressed in \( \text{GQ}' \).

**Proof.** Let \( q, m \geq 1 \). We use Corollary 52 to show that \( \text{CSP}(\mathcal{B}) \) cannot be expressed by a \( q \)-nested width \( m \) guarded query. Let \( k \geq 1 \). We construct an unsatisfiable instance \( \mathfrak{A} \) of \( \text{CSP}(\mathcal{B}) \) such that Duplicator wins the \( q \) nested width \( m \) guarded \( k \)-pebble game on \((\mathfrak{A}, \mathcal{B})\). Without loss of generality we may assume that \( m \leq k \). It will be convenient to specify \( \mathfrak{A} \) as
the canonical database of a primitive positive \( \{D,R\} \)-formula \( \phi \). Let \( \phi_0(x,y) \) be the formula \( R(x,y) \), and for \( i > 0 \) let \( \phi_i(x,y) \) be the formula
\[
\exists x_0, \ldots, x_k \left( x = x_0 \land \bigwedge_{j=0}^{k-1} \phi_{i-1}(x_j, x_{j+1}) \land R(x_0, x_k, y) \right).
\]

Let \( \phi \) be the formula \( \phi_s(x,y) \land D(x,y) \) where \( s := q + 1 \). Let \( A \) be the canonical database of \( \phi \) after transforming \( \phi \) into prenex normal form. Note that every variable of \( \phi_s(x,y) \) except \( x \) and \( x_0 \) appears exactly once as the final argument in a conjunct that involves \( x \) and \( x_0 \).

Claim. \( A \) is an unsatisfiable instance of CSP(\( B \)). This follows from the fact that \( \phi_i(x,y) \) implies \( x = y \), for every \( i \leq s \), which can be shown by a straightforward induction over \( i \).

Claim. Duplicator has a winning strategy in the \( q \) nested width \( m \) guarded \( k \)-pebble game on \( (A, B) \).

Let \( H_0 \) be the set of all partial homomorphisms \( h \) from substructures of \( A \) to \( B \) with domain size at most \( k \), and let \( H_i \), for all \( i \in \{1, \ldots, q\} \), be the set of all partial homomorphisms \( h \) from substructures of \( A \) to \( B \) with domain size at most \( k \) such that \( h(u) = h(v) \), for \( u,v \in \text{dom}(h) \), if and only if both \( u \) and \( v \) are are elements of different subformulas of \( \phi \) of the form \( \phi_{i-1} \) or are elements of different subformulas of \( \phi \) of the form \( \phi_{i-1} \) but \( \text{dom}(h) \) contains all the variables \( x_0, \ldots, x_s, x_{s+1} \) from \( \phi_0 \), for some \( 0 \leq r < s < k \) and \( u \) appears in the subformula \( \phi_{i-1}(x_r, x_{r+1}) \) and \( v \) appears in the subformula \( \phi_{i-1}(x_s, x_{s+1}) \).

Since \( \text{dom}(h) \leq k \) it is impossible that \( r = 0 \) and \( s = k - 1 \); hence, if \( x_0 \) and \( x_k \) are from \( \text{dom}(h) \), then we will have \( h(x_0) \neq h(x_k) \).

Clearly, \( H_i \) is closed under restrictions and non-empty. Now suppose that \( h \in H_i \) is such that there exists a tuple \( a \) in a relation of \( A \) whose entries contain \( \text{dom}(h) \). Let \( S \subseteq A \) be a superset of \( \text{dom}(h) \) of cardinality at most \( k \). If this relation is \( D \), then \( a \) equals \( (x,y) \), we may clearly extend \( h \) to some \( h' \in H_i \) with \( h'(x) \neq h'(y) \). Otherwise, the relation must be \( R \) and \( a \) equals \( (x_0, x_k, y) \) for some variables \( x_0, x_k, y \) from a subformula of \( \phi \) of the form \( \phi_j(x,y) \) for some \( j \leq i \). Note that \( h(x_0) = h(x_k) = h(y) \) if \( j < i \), and \( h(x_0) \neq h(x_k) \) and \( h(x_k) \neq h(y) \) otherwise. It is easy to see that in both cases we may extend \( h \) to some \( h' \in H_i \) with \( \text{dom}(h') = S \). Finally, if \( h \in H_i \) for \( i \in \{1, \ldots, q\} \) and \( S \subseteq A \) with \( |S| \leq k \) is such that \( \text{dom}(h) \subseteq S \), then \( H_{i-1} \) contains an extension \( h' \) of \( h \) with domain \( S \); if \( x \in S \) appears in a copy of \( \phi_{i-1} \) whose variables intersect \( \text{dom}(h) \), we set \( h'(x) \) to the value taken by these variables under \( h \). If \( \text{dom}(h) \) contains all the variables \( x_0, x_1, \ldots, x_s, x_{s+1} \) from \( \phi_i \) for some \( 0 \leq r < s < k \) and \( x \) appears in the subformula \( \phi_{i-1}(x_r, x_{r+1}) \) and some variable of \( \phi_{i-1}(x_r, x_{r+1}) \) appears in \( \text{dom}(h) \), then we set \( h'(x) \) to the value taken by this variable under \( h \). Otherwise, pick \( h'(x) \) to be a new value. Hence, \( H_0, H_1, \ldots, H_q \) is indeed a winning strategy for Duplicator for the \( q \) nested width \( m \) guarded \( k \)-pebble game on \( (A, B) \).

\[\blacktriangleleft\]

\[\blacktriangleright\text{Proposition 56.} \text{ The complement of CSP}(B) \text{ can be expressed in Datalog.}\]

\[\blacktriangleleft\text{Proof.} \text{ It is easy to see that CSP}(B) \text{ can be solved by a Datalog program of width } (2,3) \text{, because for a given } \tau\text{-structure } A \text{ it suffices to compute the smallest transitive reflexive binary relation } T \text{ such that for every } (x,y,z)\in R^A \text{ with } (x,y)\in T \text{ we have } (y,z)\in T. \]

\[\blacktriangleleft\text{Corollary 57.} \text{ The intersection of GSO and Datalog contains problems that cannot be expressed in GQ}.\]

\[\blacktriangleleft\text{Proof.} \text{ Since GSO is closed under negation, Proposition 54 implies that the complement of CSP}(B) \text{ is in GSO, and Proposition 55 shows that CSP}(B) \text{ is not in GQ}. \]
6.6 Separation in MSO

In this section we will prove that there are problems in MSO that can be expressed in Datalog, but that cannot be expressed in Nemodeq. The MSO sentence describes the complement of the CSP of a structure $C$ which is closely related to the structure $B$ from Section 6.5. Throughout this section, let $C$ be the $\{D,R\}$-structure $(C; D^C, R^C)$ where

$$
C := \mathbb{N} \cup \mathbb{N}^3
$$

$$
D^C := \{(x,y) \in C^2 \mid x, y \in \mathbb{N}, x \neq y\}
$$

$$
R^C := \{(x,y,z,t) \in C^4 \mid x, y, z \in \mathbb{N}, t = (x,y,z), x = y \Rightarrow y = z\}.
$$

That is, the domain $C$ contains two sorts of elements: all natural numbers and all triples of natural numbers. In words, the binary relation $D^C$ expresses disequality between natural numbers, whereas the quaternary relation $R^C$ consists of those quadruples where the first three components are natural numbers while the last component is the triple built from the first three components. Among those quadruples, $R^C$ contains those where the first three components are identical whenever the first two components are. An alternative formulation would be to say that $R^C$ contains all quadruples of the form $(x,y,z,(x,y,z))$ except those where $x = y$ and $y \neq z$.

To prove that the complement of $\text{CSP}(C)$ is in Datalog, we show that $C$ has a primitive positive interpretation in the structure $\mathcal{B}$ from the previous section and then use a known general transfer result for containment in Datalog.

**Definition 58.** Let $\sigma$ and $\tau$ be finite relational signatures, and let $d, p \in \mathbb{N}$. A $d$-dimensional interpretation $I$ of $\tau$ in $\sigma$ consists of a $\sigma$-formula $R_I(\bar{x}_1, \ldots, \bar{x}_n)$ for every $R \in \tau$ of arity $n$, where $\bar{x}_1, \ldots, \bar{x}_n$ are $d$-tuples of variables. If $\mathcal{A}$ is a $\sigma$-structure, then $I(\mathcal{A})$ is the $\tau$-structure with domain $A^d$ and for $R \in \tau$ the relation

$$
R^{I(\mathcal{A})} := \{(\bar{t}_1, \ldots, \bar{t}_n) \in (A^d)^n \mid \mathcal{A} \models R_I(\bar{t}_1, \ldots, \bar{t}_n)\}.
$$

We then say that $I$ is an interpretation of $I(\mathcal{A})$ in $\mathcal{A}$. If $\Theta$ is a set of formulas, then a $\Theta$-interpretation is an interpretation where all the interpreting formulas are from $\Theta$.

**Lemma 59.** $C$ has a 5-dimensional primitive positive interpretation in $\mathcal{B}$.

**Proof.** To define the interpretation $I$ of $C$ in $\mathcal{B}$, let $D_I(x_1, \ldots, x_5, y_1, \ldots, y_5)$ be $x_1 = x_2 \land y_1 = y_2 \land x_1 \neq y_1$. The formula $R_I(x_1, \ldots, x_5, y_1, \ldots, y_5, z_1, \ldots, z_5, t_1, \ldots, t_5)$ is given by

$$
\begin{align*}
& x_1 = x_2 \land y_1 = y_2 \land z_1 = z_2 \land t_1 \neq t_2 \\
& \land x_1 = t_3 \land x_2 = t_4 \land x_3 = t_5 \\
& \land R(x_1, y_1, z_1)
\end{align*}
$$

The idea is that 5-tuples $(t_1, \ldots, t_5)$ with $t_1 = t_2$ represent elements from the sort $\mathbb{N}$, and 5-tuples $(t_1, \ldots, t_5)$ with $t_1 \neq t_2$ represent elements from the sort $\mathbb{N}^3$.

**Corollary 60.** The complement of $\text{CSP}(C)$ is in Datalog.

---

5 For the triples inside $C$, we will use the notation $(n_1, n_2, n_3)$, to better distinguish them from tuples over $C$ which we will continue to enclose in round parentheses (…).
Proof. It is known that if a structure $\mathcal{C}'$ has a primitive positive interpretation in another structure $\mathcal{B}'$, and the complement of $\text{CSP}(\mathcal{B}')$ is in Datalog, then the complement of $\text{CSP}(\mathcal{C}')$ is in Datalog as well (proved for finite-domain structures $\mathcal{C}$ in [37]; the same proof also works for general $\mathcal{C}'$, see [8, Lemma 8.3.3]). So the statement follows immediately from Lemma 59.

We will now argue that $\text{CSP}(\mathcal{C})$ can be expressed in MSO. We first provide a characterisation for a given $\mathfrak{A}$ being in $\text{CSP}(\mathcal{B})$.

- **Lemma 61.** A finite $(D, R)$-structure $\mathfrak{A}$ is in $\text{CSP}(\mathcal{B})$ if and only if the following conditions are satisfied:

  1. There is a partition $(A', A'')$ of $A$ such that $A'$ consists of exactly those elements of $A$ occurring in the fourth position of some tuple from $R^\mathfrak{A}$, while $A''$ contains at least all elements of $A$ occurring in $D^\mathfrak{A}$ or in any of the the first three positions of some tuple from $R^\mathfrak{A}$.

  2. The binary relation $D^\mathfrak{A}$ is disjoint from the smallest equivalence relation $\approx$ over $A''$ that satisfies the following:

    - (2a) For any $(a_1, b_1, c_1, d) \in R^\mathfrak{A}$ and $(a_2, b_2, c_2, d) \in R^\mathfrak{A}$, we have $a_1 \approx a_2$ as well as $b_1 \approx b_2$ and $c_1 \approx c_2$.

    - (2b) For any $(a, b, c, d) \in R^\mathfrak{A}$ with $a \approx b$, we also have $b \approx c$.

Proof. For the “if” part, we provide a homomorphism $h : A \to C$ defined by

$$a \mapsto \begin{cases} f([a]_\approx) & \text{if } a \in A'' \\ \langle f([b]_\approx), f([c]_\approx), f([d]_\approx) \rangle & \text{whenever } (b, c, d, a) \in R^\mathfrak{A} \end{cases}$$

where $f : A'_{/\approx} \to \mathbb{N}$ is an arbitrary injection from the $\approx$-equivalence classes of $A''$ to the natural numbers. Note that (2a) ensures well-definedness of the second case.

For the “only if” part, assume a homomorphism $h$ from $\mathfrak{A}$ to $\mathfrak{B}$. W.l.o.g. we can assume $h$ to be such that it maps any $a \in A$ not participating in any of the relations to an arbitrary element of $\mathbb{N}$. We then let $A'' = h^{-1}(\mathbb{N})$ and $A' = A \setminus A''$, which by assumption satisfy Condition (1). We define an equivalence relation $\approx$ over $A''$ by letting $a \approx b$ iff $h(a) = h(b)$. We observe that $\approx$ must be disjoint from $D^\mathfrak{A}$ and that $\approx \subseteq \approx$. Therefore $\approx$ must be disjoint from $D^\mathfrak{A}$, warranting Condition (2).

We will construct an MSO sentence that describes $\text{CSP}(\mathcal{C})$ in a stepwise fashion. As a “witness” of the existence of a homomorphism $h$ from $\mathfrak{A}$ to $\mathcal{C}$, we will employ a set variable $X$ which is supposed to correspond to the set

$$\{a \in A \mid h(a) = \langle n, n, n \rangle \in \mathbb{N}^3\}.$$ 

If $X$ represented this set, $\mathfrak{A}$ would necessarily need to satisfy the MSO formula

$$\varphi_{\text{well}}(X) := \varphi_{\text{sort}}(X) \land \varphi_{\text{trig}}(X) \land \varphi_{\text{compat}}(X)$$

whose components are specified as follows:

The first conjunct $\varphi_{\text{sort}}$ prevents “type clashes” between numbers and triples (where the set variable $T$ is used to identify the elements that $h$ maps to triples):

$$\varphi_{\text{sort}}(X) := \exists T.X \subseteq T \land \forall x, y, z, t (R(x, y, z, t) \Rightarrow \neg T(x) \land \neg T(y) \land \neg T(z) \land T(t))$$

$$\land (D(x, y) \Rightarrow \neg T(x) \land \neg T(y)).$$
The second conjunct $\varphi_{\text{triag}}$ ensures that $X$ covers those $a \in A$ with $h(a) = \langle n_1, n_2, n_3 \rangle$ where $n_1 = n_2 = n_3$ is warranted because of $n_1 = n_2$ being known:

$$\varphi_{\text{triag}}(X) := \forall x, y, t. R(x, y, x, t) \land \varphi_{\text{Eq}}(x, y, X) \Rightarrow X(t)$$

where $\varphi_{\text{Eq}}(x, y, X)$ is an MSO formula with two additional free first-order variables which (presuming the choice of $X$ as above) holds for every pair $(a_1, a_2) \in A^2$ for which the above Datalog program would derive the $E_{\text{q}}$ predicate:

$$\varphi_{\text{Eq}}(x, y, X) := \forall Y. (Y(x) \land \varphi_{\text{propag}}(Y, X) \Rightarrow Y(y))$$

with the following formula $\varphi_{\text{propag}}(Y, X)$ enforcing that $Y$ is a set which is closed under “derived equalities”:

$$\forall x_1, \ldots, x_6, t(R(x_1, x_2, x_3, t) \land R(x_4, x_5, x_6, t)) \implies \bigwedge_{1 \leq i \leq 3} (Y(x_i) \iff Y(x_{i+3}))$$

$$\land \forall x_1, x_2, x_3, t(R(x_1, x_2, x_3, t) \land X(t)) \implies \bigwedge_{1 \leq i < j \leq 3} (Y(x_i) \iff Y(x_j)).$$

Finally, the third conjunct $\varphi_{\text{compat}}(X)$ ensures that the “derivable equalities” are not in conflict with the disequalities imposed through $D$:

$$\varphi_{\text{compat}}(X) := \forall x, y(\varphi_{\text{Eq}}(x, y, X) \Rightarrow \neg D(x, y)).$$

\begin{proposition}
A finite \{D, R\}-structure $\mathfrak{A}$ is in $\text{CSP}(\mathfrak{B})$ if and only if it satisfies the MSO sentence $\exists X. \varphi_{\text{well}}(X)$.
\end{proposition}

\textbf{Proof.} For the “only if” direction, we make a formal argument along the intuitions provided above. Assume a homomorphism $h$ from $\mathfrak{A}$ to $\mathfrak{B}$. We show that the assignment $X \mapsto A^=$ with

$$A^= := \{ a \in A \mid \{ n, n, n, h(a) \} \in R^\mathfrak{A}, n \in \mathbb{N} \}$$

validates $\varphi_{\text{well}}(X)$:

It validates $\varphi_{\text{sort}}(X)$ because one can choose $T \mapsto h^{-1}(\mathbb{N}^3)$ whereas in order to satisfy the premises of any implication inside $\varphi_{\text{sort}}(X)$, all first order variables but $t$ must be instantiated with elements of $h^{-1}(\mathbb{N})$.

Validation of $\varphi_{\text{triag}}(X)$ can be obtained from the fact that, for any $(a_x, a_y, a_z, a_t) \in R^\mathfrak{A}$ satisfying $h(a_x) = h(a_y)$ it must also hold that $h(a_y) = h(a_z)$ by virtue of $h$ being a homomorphism into $\mathfrak{B}$ – where it remains to show that $\varphi_{\text{Eq}}(a_x, a_y, A^=)$ indeed implies $h(a_x) = h(a_y)$. To see that this is true, consider the case where $Y$ is mapped to the set $A_x = h^{-1}(h(a_x))$. Then the implication’s consequence indeed ensures $h(a_x) = h(a_y)$, provided that the premise is found to be true. The premise’s first conjunct holds by construction, whence it remains to show that $\varphi_{\text{propag}}(A_x)$ also holds true, which – in view of our chosen assignment for $X$ – again follows from the fact that $h$ is a homomorphism into $\mathfrak{B}$. Finally, validation of $\varphi_{\text{compat}}(X)$ is established by recalling that $\varphi_{\text{Eq}}(a_x, a_y, A^=)$ implies $h(a_x) = h(a_y)$ (see above) and therefore $(h(a_x), h(a_y)) \notin D^\mathfrak{B}$ by definition.

For the “if” direction, assume that some assignment $X \mapsto A_X \subseteq A$ validates $\varphi_{\text{well}}(X)$ for $\mathfrak{A}$. We will use Lemma 61 to argue that $\mathfrak{A}$ is in $\text{CSP}(\mathfrak{B})$. Let $A'' = \{ a_4 \mid (a_1, a_2, a_3, a_4) \in R^\mathfrak{A} \}$ and let $A' = A \setminus A''$. Then, by virtue of $\varphi_{\text{sort}}$, the partition $(A', A'')$ satisfies Condition (1) of Lemma 61. Satisfaction of the Condition (2) would be an immediate consequence of $\varphi_{\text{compat}}(X)$ if one could establish that the binary relation $E_{\text{q}}A_X := \{(a_1, a_2) \mid \ldots\}$
$\varphi_{\text{Eq}}(a_1, a_2, A_X)$ contains $\approx$. This is achieved by arguing that $\text{Eq}_{A_X}$ is an equivalence relation and satisfies the two subitems in Lemma 61 defining $\approx$. The former is a result of the structure of $\varphi_{\text{Eq}}$ as an undirected reachability check. The latter is enforced through $\varphi_{\text{propag}}$ and $\varphi_{\text{triag}}$ which together ensure the two subconditions (2a) and (2b).

The proof of the following proposition is similar to the proof of Proposition 55.

**Proposition 63.** The complement of CSP(}}</span>Cannot be expressed in GQ⁺.

**Proof.** Let $q, m, k \in \mathbb{N}$ be such that $q, m \geq 1$ and $k \geq m$. We construct an unsatisfiable instance $\mathfrak{A}$ of CSP(</span>Cannot be expressed in GQ⁺) such that Duplicator wins the $q$ nested width $m$ guarded $k$-pebble game on $(\mathfrak{A}, \mathfrak{C})$. Let $\phi'_i$ be as defined in the proof of Proposition 55, but replacing $R(x, y, z)$ by $R(x, y, z, t)$ where $t$ is a fresh variable. Let $\mathfrak{A}$ be the canonical database of $\phi := \phi_{q+1}(x, y) \land D(x, y)$ after transforming it into prenex normal form. Similarly as in the proof of Proposition 55, it is straightforward to show that $\mathfrak{A}$ does not have a homomorphism to $\mathfrak{C}$. We need to show that Duplicator has a winning strategy in the $q$ nested width $m$ guarded $k$-pebble game on $(\mathfrak{A}, \mathfrak{C})$. Let $\mathcal{H}_0$ be the set of all partial homomorphisms $h$ from substructures of $\mathfrak{A}$ to $\mathfrak{C}$ with domain size at most $k$. Let $\mathcal{H}_i$, for all $i \in \{1, \ldots, q\}$, be the set of all partial homomorphisms $h$ from substructures of $\mathfrak{A}$ to $\mathfrak{C}$ with domain size at most $k$ defined as follows. If $u, v \in \text{dom}(h)$ are variables of $\phi$ that do not appear as the last argument of any atomic formula $R(x, y, z, t)$ in $\phi$, then we require that $h(u) = h(v)$ if and only if both $u$ and $v$ are part of the same subformula of $\phi_{q+1}(x, y) \land D(x, y)$ of the form $\phi_{i-1}$, or $\text{dom}(h)$ contains all the variables $x_r, \ldots, x_s, x_{s+1}$ from $\phi_i$ for some $0 \leq r < s < k$ and $u$ appears in the subformula $\phi_{i-1}(x_r, x_{r+1})$ and $v$ appears in the subformula $\phi_{i-1}(x_s, x_{s+1})$. Let $t, t' \in \text{dom}(h)$ be such that $\phi$ contains conjunctions $R(x, y, z, t)$ and $R(x', y', z', t')$ then these conjunctions are unique by the construction of $\phi$; in this case, $h(t) = h(t')$ if and only if $h(x) = h(x')$, $h(y) = h(y')$, and $h(z) = h(z')$. Otherwise, $h(t)$ must be distinct from all other points in the image of $h$.

Since $\text{dom}(h) \leq k$ it is impossible that $r = 0$ and $s = k - 1$; hence, if $x_0$ and $x_k$ are from $\text{dom}(h)$, then $h(x_0) \neq h(x_k)$. Clearly, $\mathcal{H}_i$ is closed under restrictions and non-empty. Now suppose that $h \in \mathcal{H}_i$ is such that there exists a tuple $a$ in a relation of $\mathfrak{A}$ whose entries contain $\text{dom}(h)$. Let $S \subseteq A$ be a superset of $\text{dom}(h)$ of cardinality at most $k$. If this relation is $D$, then $a$ equals $(x, y)$ and we may clearly extend $h$ to some $h' \in \mathcal{H}_i$ with $h'(x) \neq h'(y)$. Otherwise, the relation must be $R$ and $a$ equals $(x_0, x_k, y, t)$ for some variables $x_0, x_k, y, t$ from a subformula $\phi$ of the form $\phi_j(x, y)$ for some $j \leq i$. Note that $h(x_0) = h(x_k) = h(y)$ if $j < i$, and $h(x_0) \neq h(x_k)$ and $h(x_k) \neq h(y)$ otherwise. It is easy to see that in both cases we may extend $h$ to some $h' \in \mathcal{H}_i$ with domain $S$. Finally, if $h \in \mathcal{H}_i$ for $i \in \{1, \ldots, q\}$ and $S \subseteq A$ with $|S| \leq k$ is such that $\text{dom}(h) \subseteq S$, then $\mathcal{H}_{i-1}$ contains an extension $h'$ of $h$ with domain $S$: if $x \in S$ appears in a copy of $\phi_{i-1}$ whose variables intersect $\text{dom}(h)$, we set $h'(x)$ to the value taken by these variables under $h$. If $\text{dom}(h)$ contains all the variables $x_r, \ldots, x_s, x_{s+1}$ from $\phi_i$ for some $0 \leq r < s < k$ and $x$ appears in the subformula $\phi_{i-1}(x_r, x_{r+1})$ and some variable of $\phi_{i-1}(x_r, x_{r+1})$ appears in $\text{dom}(h)$, then we set $h'(x)$ to the value taken by this variable under $h$. Otherwise, pick $h'(x)$ to be a new value. Hence, $\mathcal{H}_0, \mathcal{H}_1, \ldots, \mathcal{H}_q$ is indeed a winning strategy for Duplicator for the $q$ nested width $m$ guarded $k$ pebble game on $(\mathfrak{A}, \mathfrak{C})$.\end{itemize}

**Corollary 64.** The intersection of MSO and Datalog contains problems that cannot be expressed in GQ⁺.

**Proof.** We already know that the complement of CSP(</span>Cannot be expressed in GQ⁺) is in Datalog (Corollary 60), but not in GQ⁺ (Proposition 63). Proposition 62 shows that CSP(</span>Cannot be expressed in GQ⁺) is in MSO; then, as MSO
is closed under negation, the complement of $\text{CSP}(\mathfrak{B})$ is MSO-expressible as well.

\section{Conclusion, Open Problems, and Prospect}

We provided a game-theoretic characterisation of the 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 $\tau$-structures in GSO whose complement is closed under homomorphisms is a finite union of CSPs.

Our results imply that the so-called universal-algebraic approach, which has eventually led to the classification of finite-domain CSPs in Datalog \cite{Ganian2016}, can be applied to study problems that are simultaneously in GSO and in Datalog (see \cite{Ganian2016}). They might also pave the way towards a syntactic characterisation of GSO \cap Datalog and of MSO \cap Datalog; however, we showed that the class of nested guarded queries from \cite{Bodirsky2013} is not expressive enough for this purpose. See Figure 4 for an overview of the considered logic, their inclusions, and references to examples that show that the inclusions are strict.

We state some concrete open problems in the context:

1. Is there a finite structure whose CSP is in Datalog, but not in Nemodeq? Also the expressive power of frontier-guarded Datalog, GQ, and GQ$^+$ for finite-domain CSPs appears to be unexplored.
2. It is known that singleton linear arc consistency (SLAC) [36] captures the intersection of finite-domain CSPs with Datalog. It would be interesting to define an appropriate notion of singleton linear arc consistency for CSPs for ω-categorical structures; can it be used to precisely characterise the intersection of MSO and Datalog?
3. Is there a CSP of a reduct of a finitely bounded homogeneous structure which is not expressible in GSO?
4. Is every CSP in MSO ∩ Datalog the CSP of a reduct of a finitely bounded homogeneous structure?
5. Is every CSP in existential MSO also in MMSNP?

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 [13] so, by virtue of our results, we immediately know they must be (complements of) ω-categorical CSPs.

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