Monadic Datalog over Finite Structures with Bounded Treewidth

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Abstract

Bounded treewidth and Monadic Second Order (MSO) logic have proved to be key concepts in establishing fixed-parameter tractability results. Indeed, by Courcelle’s Theorem we know: Any property of finite structures, which is expressible by an MSO sentence, can be decided in linear time (data complexity) if the structures have bounded treewidth. In principle, Courcelle’s Theorem can be applied directly to construct concrete algorithms by transforming the MSO evaluation problem into a tree language recognition problem. The latter can then be solved via a finite tree automaton (FTA). However, this approach has turned out to be problematical, since even relatively simple MSO formulae may lead to a “state explosion” of the FTA.

In this work we propose monadic datalog (i.e., datalog where all intentional predicate symbols are unary) as an alternative method to tackle this class of fixed-parameter tractable problems. We show that if some property of finite structures is expressible in MSO then this property can also be expressed by means of a monadic datalog program over the structure plus the tree decomposition. Moreover, we show that the resulting fragment of datalog can be evaluated in linear time (both w.r.t. the program size and w.r.t. the data size). This new approach is put to work by devising new algorithms for the 3-Colorability problem of graphs and for the PRIMALITY problem of relational schemas (i.e., testing if some attribute in a relational schema is part of a key). We also report on experimental results with a prototype implementation.

1 Introduction

Over the past decade, parameterized complexity has evolved as an important subdiscipline in the field of computational complexity, see [8,14]. In particular, it has been shown that many hard problems become tractable if some problem parameter is fixed or bounded by a constant. In the arena of graphs and, more generally, of finite structures, the treewidth is one such parameter which has served as the key to many fixed-parameter tractability (FPT) results. The most prominent method for establishing the FPT in case of bounded treewidth is via Courcelle’s Theorem, see [5]: Any property of finite structures, which is expressible by a

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Monadic Second Order (MSO) sentence, can be decided in linear time (data complexity) if the treewidth of the structures is bounded by a fixed constant.

Recipes as to how one can devise concrete algorithms based on Courcelle’s Theorem can be found in the literature, see [2][13]. The idea is to first translate the MSO evaluation problem over finite structures into an equivalent MSO evaluation problem over colored binary trees. This problem can then be solved via the correspondence between MSO over trees and finite tree automata (FTA), see [29][6]. In theory, this generic method of turning an MSO description into a concrete algorithm looks very appealing. However, in practice, it has turned out that even relatively simple MSO formulae may lead to a “state explosion” of the FTA, see [15][26]. Consequently, it was already stated in [21] that the algorithms derived via Courcelle’s Theorem are “useless for practical applications”. The main benefit of Courcelle’s Theorem is that it provides “a simple way to recognize a property as being linear time computable”. In other words, proving the FPT of some problem by showing that it is MSO expressible is the starting point (rather than the end point) of the search for an efficient algorithm.

In this work we propose monadic datalog (i.e., datalog where all intensional predicate symbols are unary) as a practical tool for devising efficient algorithms in situations where the FPT has been shown via Courcelle’s Theorem. Above all, we prove that if some property of finite structures is expressible in MSO then this property can also be expressed by means of a monadic datalog program over the structure plus the tree decomposition. Hence, in the first place, we prove an expressivity result rather than a mere complexity result. However, we also show that the resulting fragment of datalog can be evaluated in linear time (both w.r.t. the program size and w.r.t. the data size). We thus get the corresponding complexity result (i.e., Courcelle’s Theorem) as a corollary of this MSO-to-datalog transformation.

Our MSO-to-datalog transformation for finite structures with bounded treewidth generalizes a result from [16] where it was shown that MSO on trees has the same expressive power as monadic datalog on trees. Several obstacles had to be overcome to prove this generalization:

- First of all, we no longer have to deal with a single universe, namely the universe of trees whose domain consists of the tree nodes. Instead, we now have to deal with – and constantly switch between – two universes, namely the relational structure (with its own signature and its own domain) on the one hand, and the tree decomposition (with appropriate predicates expressing the tree structure and with the tree nodes as a separate domain) on the other hand.

- Of course, not only the MSO-to-datalog transformation itself had to be lifted to the case of two universes. Also important prerequisites of the results in [16] (notably several results on MSO-equivalences of tree structures shown in [28]) had to be extended to this new situation.

- Apart from switching between the two universes, it is ultimately necessary to integrate both universes into the monadic datalog program. For this purpose, both the signature and the domain of the finite structure have to be appropriately extended.

- It has turned out that previous notions of standard or normal forms of tree decompositions (see [8][13]) are not suitable for our purposes. We therefore have to introduce a modified version of “normalized tree decompositions”, which is then further refined as we present new algorithms based on monadic datalog.

In the second part of this paper, we put monadic datalog to work by presenting new algorithms for the 3-Colorability problem of graphs and for the PRIMALITY problem of relational schemas (i.e., testing if some attribute in a relational schema is part of a key). Both problems are well-known to be intractable (e.g., see [25] for PRIMALITY). It is folklore that the 3-Colorability problem can be expressed by an MSO sentence. In [13], it was shown that PRIMALITY is MSO expressible. Hence, in case of bounded treewidth, both problems become tractable. However, two attempts to tackle these problems via the standard MSO-to-FTA approach turned out to be very problematical: We experimented with a prototype implementation using MONA (see [22]) for the MSO model checking, but we ended up with “out-of-memory” errors already for really small input data (see Section 6). Alternatively, we made an attempt to directly implement the MSO-to-FTA mapping proposed in [13]. However, the “state explosion” of the resulting FTA – which tends to
occur already for comparatively simple formulae (cf. [26]) – led to failure yet before we were able to feed any input data to the program.

In contrast, the experimental results with our new datalog approach look very promising, see Section 6. By the experience gained with these experiments, the following advantages of datalog compared with MSO became apparent:

- **Level of declarativity.** MSO as a logic has the highest level of declarativity which often allows one very elegant and succinct problem specifications. However, MSO does not have an operational semantics. In order to turn an MSO specification into an algorithm, the standard approach is to transform the MSO evaluation problem into a tree language recognition problem. But the FTA clearly has a much lower level of declarativity and the intuition of the original problem is usually lost when an FTA is constructed. In contrast, the datalog program with its declarative style often reflects both the *intuition of the original problem and of the algorithmic solution*. This intuition can be exploited for defining heuristics which lead to problem-specific optimizations.

- **General optimizations.** A lot of research has been devoted to generally applicable (i.e., not problem-specific) optimization techniques of datalog (see e.g. [4]). In our implementation (see Section 6), we make heavy use of these optimization techniques, which are not available in the MSO-to-FTA approach.

- **Flexibility.** The generic transformation of MSO formulae to monadic datalog programs (given in Section 4) inevitably leads to programs of exponential size w.r.t. the size of the MSO-formula and the treewidth. However, as our programs for 3-Colorability and PRIMALITY demonstrate, many relevant properties can be expressed by really short programs. Moreover, as we will see in Section 5, also datalog provides us with a *certain level of succinctness*. In fact, we will be able to express a big monadic datalog program by a small non-monadic program.

- **Required transformations.** The problem of a “state explosion” reported in [26] already refers to the transformation of (relatively simple) MSO formulae on trees to an FTA. If we consider MSO on structures with bounded treewidth the situation gets even worse, since the original (possibly simple) MSO formula over a finite structure first has to be transformed into an equivalent MSO formula over trees. This transformation (e.g., by the algorithm in [13]) leads to a much more complex formula (in general, even with additional quantifier alternations) than the original formula. In contrast, our approach works with monadic datalog programs on finite structures which need no further transformation. Each program can be executed as it is.

- **Extending the programming language.** One more aspect of the flexibility of datalog is the possibility to define new built-in predicates if they admit an efficient implementation by the interpreter. Another example of a useful language extension is the introduction of generalized quantifiers. For the theoretical background of this concept, see [11, 12].

Some applications require a fast execution which cannot always be guaranteed by an interpreter. Hence, while we propose a logic programming approach, one can of course go one step further and implement our algorithms directly in Java, C++, etc. following the same paradigm.

The paper is organized as follows. After recalling some basic notions and results in Section 2 we prove several results on the MSO-equivalence of substructures induced by subtrees of a tree decomposition in Section 3. In Section 4, it is shown that any MSO formula with one free individual variable over structures with bounded treewidth can be transformed into an equivalent monadic datalog program. In Section 5 we put monadic datalog to work by presenting new FPT algorithms for the 3-Colorability problem and for the PRIMALITY problem in case of bounded treewidth. In Section 6, we report on experimental results with a prototype implementation. A conclusion is given in Section 7.
2 Preliminaries

2.1 Relational Schemas and Primalty

We briefly recall some basic notions and results from database design theory (for details, see [25]). In particular, we shall define the PRIMALITY problem, which will serve as a running example throughout this paper.

A relational schema is denoted as \((R, F)\) where \(R\) is the set of attributes, and \(F\) the set of functional dependencies (FDs, for short) over \(R\). W.l.o.g., we only consider FDs whose right-hand side consists of a single attribute. Let \(f \in F\) with \(f : Y \rightarrow A\). We refer to \(Y \subseteq R\) and \(A \in R\) as \(\text{lhs}(f)\) and \(\text{rhs}(f)\), respectively. The intended meaning of an FD \(f : Y \rightarrow A\) is that, in any valid database instance of \((R, F)\), the value of the attribute \(A\) is uniquely determined by the value of the attributes in \(Y\). It is convenient to denote a set \(\{A_1, A_2, \ldots, A_n\}\) of attributes as a string \(A_1A_2\ldots A_n\). For instance, we write \(f : ab \rightarrow c\) rather than \(f : \{a, b\} \rightarrow c\).

For any \(X \subseteq R\), we write \(X^+\) to denote the closure of \(X\), i.e., the set of all attributes determined by \(X\). An attribute \(A\) is contained in \(X^+\) if and only if for some sequence of attributes \(X_1, \ldots, X_m\) in \(X\) there exists an FD \(f_i \in F\) with \(\text{lhs}(f_i) \subseteq X_i \cup \{A\} \) and \(\text{rhs}(f_i) = X_{i+1}\). If \(X^+ = R\) then \(X\) is called a superkey. If \(X\) is minimal with this property, then \(X\) is a key. An attribute \(A\) is called prime if it is contained in at least one key in \((R, F)\). An efficient algorithm for testing the primitivity of an attribute is crucial in database design since it is an indispensable prerequisite for testing if a schema is in third normal form. However, given a relational schema \((R, F)\) and an attribute \(A \in R\), it is NP-complete to test if \(A\) is prime (cf. [25]).

We shall consider two variants of the PRIMALITY problem in this paper (see Section 5.2 and 5.3, respectively): the decision problem (i.e., given a relational schema \((R, F)\) and an attribute \(A \in R\), is \(A\) prime in \((R, F)\)?) and the enumeration problem (i.e., given a relational schema \((R, F)\), compute all prime attributes in \((R, F)\)).

**Example 2.1** Consider the relational schema \((R, F)\) with \(R = abcd\) and \(F = \{f_1 : ab \rightarrow c, f_2 : c \rightarrow b, f_3 : cd \rightarrow e, f_4 : de \rightarrow g, f_5 : g \rightarrow e\}\). It can be easily checked that there are two keys for the schema: \(abd\) and \(acd\). Thus the attributes \(a, b, c\) and \(d\) are prime, while \(e\) and \(g\) are not prime.

2.2 Finite Structures and Treewidth

Let \(\tau = \{R_1, \ldots, R_K\}\) be a set of predicate symbols. A **finite structure** \(\mathcal{A}\) over \(\tau\) (a \(\tau\)-structure, for short) is given by a finite domain \(A = \text{dom}(\mathcal{A})\) and relations \(R_i^\mathcal{A} \subseteq A^n\), where \(n\) denotes the arity of \(R_i\) in \(\tau\). A finite structure may also be given in the form \((\mathcal{A}, \bar{a})\) where, in addition to \(\mathcal{A}\), we have distinguished elements \(\bar{a} = (a_0, \ldots, a_w)\) from \(\text{dom}(\mathcal{A})\). Such distinguished elements are required for interpreting formulae with free variables.

A **tree decomposition** \(T\) of a \(\tau\)-structure \(\mathcal{A}\) is defined as a pair \((T, (A_t)_{t \in T})\) where \(T\) is a tree and each \(A_t\) is a subset of \(A\) with the following properties: (1) Every \(a \in A\) is contained in some \(A_t\). (2) For every \(R_i \in \tau\) and every tuple \((a_1, \ldots, a_n) \in R_i^\mathcal{A}\), there exists some node \(t \in T\) with \(\{a_1, \ldots, a_n\} \subseteq A_t\). (3) For every \(a \in A\), the set \(\{t \mid a \in A_t\}\) induces a subtree of \(T\).

The third condition is usually referred to as the connectedness condition. The sets \(A_t\) are called the bags (or blocks) of \(T\). The **width** of a tree decomposition \((T, (A_t)_{t \in T})\) is defined as \(\max\{|A_t| \mid t \in T\} - 1\). The **treewidth** of \(\mathcal{A}\) is the minimal width of all tree decompositions of \(\mathcal{A}\). It is denoted as \(\text{tw}(\mathcal{A})\). Note that trees and forests are precisely the structures with treewidth 1.

For given \(w \geq 1\), it can be decided in linear time if some structure has treewidth \(\leq w\). Moreover, in case of a positive answer, a tree decomposition of width \(w\) can be computed in linear time, see [3].

In this paper, we assume that a relational schema \((R, F)\) is given as a \(\tau\)-structure with \(\tau = \{fd, att, lh, rh\}\). The intended meaning of these predicates is as follows: \(fd(f)\) means that \(f\) is an FD and \(att(b)\) means that \(b\) is an attribute. \(lh(b, f)\) (resp. \(rh(b, f)\)) means that \(b\) occurs in \(\text{lhs}(f)\) (resp. \(\text{rhs}(f)\)). The treewidth of \((R, F)\) is then defined as the treewidth of this \(\tau\)-structure.
Example 2.2 Recall the relational schema \((R, F)\) with \(R = abcdg\) and \(F = \{f_1: ab \rightarrow c, f_2: c \rightarrow b, f_3: cd \rightarrow e, f_4: de \rightarrow g, f_5: g \rightarrow e\}\) from Example 2.1. This schema is represented as the following \(\tau\)-structure with \(\tau = \{fd, att, lh, rh\}: A = (A, fd^A, att^A, lh^A, rh^A)\) with \(A = R, fd^A = \{f_1, f_2, f_3, f_4, f_5\}, att^A = \{a, b, c, d, e, g\}, lh^A = \{(a, f_1), (b, f_1), (c, f_2), (c, f_3), (d, f_3), (d, f_4), (e, f_4), (g, f_5)\}, rh^A = \{(c, f_1), (b, f_2), (c, f_3), (g, f_4), (e, f_5)\}.\)

A tree decomposition \(T\) of this structure is given in Figure 1. Note that the maximal size of the bags in \(T\) is 3. Hence, the tree-width is \(\leq 2\). On the other hand, it is easy to check that the tree-width of \(T\) cannot be smaller than 2: In order to see this, we consider the tuples in \(lh^A\) and \(rh^A\) as edges of an undirected graph. Then the edges corresponding to \((b, f_1), (c, f_2) \in lh^A\) and \((b, f_2), (c, f_1) \in rh^A\) form a cycle in this graph. However, as we have recalled above, only trees and forests have treewidth 1. The tree decomposition in Figure 1 is, therefore, optimal and we have \(tw(F) = tw(A) = 2\).

Remark. A relational schema \((R, F)\) defines a hypergraph \(H(R, F)\) whose vertices are the attributes in \(R\) and whose hyperedges are the sets of attributes jointly occurring in at least one FD in \(F\). Recall that the incidence graph of a hypergraph \(H\) contains as nodes the vertices and hyperedges of \(H\). Moreover, two nodes \(v\) and \(h\) (corresponding to a vertex \(v\) and a hyperedge \(h\) in \(H\)) are connected in this graph iff (in the hypergraph \(H\)) \(v\) occurs in \(h\). It can be easily verified that the treewidth of the above described \(\tau\)-structure and of the incidence graph of the hypergraph \(H(R, F)\) coincide.

In this paper, we consider the following form of normalized tree decompositions, which is similar to the normal form introduced in Theorem 6.72 of [3]:

Definition 2.3 Let \(A\) be an arbitrary structure with tree decomposition \(T\) of width \(w\). We call \(T\) normalized if the conditions 1 – 4 are fulfilled: (1) The bags are considered as tuples of \(w + 1\) pairwise distinct elements \((a_0, \ldots, a_w)\) rather than sets. (2) Every internal node \(t \in T\) has either 1 or 2 child nodes. (3) If a node \(t\) with bag \((a_0, \ldots, a_w)\) has one child node, then the bag of the child is either obtained via a permutation of \((a_0, \ldots, a_w)\) or by replacing \(a_0\) with another element \(a'_0\). We call such a node \(t\) a permutation node or an element replacement node, respectively. (4) If a node \(t\) has two child nodes then these child nodes have identical bags as \(t\). In this case, we call \(t\) a branch node.

Proposition 2.4 Let \(A\) be an arbitrary structure with tree decomposition \(T\) of width \(w\). W.l.o.g., we may assume that the domain \(\text{dom}(A)\) has at least \(w + 1\) elements. Then \(T\) can be transformed in linear time into a normalized tree decomposition \(T'\), s.t. \(T\) and \(T'\) have identical width.

Proof. We can transform an arbitrary tree decomposition \(T\) into a normalized tree decomposition \(T'\) by the following steps (1) - (5). Clearly this transformation works in in linear time and preserves the width.

1. All bags can be padded to the “full” size of \(w + 1\) elements by adding elements from a neighboring bag, e.g.: Let \(s\) and \(s'\) be adjacent nodes and let \(A_s\) have \(w + 1\) elements (in a tree decomposition of width \(w\), at least one such node exists) and let \(|A_{s'}| = w' + 1\) with \(w' < w\). Then \(|A_s \setminus A_{s'}| \geq (w - w')\) and we may simply add \((w - w')\) elements from \(A_s \setminus A_{s'}\) to \(A_{s'}\) without violating the connectedness condition.

2. Suppose that some internal node \(s\) has \(k + 2\) child nodes \(t_1, \ldots, t_{k+2}\) with \(k > 0\). It is a standard technique to turn this part of the tree into a binary tree by inserting copies of \(s\) into the tree, i.e., we introduce \(k\) nodes \(s_1, \ldots, s_k\) with \(A_{s_i} = A_s\), s.t. the second child of \(s\) is \(s_1\), the second child of \(s_1\) is \(s_2\), the second child of \(s_2\) is \(s_3\), etc. Moreover, \(t_1\) remains the first child of \(s\), while \(t_2\) becomes the first child of \(s_1\), \(t_3\)
becomes the first child of \( s_2, \ldots, s_{k+1} \) becomes the first child of \( s_k \). Finally, \( t_{k+2} \) becomes the second child of \( s_k \). Clearly, the connectedness condition is preserved by this construction.

(3) If an internal node \( s \) has two children \( t_1 \) and \( t_2 \), s.t. the bags of \( s, t_1 \), and \( t_2 \) are not identical, then we simply insert a copy \( s_1 \) of \( s \) between \( s \) and \( t_1 \) and another copy \( s_2 \) of \( s \) between \( s \) and \( t_2 \).

(4) Let \( s \) be the parent of \( s' \) and let \( |A_s \setminus A_{s'}| = k \) with \( k > 1 \). Then we can obviously “interpolate” \( s \) and \( s' \) by new nodes \( s_1, \ldots, s_{k-1} \), s.t. \( s_{k-1} \) is the new parent of \( s' \), \( s_{k-2} \) is the parent of \( s_{k-1} \), \ldots, \( s \) is the parent of \( s_1 \). Moreover, the bags \( A_{s_1} \) can be defined in such a way that the bags of any two neighboring nodes differ in exactly one element, e.g., \( |A_s \setminus A_{s_1}| = |A_{s_1} \setminus A_s| = 1 \).

(5) Let the bags of any two neighboring nodes \( s \) and \( s' \) differ by one element, i.e., \( \exists a \in A_s \setminus A_{s'} \) and \( \exists a' \in A_{s'} \setminus A_s \). Then we can insert two “interpolation nodes” \( t \) and \( t' \), s.t. \( A_t \) has the same elements as \( A_s \) with \( a \) at position 0. Likewise, \( A_{t'} \) has the same elements as \( A_{s'} \) but with \( a' \) at position 0. \( \square \)

**Example 2.5** The tree decomposition \( T \) in Figure 1 is clearly not normalized. In contrast, tree decomposition \( T' \) in Figure 2 is normalized in the above sense. Let us ignore the node identifiers \( s_1, \ldots, s_{22} \) for the moment. Note the \( T \) and \( T' \) have identical width.

![Figure 2: Normalized tree decomposition \( T' \) of schema \((R,F)\) in Example 2.1](image)

### 2.3 Monadic Second Order Logic

We assume some familiarity with Monadic Second Order logic (MSO), see e.g. [9, 24]. MSO extends First Order logic (FO) by the use of *set variables* (usually denoted by upper case letters), which range over sets of domain elements. In contrast, the *individual variables* (which are usually denoted by lower case letters) range over single domain elements. An FO-formula \( \varphi \) over a \( \tau \)-structure has as atomic formulae either atoms with some predicate symbol from \( \tau \) or equality atoms. An MSO-formula \( \varphi \) over a \( \tau \)-structure may additionally have atoms whose predicate symbol is a monadic predicate variable. For the sake of readability, we denote such an atom usually as \( a \in X \) rather than \( X(a) \). Likewise, we use set operators \( \subseteq \) and \( \subset \) with the obvious meaning.

The *quantifier depth* of an MSO-formula \( \varphi \) is defined as the maximum degree of nesting of quantifiers (both for individual variables and set variables) in \( \varphi \). In this work, we will mainly encounter MSO formulae with free individual variables. A formula \( \varphi(x) \) with exactly one free individual variable is called a *unary query*. More generally, let \( \varphi(\bar{x}) \) with \( \bar{x} = (x_0, \ldots, x_w) \) for some \( w \geq 0 \) be an MSO formula with free variables \( \bar{x} \). Furthermore, let \( \mathcal{A} \) be a \( \tau \)-structure and \( \bar{a} = (a_0, \ldots, a_w) \) be distinguished domain elements. We write \( (\mathcal{A}, \bar{a}) \models \varphi(\bar{x}) \) to denote that \( \varphi(\bar{a}) \) evaluates to true in \( \mathcal{A} \). Usually, we refer to \((\mathcal{A}, \bar{a})\) simply as a “structure” rather than a “structure with distinguished domain elements”.

6
Example 2.6 It was shown in [18] that primality can be expressed in MSO. We give a slightly different MSO-formula \( \varphi(x) \) here, which is better suited for our purposes in Section 5, namely

\[
\varphi(x) = (\exists Y)[Y \subseteq R \land \text{Closed}(Y) \land x \notin Y \land \text{Closure}(Y \cup \{x\}, R)]
\]

with

\[
\text{Closed}(Y) \equiv \{fe(f) \rightarrow (\exists b)((rh(b, f) \land b \in Y) \lor (lh(b, f) \land b \notin Y))\}
\]

and

\[
\text{Closure}(Y, Z) \equiv Y \subseteq Z \land \text{Closed}(Z) \land \sim(\exists Z')[Y \subseteq Z' \land Z' \subset Z \land \text{Closed}(Z')].
\]

This formula expresses the following characterization of primality: An attribute \( a \) is prime, if there exists an attribute set \( Y \subseteq R \), s.t. \( Y \) is closed w.r.t. \( F \) (i.e., \( Y^+ = Y \)), \( a \notin Y \) and \( (Y \cup \{a\})^+ = R \). In other words, \( Y \cup \{a\} \) is a superkey but \( Y \) is not.

Recall the \( \tau \)-structure \( A \) from Example 2.2 representing a relational schema. It can be easily verified that \( (A, a) \models \varphi(x) \) and \( (A, e) \not\models \varphi(x) \) hold.

We call two structures \( (A, \bar{a}) \) and \( (B, \bar{b}) \) \( k \)-equivalent and write \( (A, \bar{a}) \equiv_k^{MSO} (B, \bar{b}) \), iff for every MSO-formula \( \varphi \) of quantifier depth \( \leq k \), the equivalence \( (A, \bar{a}) \models \varphi \iff (B, \bar{b}) \models \varphi \) holds. By definition, \( \equiv_k^{MSO} \) is an equivalence relation. For any \( k \), the relation \( \equiv_k^{MSO} \) has only finitely many equivalence classes. These equivalence classes are referred to as \( k \)-types or simply as types. The \( \equiv_k^{MSO} \)-equivalence between two structures can be effectively decided. There is a nice characterization of \( \equiv_k^{MSO} \)-equivalence by Ehrenfeucht-Fraïssé games: The \( k \)-round MSO-game on two structures \( (A, \bar{a}) \) and \( (B, \bar{b}) \) is played between two players – the spoiler and the duplicator. In each of the \( k \) rounds, the spoiler can choose between a point move and a set move. If, in the \( i \)-th round, he makes a point move, then he selects some element \( c_i \in \text{dom}(A) \) or some element \( d_i \in \text{dom}(B) \). The duplicator answers by choosing an element in the opposite structure. If, in the \( i \)-th round, the spoiler makes a set move, then he selects a set \( P_i \subseteq \text{dom}(A) \) or a set \( Q_i \subseteq \text{dom}(B) \). The duplicator answers by choosing a set of domain elements in the opposite structure. Suppose that, in \( k \) rounds, the domain elements \( c_1, \ldots, c_m \) and \( d_1, \ldots, d_n \) from \( \text{dom}(A) \) and \( \text{dom}(B) \), respectively, were chosen in the point moves. Likewise, suppose that the subsets \( P_1, \ldots, P_n \) and \( Q_1, \ldots, Q_m \) of \( \text{dom}(A) \) and \( \text{dom}(B) \), respectively, were chosen in the set moves. The duplicator wins this game, if the mapping which maps each \( c_i \) to \( d_i \) is a partial isomorphism from \( (A, \bar{a}, P_1, \ldots, P_n) \) to \( (B, \bar{b}, Q_1, \ldots, Q_n) \). We say that the duplicator has a winning strategy in the \( k \)-round MSO-game on \( (A, \bar{a}) \) and \( (B, \bar{b}) \) if he can win the game for any possible moves of the spoiler.

The following relationship between \( \equiv_k^{MSO} \)-equivalence and \( k \)-round MSO-games holds: Two structures \( (A, \bar{a}) \) and \( (B, \bar{b}) \) are \( k \)-equivalent iff the duplicator has a winning strategy in the \( k \)-round MSO-game on \( (A, \bar{a}) \) and \( (B, \bar{b}) \), see [9, 24].

2.4 Datalog

We assume some familiarity with datalog, see e.g. [1, 4, 30]. Syntactically, a datalog program \( P \) is a set of function-free Horn clauses. The (minimal-model) semantics can be defined as the least fixpoint of applying the immediate consequence operator. Predicates occurring only in the body of rules in \( P \) are called extensional, while predicates occurring also in the head of some rule are called intensional.

Let \( A \) be a \( \tau \)-structure with domain \( A \) and relations \( R_1^A, \ldots, R_K^A \) with \( R_i^A \subseteq A^\alpha \), where \( \alpha \) denotes the arity of \( R_i \in \tau \). In the context of datalog, it is convenient to think of the relations \( R_i^A \) as sets of ground atoms. The set of all such ground atoms of a structure \( A \) is referred to as the extensional database (EDB) of \( A \), which we shall denote as \( E(A) \) (or simply as \( A \), if no confusion is possible). We have \( R_i(\bar{a}) \in E(A) \) iff \( \bar{a} \in R_i^A \).

Evaluating a datalog program \( P \) over a structure \( A \) comes down to computing the least fixpoint of \( P \cup A \). Concerning the complexity of datalog, we are mainly interested in the combined complexity (i.e., the complexity w.r.t. the size of the program \( P \) plus the size of the data \( A \)). In general, the combined complexity of datalog is EXPTIME-complete (implicit in [31]). However, there are some fragments which can be evaluated much more efficiently. (1) Propositional datalog (i.e., all rules are ground) can be evaluated in linear time (combined complexity), see [7, 27]. (2) The guarded fragment of datalog (i.e., every rule \( r \) contains an extensional atom \( B \) in the body, s.t. all variables occurring in \( r \) also occur in \( B \)) can be evaluated in time \( O(|P| \ast |A|) \). (3) Monadic datalog (i.e., all intensional predicates are unary) is NP-complete (combined complexity), see [16].
3 Induced substructures

In this section, we study the $k$-types of substructures induced by certain subtrees of a tree decomposition (see Definitions 3.1 and 3.2). Moreover, it is convenient to introduce some additional notation in Definition 3.4 below.

**Definition 3.1** Let $T$ be a tree and $t$ a node in $T$. Then we denote the subtree rooted at $t$ as $T_t$. Moreover, analogously to [28], we write $\overline{T}_t$ to denote the envelope of $T_t$. This envelope is obtained by removing all of $T_t$ from $T$ except for the node $t$.

Likewise, let $T = \langle T, (A_s)_{s \in T} \rangle$ be a tree decomposition of a finite structure. Then we define $T_t = \langle T_t, (A_s)_{s \in T_t} \rangle$ and $\overline{T}_t = \langle \overline{T}_t, (A_s)_{s \in \overline{T}_t} \rangle$.

In other words, $t$ is the root node in $T_t$ while, in $\overline{T}_t$, it is a leaf node. Clearly, the only node occurring in both $T_t$ and $\overline{T}_t$ is $t$.

**Definition 3.2** Let $A$ be a finite structure and let $T = \langle T, (A_t)_{t \in T} \rangle$ be a tree decomposition of $A$. Moreover, let $s$ be a node in $T$ with bag $A_s = \bar{a} = (a_0, \ldots, a_w)$ and let $S$ be one of the subtrees $T_s$ or $\overline{T}_s$ of $T$.

Then we write $I(A, S, s)$ to denote the structure $(A', \bar{a})$, where $A'$ is the substructure of $A$ induced by the elements occurring in the bags of $S$.

**Example 3.3** Recall the relational schema $(R, F)$ represented by the structure $A$ from Example 2.2 with (normalized) tree decomposition $T'$ in Figure 2. Consider, for instance, the node $s$ in $T'$, as depicted in Figure 3, with bag $A_s = (b, c)$. Then the induced substructure $I(A, T'_s, s)$ is the substructure of $A$ which is induced by the elements occurring in the bags of $T'_s$, whereas $I(A, \overline{T'_s}, s)$ the substructure of $A$ which is induced by the elements occurring in the bags of $\overline{T'_s}$.

**Figure 3:** Induced substructures $T'_s$ and $\overline{T'_s}$ of the tree decomposition $T$ w.r.t. the node $s$.

**Definition 3.4** Let $w \geq 1$ be a natural number and let $A$ and $B$ be finite structures over some signature $\tau$. Moreover, let $(a_0, \ldots, a_w)$ (resp. $(b_0, \ldots, b_w)$) be a tuple of pairwise distinct elements in $A$ (resp. $B$).

We call $(a_0, \ldots, a_w)$ and $(b_0, \ldots, b_w)$ equivalent and write $(a_0, \ldots, a_w) \equiv (b_0, \ldots, b_w)$, iff for any predicate symbol $R \in \tau$ with arity $\alpha$ and for all tuples $(i_1, \ldots, i_\alpha) \in \{0, \ldots, w\}^\alpha$, the equivalence $R^A(a_{i_1}, \ldots, a_{i_\alpha}) \Leftrightarrow R^B(b_{i_1}, \ldots, b_{i_\alpha})$ holds.
We are now ready to generalize results from [28] (dealing with trees plus a distinguished node) to the case of finite structures of bounded treewidth over an arbitrary signature \( \tau \). In the three lemmas below, let \( k \geq 0 \) and \( w \geq 1 \) be arbitrary natural numbers \( \tau \) be an arbitrary signature.

**Lemma 3.5** Let \( A \) and \( B \) be \( \tau \)-structures, let \( S \) (resp. \( T \)) be a normalized tree decomposition of \( A \) (resp. of \( B \)) of width \( w \), and let \( s \) (resp. \( t \)) be an internal node in \( S \) (resp. in \( T \)).

1. **permutation nodes.** Let \( s' \) (resp. \( t' \)) be the only child of \( s \) in \( S \) (resp. of \( t \) in \( T \)). Moreover, let \( \bar{a}, \bar{a}', \bar{b}, \) and \( \bar{b}' \) denote the bags at the nodes \( s, s', t, \) and \( t', \) respectively.

   If \( \mathcal{I}(A, S_{s'}, s') \equiv_k \mathcal{I}(B, T_{t'}, t') \) and there exists a permutation \( \pi \), s.t. \( \bar{a} = \pi(\bar{a}') \) and \( \bar{b} = \pi(\bar{b}') \)

   then \( \mathcal{I}(A, S_s, s) \equiv_k \mathcal{I}(B, T_t, t) \).

2. **element replacement nodes.** Let \( s' \) (resp. \( t' \)) be the only child of \( s \) in \( S \) (resp. of \( t \) in \( T \)). Moreover, let \( \bar{a} = (a_0, a_1, \ldots, a_w), \bar{a}' = (a'_0, a_1, \ldots, a_w), \bar{b} = (b_0, b_1, \ldots, b_w), \) and \( \bar{b}' = (b'_0, b_1, \ldots, b_w) \) denote the bags at the nodes \( s, s', t, \) and \( t', \) respectively.

   If \( \mathcal{I}(A, S_{s'}, s') \equiv_k \mathcal{I}(B, T_{t'}, t') \) and \( \bar{a} \equiv \bar{b} \) then \( \mathcal{I}(A, S_s, s) \equiv_k \mathcal{I}(B, T_t, t) \).

3. **branch nodes.** Let \( s_1 \) and \( s_2 \) (resp. \( t_1 \) and \( t_2 \)) be the children of \( s \) in \( S \) (resp. of \( t \) in \( T \)).

   If \( \mathcal{I}(A, S_{s_1}, s_1) \equiv_k \mathcal{I}(B, T_{t_1}, t_1) \) and \( \mathcal{I}(A, S_{s_2}, s_2) \equiv_k \mathcal{I}(B, T_{t_2}, t_2) \)

   then \( \mathcal{I}(A, S_s, s) \equiv_k \mathcal{I}(B, T_t, t) \).

**Proof.**

1. Let \( \mathcal{I}(A, S_{s'}, s') \equiv_k \mathcal{I}(B, T_{t'}, t') \). Hence, there exists a winning strategy of the duplicator on these structures. Moreover, \( (a_0, \ldots, a_w) \) and \( (b_0, \ldots, b_w) \) are obtained from \( (a'_0, \ldots, a'_w) \) by identical permutations. Thus the duplicator’s winning strategy on the structures \( \mathcal{I}(A, S_{s'}, s') \) and \( \mathcal{I}(B, T_{t'}, t') \) is also a winning strategy on \( \mathcal{I}(A, S_s, s) \) and \( \mathcal{I}(B, T_t, t) \).

2. Let \( \mathcal{I}(A, S_{s'}, s') \equiv_k \mathcal{I}(B, T_{t'}, t') \). Hence, there exists a winning strategy of the duplicator on these structures. The duplicator extends this strategy to the structures \( \mathcal{I}(A, S_s, s) \) and \( \mathcal{I}(B, T_t, t) \) in the following way. (We only consider moves of the spoiler in \( \mathcal{I}(A, S_s, s) \).) Moves in \( \mathcal{I}(B, T_t, t) \) are treated analogously. Any point or set move which is entirely in \( \mathcal{I}(A, S_{s'}, s') \) is answered according to the winning strategy on the substructures \( \mathcal{I}(A, S_{s'}, s') \) and \( \mathcal{I}(B, T_{t'}, t') \). For moves involving \( a_0 \), we proceed as follows. If the duplicator picks \( a_0 \) in a point move, then the duplicator answers with \( b_0 \). Likewise, if the spoiler makes a set move of the form \( P \cup \{a_0\} \), where \( P \) is a subset of the elements in \( \mathcal{I}(A, S_s, s') \) then the duplicator answers with \( Q \cup \{b_0\} \), where \( Q \) is the duplicator’s answer to \( P \) in the game played on the substructures \( \mathcal{I}(A, S_{s'}, s') \) and \( \mathcal{I}(B, T_{t'}, t') \).

   Let \( c_1, \ldots, c_m \) and \( d_1, \ldots, d_m \) be the elements selected in point moves and \( P_1, \ldots, P_n \) and \( Q_1, \ldots, Q_n \) be the sets selected in set moves. By the above definition of the duplicator’s strategy, every move involving \( a_0 \) is answered by the analogous move involving \( b_0 \). For all other elements, the selected elements clearly define a partial isomorphism on the structures \( \mathcal{I}(A, S_s, s) \) and \( \mathcal{I}(B, T_t, t) \) extended by the selected sets. It remains to verify that the selected elements also define a partial isomorphism on the structures \( \mathcal{I}(A, S_s, s) \) and \( \mathcal{I}(B, T_t, t) \) extended by the selected sets. In particular, we have to verify that all relations \( R \in \tau \) are preserved by the selected elements. For any tuples of elements not involving \( a_0 \) (resp. \( b_0 \)), this is guaranteed by the fact that the winning strategy on \( \mathcal{I}(A, S_s, s) \) and \( \mathcal{I}(B, T_t, t) \) is taken over to the structures \( \mathcal{I}(A, S_s, s) \) and \( \mathcal{I}(B, T_t, t) \). On the other hand, by the connectedness condition of tree decompositions, we can be sure that the only relations on \( \mathcal{I}(A, S_s, s) \) (resp. \( \mathcal{I}(B, T_t, t) \)) involving \( a_0 \) (resp. \( b_0 \)) are with elements in the bag \( (a_0, \ldots, a_w) \) (resp. \( (b_0, \ldots, b_w) \)). But then, by the equivalence \( (a_0, \ldots, a_w) \equiv (b_0, \ldots, b_w) \), the preservation of \( R \in \tau \) is again guaranteed.

3. By the definition of branch nodes, the three nodes \( s, s_1, s_2 \) have identical bags, say \( (a_0, \ldots, a_w) \). In particular, since the bag of \( s \) introduces no new elements, all elements contained in \( \mathcal{I}(A, S_s, s) \) are either contained in \( \mathcal{I}(A, S_{s_1}, s_1) \) or in \( \mathcal{I}(A, S_{s_2}, s_2) \). Moreover, by the connectedness condition, only the elements \( a_0, \ldots, a_w \) occur in both substructures. Of course, the analogous observation holds for \( t, t_1, t_2 \), and \( \mathcal{I}(B, T_t, t) \).
By assumption, \( \mathcal{I}(A, S_{s_1}, s_1) \equiv_k^{MSO} \mathcal{I}(B, T_{i_0}, t_2) \) and \( \mathcal{I}(A, S_{s_2}, s_2) \equiv_k^{MSO} \mathcal{I}(B, T_{i_1}, t_2) \). We define the duplicator’s strategy on \( \mathcal{I}(A, S_s, s) \) and \( \mathcal{I}(B, T_t, t) \) by simply combining the winning strategies on the substructures in the obvious way (Again we only consider moves of the spoiler in \( \mathcal{I}(A, S_s, s) \)), i.e., if the spoiler picks some element \( c \) of \( \mathcal{I}(A, S_s, s) \) then the chosen element \( c \) is in \( \mathcal{I}(A, S_{s_i}, s_i) \) for some \( i \in \{1, 2\} \). Hence, the duplicator simply answers according to his winning strategy in the game on \( \mathcal{I}(A, S_{s_i}, s_i) \) and \( \mathcal{I}(B, T_i, t_i) \). On the other hand, suppose that the spoiler picks a set \( P \). Then \( P \) is of the form \( P = P_1 \cup P_2 \), where \( P_1 \) contains only elements in \( \mathcal{I}(A, S_{s_i}, s_i) \). Thus, the duplicator simply answers with \( Q = Q_1 \cup Q_2 \), where \( Q_i \) is the answer to \( P_i \) according to the winning strategy in the game on \( \mathcal{I}(A, S_{s_i}, s_i) \) and \( \mathcal{I}(B, T_i, t_i) \).

It remains to verify that the selected vertices indeed define a partial isomorphism on the structures \( \mathcal{I}(A, S_s, s) \) and \( \mathcal{I}(B, T_t, t) \) extended by the selected sets. Again, the only interesting point is that every relation \( R \in \tau \) is preserved by the elements selected in the point moves. If all elements in a tuple \( \vec{c} \) (resp. \( \vec{d} \)) come from the same substructure \( \mathcal{I}(A, S_{s_i}, s_i) \) (resp. \( \mathcal{I}(B, T_{i_0}, t_2) \)), then this is clearly fulfilled due to the fact that the duplicator’s winning strategy on the substructures \( \mathcal{I}(A, S_{s_i}, s_i) \) and \( \mathcal{I}(B, T_{i_1}, t_1) \) is taken over unchanged to the game on \( \mathcal{I}(A, S_s, s) \) and \( \mathcal{I}(B, T_t, t) \). On the other hand, by the connectedness condition, we can be sure that the only relations between elements from different substructures \( \mathcal{I}(A, S_{s_1}, s_1) \) and \( \mathcal{I}(A, S_{s_2}, s_2) \) (resp. \( \mathcal{I}(B, T_{i_0}, t_1) \) and \( \mathcal{I}(B, T_{i_2}, t_2) \)) are elements in the bag \((a_0, \ldots, a_w)\) (resp. \((b_0, \ldots, b_w)\)) of \( s_1 \) and \( s_2 \) (resp. \( t_1 \), \( t_2 \), and \( t \)). But then, by the equivalences \( \mathcal{I}(A, S_{s_1}, s_1) \equiv_k^{MSO} \mathcal{I}(B, T_{i_1}, t_1) \) and \( \mathcal{I}(A, S_{s_2}, s_2) \equiv_k^{MSO} \mathcal{I}(B, T_{i_2}, t_2) \), the preservation of \( R \in \tau \) is again guaranteed.

\[\blacksquare\]

**Lemma 3.6** Let \( A \) and \( B \) be \( \tau \)-structures, let \( S \) (resp. \( T \)) be a normalized tree decomposition of \( A \) (resp. of \( B \)) of width \( w \), and let \( s \) (resp. \( t \)) be an internal node in \( S \) (resp. in \( T \)).

(1) permutation nodes. Let \( s' \) (resp. \( t' \)) be the only child of \( s \) in \( S \) (resp. of \( t \) in \( T \)). Moreover, let \( \bar{a}, \bar{a}', \bar{b}, \bar{b}' \) denote the bags at the nodes \( s', t, \) and \( t' \), respectively.

If \( \mathcal{I}(A, S_s, s) \equiv_k^{MSO} \mathcal{I}(B, T_t, t) \) and there exists a permutation \( \pi \), s.t. \( \bar{a} = \pi(\bar{a}') \) and \( \bar{b} = \pi(\bar{b}') \) then \( \mathcal{I}(A, S_{s'}, s') \equiv_k^{MSO} \mathcal{I}(B, T_{t'}, t') \).

(2) element replacement nodes. Let \( s' \) (resp. \( t' \)) be the only child of \( s \) in \( S \) (resp. of \( t \) in \( T \)). Moreover, let \( \bar{a} = (a_0, a_1, \ldots, a_w), \bar{a}' = (a_0', a_1', \ldots, a_w'), \bar{b} = (b_0, b_1, \ldots, b_w), \) and \( \bar{b}' = (b_0', b_1', \ldots, b_w') \) denote the bags at the nodes \( s', t, \) and \( t', \) respectively.

If \( \mathcal{I}(A, S_s, s) \equiv_k^{MSO} \mathcal{I}(B, T_t, t) \) and \( \bar{a'} \equiv \bar{b'} \) then \( \mathcal{I}(A, S_{s'}, s') \equiv_k^{MSO} \mathcal{I}(B, T_{t'}, t') \).

(3) branch nodes. Let \( s_1 \) and \( s_2 \) (resp. \( t_1 \) and \( t_2 \)) be the children of \( s \) in \( S \) (resp. of \( t \) in \( T \)).

If \( \mathcal{I}(A, S_{s_1}, s_1) \equiv_k^{MSO} \mathcal{I}(B, T_{t_1}, t_1) \) and \( \mathcal{I}(A, S_{s_2}, s_2) \equiv_k^{MSO} \mathcal{I}(B, T_{t_2}, t_2) \) then \( \mathcal{I}(A, S_{s_1}, s_1) \equiv_k^{MSO} \mathcal{I}(B, T_{t_1}, t_1) \).

If \( \mathcal{I}(A, S_{s_2}, s_2) \equiv_k^{MSO} \mathcal{I}(B, T_{t_2}, t_2) \) then \( \mathcal{I}(A, S_{s_1}, s_1) \equiv_k^{MSO} \mathcal{I}(B, T_{t_1}, t_1) \).

**Proof.** The proof is by Ehrenfeucht-Fraïssé games, analogously to Lemma 3.5 \(\blacksquare\)

**Lemma 3.7** Let \( A \) and \( B \) be \( \tau \)-structures, let \( S \) (resp. \( T \)) be a normalized tree decomposition of \( A \) (resp. of \( B \)) of width \( w \), and let \( s \) (resp. \( t \)) be an arbitrary node in \( S \) (resp. in \( T \)), whose bag is \((a_0, \ldots, a_w)\) (resp. \((b_0, \ldots, b_w)\)).

If \( \mathcal{I}(A, S_s, s) \equiv_k^{MSO} \mathcal{I}(B, T_t, t) \) and \( \mathcal{I}(A, S_s, s) \equiv_k^{MSO} \mathcal{I}(B, T_t, t) \) then \( \mathcal{I}(A, S_s, s) \equiv_k^{MSO} \mathcal{I}(B, T_t, t) \) for every \( i \in \{0, \ldots, w\} \).

**Proof.** Again, the proof is by Ehrenfeucht-Fraïssé games, analogously to Lemma 3.5 \(\blacksquare\)

**Discussion.** Lemma 3.5 provides the intuition how to determine the \( k \)-type of the substructure induced by a subtree \( S_s \) via a bottom-up traversal of the tree decomposition \( S \). The three cases in the lemma refer to the three kinds of nodes which the root node \( s \) of this subtree can have. The essence of the lemma is that the type of the structure induced by \( S_s \) is fully determined by the type of the structure induced by the subtree rooted at the child node(s) plus the relations between elements in the bag at node \( s \). Of course, this is no
big surprise. Analogously, Lemma 3.6 deals with the $k$-type of the substructure induced by a subtree $S$, which can be obtained via a top-down traversal of $S$. Finally, Lemma 3.7 shows how the $k$-type of the substructures induced by $S$ and $S'$ fully determines the type of the entire structure $A$ extended by some domain element from the bag of $s$.

## 4 Monadic Datalog

In this section, we introduce two restricted fragments of datalog, namely monadic datalog over finite structures with bounded treewidth and the quasi-guarded fragment of datalog. Let $\tau = \{ R_1, \ldots, R_K \}$ be a set of predicate symbols and let $w \geq 1$ denote the treewidth. Then we define the following extended signature $\tau_{td}$.

$$
\tau_{td} = \tau \cup \{ \text{root, leaf, child}_1, \text{child}_2, \text{bag} \}
$$

where the unary predicates root, and leaf as well as the binary predicates child$_1$ and child$_2$ are used to represent the tree $T$ of the normalized tree decomposition in the obvious way. For instance, we write child$_1(s_1, s)$ to denote that $s_1$ is either the first child or the only child of $s$. Finally, bag has arity $w + 2$, where bag$(t, a_0, \ldots, a_w)$ means that the bag at node $t$ is $(a_0, \ldots, a_w)$.

**Definition 4.1** Let $\tau$ be a set of predicate symbols and let $w \geq 1$. A monadic datalog program over $\tau$-structures with treewidth $w$ is a set of datalog rules where all extensional predicates are from $\tau_{td}$ and all intensional predicates are unary.

For any $\tau$-structure $A$ with normalized tree decomposition $T = (T, (A_t)_{t \in T})$ of width $w$, we denote by $A_{td}$ the $\tau_{td}$-structure representing $A$ plus $T$ as follows: The domain of $A_{td}$ is the union of $\text{dom}(A)$ and the nodes of $T$. In addition to the relations $R_i^{A}$ with $R_i \in \tau$, the structure $A_{td}$ also contains relations for each predicate root, leaf, child$_1$, child$_2$, and bag thus representing the tree decomposition $T$. By 3, one can compute $A_{td}$ from $A$ in linear time w.r.t. the size of $A$. Hence, the size of $A_{td}$ (for some reasonable encoding, see e.g. 13) is also linearly bounded by the size of $A$.

**Example 4.2** Recall the relational schema $(R, F)$ represented by the structure $A$ from Example 2.2 with normalized tree decomposition $T'$ in Figure 2. The domain of $A_{td}$ is the union of $\text{dom}(A)$ and the tree nodes $\{s_1, \ldots, s_{22}\}$. The corresponding $\tau_{td}$ structure $A_{td}$ representing the relational schema plus tree decomposition $T'$ is made up by the following set of ground atoms: root$(s_1)$, leaf$(s_{12})$, leaf$(s_{14})$, leaf$(s_{19})$, child$_1$(s$_2$, s$_1$), child$_2$(s$_3$, s$_1$), . . . , bag$(s_1, f_3, d, e)$, . . .

As we recalled in Section 2.2, the evaluation of monadic datalog is NP-complete (combined complexity). However, the target of our transformation from MSO to datalog will be a further restricted fragment of datalog, which we refer to as “quasi-guarded”. The evaluation of this fragment can be easily shown to be tractable.

**Definition 4.3** Let $B$ be an atom and $y$ a variable in some rule $r$. We call $y$ “functionally dependent” on $B$ if in every ground instantiation $r'$ of $r$, the value of $y$ is uniquely determined by the value of $B$.

We call a datalog program $P$ “quasi-guarded” if every rule $r$ contains an extensional atom $B$, s.t. every variable occurring in $r$ either occurs in $B$ or is functionally dependent on $B$.

**Theorem 4.4** Let $P$ be a quasi-guarded datalog program and let $A$ be a finite structure. Then $P$ can be evaluated over $A$ in time $O(|P| + |A|)$, where $|P|$ denotes the size of the datalog program and $|A|$ denotes the size of the data.
Proof. Let \( r \) be a rule in the program \( \mathcal{P} \) and let \( B \) be the “quasi-guard” of \( r \), i.e., all variables in \( r \) either occur in \( B \) or are functionally dependent on \( B \). In order to compute all possible ground instances \( r' \) of \( r \) over \( \mathcal{A} \), we first instantiate \( B \). The maximal number of such instantiations is clearly bounded by \( |\mathcal{A}| \). Since all other variables occurring in \( r \) are functionally dependent on the variables in \( B \), in fact the number of all possible ground instantiations \( r' \) of \( r \) is bounded by \( |\mathcal{A}| \).

Hence, in total, the ground program \( \mathcal{P}' \) consisting of all possible ground instantiations of the rules in \( \mathcal{P} \) has size \( O(|\mathcal{P}||\mathcal{A}|) \) and also the computation of these ground rules fits into the linear time bound. As we recalled in Section 2.13 the ground program \( \mathcal{P}' \) can be evaluated over \( \mathcal{A} \) in time \( O(|\mathcal{P}'| + |\mathcal{A}|) = O(|\mathcal{P}||\mathcal{A}| + |\mathcal{A}|) = O(|\mathcal{P}||\mathcal{A}|) \). □

Before we state the main result concerning the expressive power of monadic datalog over structures with bounded treewidth, we introduce the following notation. In order to simplify the exposition below, we assume that all predicates \( R_i \in \tau \) have the same arity \( r \). First, this can be easily achieved by copying columns in relations with smaller arity. Moreover, it is easily seen that the results also hold without this restriction.

It is convenient to use the following abbreviations. Let \( \bar{a} = (a_0, \ldots, a_w) \) be a tuple of domain elements. Then we write \( \mathcal{R}(\bar{a}) \) to denote the set of all ground atoms with predicates in \( \tau = \{R_1, \ldots, R_K\} \) and arguments in \( \{a_0, \ldots, a_w\} \), i.e.,

\[
\mathcal{R}(\bar{a}) = \bigcup_{i=1}^K \bigcup_{j_1=0}^w \cdots \bigcup_{j_w=0}^w \{R_i(a_{j_1}, \ldots, a_{j_w})\}
\]

Let \( \mathcal{A} \) be a structure with tree decomposition \( \mathcal{T} \) and let \( s \) be a node in \( \mathcal{T} \) whose bag is \( \bar{a} = (a_0, \ldots, a_w) \). Then we write \( (\mathcal{A}, s) \) as a short-hand for the structure \( (\mathcal{A}, \bar{a}) \) with distinguished constants \( \bar{a} = (a_0, \ldots, a_w) \).

Theorem 4.5 Let \( \tau \) and \( w \geq 1 \) be arbitrary but fixed. Every MSO-definable unary query over \( \tau \)-structures of treewidth \( w \) is also definable in the quasi-guarded fragment of monadic datalog over \( \tau_{td} \).

Proof. Let \( \varphi(x) \) be an arbitrary MSO formula with free variable \( x \) and quantifier depth \( k \). We have to construct a monadic datalog program \( \mathcal{P} \) with distinguished predicate \( \varphi \) which defines the same query.

W.l.o.g., we only consider the case of structures whose domain has \( \geq w + 1 \) elements. We maintain two disjoint sets of \( k \)-types \( \Theta^1 \) and \( \Theta^\downarrow \), representing \( k \)-types of structures \( (\mathcal{A}, \bar{a}) \) of the following form: \( \mathcal{A} \) has a tree decomposition \( \mathcal{T} \) of width \( w \) and \( \bar{a} \) is the bag of some node \( s \) in \( \mathcal{T} \). Moreover, for \( \Theta^\downarrow \), we require that \( s \) is the root of \( \mathcal{T} \) while, for \( \Theta^1 \), we require that \( s \) is a leaf node of \( \mathcal{T} \). We maintain for each type \( \vartheta \) a witness \( W(\vartheta) = (\mathcal{A}, T, s) \). The types in \( \Theta^1 \) and \( \Theta^\downarrow \) will serve as predicate names in the monadic datalog program to be constructed. Initially, \( \Theta^1 = \Theta^\downarrow = \mathcal{P} = \emptyset \).

1. “Bottom-up” construction of \( \Theta^1 \).

Base case. Let \( a_0, \ldots, a_w \) be pairwise distinct elements and let \( S \) be a tree decomposition consisting of a single node \( s \), whose bag is \( A_s = (a_0, \ldots, a_w) \). Then we consider all possible structures \( (\mathcal{A}, s) \) with this tree decomposition. In particular, \( \text{dom}(\mathcal{A}) = \{a_0, \ldots, a_w\} \). We get all possible structures with tree decomposition \( S \) by letting the EDB \( \mathcal{E}(\mathcal{A}) \) be any subset of \( \mathcal{R}(\bar{a}) \). For every such structure \( (\mathcal{A}, s) \), we check if there exists a type \( \vartheta \) \( \in \Theta^1 \) with \( W(\vartheta) = (\mathcal{B}, \mathcal{T}, t), s.t. (\mathcal{A}, s) \equiv^MSO_k (\mathcal{B}, t) \). If such a \( \vartheta \) exists, we take it. Otherwise we invent a new token \( \vartheta \), add it to \( \Theta^1 \) and set \( W(\vartheta) := (\mathcal{A}, \mathcal{S}, s) \). In any case, we add the following rule to the program \( \mathcal{P} \):

\[
\vartheta(v) \leftarrow \text{bag}(v, x_0, \ldots, x_w), \text{leaf}(v), \{R_i(x_{j_1}, \ldots, x_{j_w}) \mid R(a_{j_1}, \ldots, a_{j_w}) \in \mathcal{E}(\mathcal{A}), \} \}
\{
\neg R_i(x_{j_1}, \ldots, x_{j_w}) \mid R(a_{j_1}, \ldots, a_{j_w}) \notin \mathcal{E}(\mathcal{A}) \}.
\]

Induction step. We construct new structures by extending the tree decompositions of existing witnesses in “bottom-up” direction, i.e., by introducing a new root node. This root node may be one of three kinds of nodes.
(a) Permutation nodes. For each $\vartheta' \in \Theta^1$, let $W(\vartheta') = (A, S', s')$ with bag $A_{s'} = (a_0, \ldots, a_w)$ at the root $s'$ in $S'$. Then we consider all possible triples $(A, S, s)$, where $S$ is obtained from $S'$ by appending $s'$ to a new root node $s$, s.t. $s$ is a permutation node, i.e., there exists some permutation $\pi$, s.t. $A_s = (a_{\pi(0)}, \ldots, a_{\pi(w)})$

For every such structure $(A, s)$, we check if there exists a type $\vartheta \in \Theta^1$ with $W(\vartheta) = (B, T, t)$, s.t. $(A, s) \equiv^k_{MSO} (B, t)$. If such a $\vartheta$ exists, we take it. Otherwise we invent a new token $\vartheta$, add it to $\Theta^1$ and set $W(\vartheta) := (A, S, s)$. In any case, we add the following rule to the program $P$:

$$\vartheta(v) \leftarrow \text{bag}(v, x_{\pi(0)}, \ldots, x_{\pi(w)}), \text{child}_1(v', v), \vartheta'(v'), \text{bag}(v', x_0, \ldots, x_w).$$

(b) Element replacement nodes. For each $\vartheta' \in \Theta^1$, let $W(\vartheta') = (A', S', s')$ with bag $A_{s'} = (a_0', a_1', \ldots, a_w')$ at the root $s'$ in $S'$. Then we consider all possible triples $(A, S, s)$, where $S$ is obtained from $S'$ by appending $s'$ to a new root node $s$, s.t. $s$ is an element replacement node. For the tree decomposition $S$, we thus invent some new element $a_0$ and set $A_s = (a_0, a_1, \ldots, a_w)$. For this tree decomposition $S$, we consider all possible structures $A$ with $\text{dom}(A) = \text{dom}(A') \cup \{a_0\}$ where the EDB $E(A')$ is extended to the EDB $E(A)$ by new ground atoms from $R(a)$, s.t. $a_0$ occurs as argument of all ground atoms in $E(A') \setminus E(A')$.

For every such structure $(A, s)$, we check if there exists a type $\vartheta \in \Theta^1$ with $W(\vartheta) = (B, T, t)$, s.t. $(A, s) \equiv^k_{MSO} (B, t)$. If such a $\vartheta$ exists, we take it. Otherwise we invent a new token $\vartheta$, add it to $\Theta^1$ and set $W(\vartheta) := (A, S, s)$. In any case, we add the following rule to the program $P$:

$$\vartheta(v) \leftarrow \text{bag}(v, x_0, x_1, \ldots, x_w), \text{child}_1(v', v), \vartheta'(v'), \text{bag}(v', x_0, x_1, \ldots, x_w), \{R_i(x_j, \ldots, x_j) \mid R(a_j, \ldots, a_j) \in E(A)\}, \{\neg R_i(x_j, \ldots, x_j) \mid R(a_j, \ldots, a_j) \not\in E(A)\}.$$

(c) Branch nodes. Let $\vartheta_1, \vartheta_2$ be two (not necessarily distinct) types in $\Theta^1$ with $W(\vartheta_1) = (A_1, S_1, s_1)$ and $W(\vartheta_2) = (A_2, S_2, s_2)$. Let $A_{s_1} = (a_0, \ldots, a_w)$ and $A_{s_2} = (b_0, \ldots, b_w)$, respectively. Moreover, let $\text{dom}(A_1) \cap \text{dom}(A_2) = \emptyset$.

Let $\delta$ be a renaming function with $\delta = \{a_0 \leftarrow b_0, \ldots, a_w \leftarrow b_w\}$. By applying $\delta$ to $(A_2, S_2, s_2)$, we obtain a new triple $(A_2', S_2', s_2)$ with $A_{s_2}' = A_2\delta$ and $S_{s_2}' = S_2\delta$. In particular, we thus have $A_{s_2}'\delta = (a_0, \ldots, a_w)$. Clearly, $(A_2, S_2, s_2) \equiv^k_{MSO} (A_2', S_2', s_2)$ holds.

For every such pair $(A_1, S_1, s_1)$ and $(A_2', S_2', s_2)$, we check if the EDBs are inconsistent, i.e., $E(A_1) \cap R(\bar{a}) \neq E(A_2') \cap R(\bar{a})$. If this is the case, then we ignore this pair. Otherwise, we construct a new tree decomposition $S$ with a new root node $s$, whose child nodes are $s_1$ and $s_2$. As the bag of $s$, we set $A_s = A_{s_1} = A_{s_2}'$. By construction, $S$ is a normalized tree decomposition of the structure $A$ with $\text{dom}(A) = \text{dom}(A_1) \cup \text{dom}(A_2')$ and EDB $E(A) = E(A_1) \cup E(A_2')$.

As in the cases above, we have to check if there exists a type $\vartheta \in \Theta^1$ with $W(\vartheta) = (B, T, t)$, s.t. $(A, s) \equiv^k_{MSO} (B, t)$. If such a $\vartheta$ exists, we take it. Otherwise we invent a new token $\vartheta$, add it to $\Theta^1$ and set $W(\vartheta) := (A, S, s)$. In any case, we add the following rule to the program $P$:

$$\vartheta(v) \leftarrow \text{bag}(v, x_0, x_1, \ldots, x_w), \text{child}_1(v_1, v), \vartheta_1(v_1), \text{child}_2(v_2, v), \vartheta_2(v_2), \text{bag}(v_1, x_0, x_1, \ldots, x_w), \text{bag}(v_2, x_0, x_1, \ldots, x_w).$$

2. “Top-down” construction of $\Theta^1$.

Base Case. Let $a_0, \ldots, a_w$ be pairwise distinct elements and let $S$ be a tree decomposition consisting of a single node $s$, whose bag is $A_s = (a_0, \ldots, a_w)$. Then we consider all possible structures $(A, s)$ with this tree decomposition. In particular, $\text{dom}(A) = \{a_0, \ldots, a_w\}$. We get all possible structures with tree decomposition $S$ by letting the EDB $E(A)$ be any subset of $R(\bar{a})$. For every such structure $(A, s)$, we check if there exists a type $\vartheta \in \Theta^1$ with $W(\vartheta) = (B, T, t)$, s.t. $(A, s) \equiv^k_{MSO} (B, t)$. If such a $\vartheta$ exists, we take it. Otherwise we invent a new token $\vartheta$, add it to $\Theta^1$ and set $W(\vartheta) := (A, S, s)$. In any case, we add the following rule to the program $P$:
\[ \vartheta(v) \leftarrow \text{bag}(v, x_0, \ldots, x_w), \text{root}(v), \{ R_i(x_j, \ldots, x_{j'}) \mid R(a_{j1}, \ldots, a_{j'}) \in \mathcal{E}(A) \}, \{ \neg R_i(x_j, \ldots, x_{j'}) \mid R(a_{j1}, \ldots, a_{j'}) \not\in \mathcal{E}(A) \}. \]

**INDUCTION STEP.** We construct new structures by extending the tree decompositions of existing witnesses in "top-down" direction, i.e., by introducing a new leaf node \( s \) and appending it as new child to a former leaf node \( s' \). The node \( s' \) may thus become one of three kinds of nodes in a normalized tree decomposition.

(a) Permutation nodes. For each \( \vartheta' \in \Theta_1 \), let \( W(\vartheta') = \langle A, S', s' \rangle \) with bag \( A_{s'} = (a_{01}, \ldots, a_{w1}) \) at some leaf node \( s' \) in \( S' \). Then we consider all possible triples \( \langle A, S, s \rangle \), where \( S \) is obtained from \( S' \) by appending \( s \) as a new child of \( s' \), s.t. \( s' \) is a permutation node, i.e., there exists some permutation \( \pi \), s.t. \( A_s = (a_{\pi(0)}, \ldots, a_{\pi(w)}) \).

For every such structure \( \langle A, s \rangle \), we check if there exists a type \( \vartheta \in \Theta_1 \) with \( W(\vartheta) = \langle B, T, t \rangle \), s.t. \( \langle A, s \rangle \equiv_{k}\mathcal{MSO}_{k} \langle B, t \rangle \). If such a \( \vartheta \) exists, we take it. Otherwise we invent a new token \( \vartheta \), add it to \( \Theta_1 \) and set \( W(\vartheta) := \langle A, S, s \rangle \). In any case, we add the following rule to the program \( P \):

\[ \vartheta(v) \leftarrow \text{bag}(v, x_{\pi(0)}, \ldots, x_{\pi(w)}), \text{child}_1(v, v'), \vartheta'(v'), \text{bag}(v', x_0, \ldots, x_w). \]

(b) Element replacement nodes. For each \( \vartheta' \in \Theta_1 \), let \( W(\vartheta') = \langle A', S', s' \rangle \) with bag \( A_{s'} = (a_{01}', a_{11}, \ldots, a_{w1}) \) at leaf node \( s' \) in \( S' \). Then we consider all possible triples \( \langle A, S, s \rangle \), where \( S \) is obtained from \( S' \) by appending \( s \) as new child of \( s' \), s.t. \( s' \) is an element replacement node. For the tree decomposition \( S \), we thus invent some new element \( a_0 \) and set \( A_s = (a_0, a_{11}, \ldots, a_{w1}) \). For this tree decomposition \( S \), we consider all possible structures \( A \) with \( \text{dom}(\vartheta) = \text{dom}(A') \cup \{ a_0 \} \) where the EDB \( \mathcal{E}(A') \) is extended to the EDB \( \mathcal{E}(A) \) by new ground atoms from \( \mathcal{R}(\vartheta) \), s.t. \( a_0 \) occurs as argument of all ground atoms in \( \mathcal{E}(A) \setminus \mathcal{E}(A') \).

For every such structure \( \langle A, s \rangle \), we check if there exists a type \( \vartheta \in \Theta_1 \) with \( W(\vartheta) = \langle B, T, t \rangle \), s.t. \( \langle A, s \rangle \equiv_{k}\mathcal{MSO}_{k} \langle B, t \rangle \). If such a \( \vartheta \) exists, we take it. Otherwise we invent a new token \( \vartheta \), add it to \( \Theta_1 \) and set \( W(\vartheta) := \langle A, S, s \rangle \). In any case, we add the following rule to the program \( P \):

\[ \vartheta(v) \leftarrow \text{bag}(v, x_0, x_1, \ldots, x_w), \text{child}_1(v, v'), \vartheta'(v'), \text{bag}(v', x_0, x_1, \ldots, x_w), \{ R_i(x_j, \ldots, x_{j'}) \mid R(a_{j1}, \ldots, a_{j'}) \in \mathcal{E}(A) \}, \{ \neg R_i(x_j, \ldots, x_{j'}) \mid R(a_{j1}, \ldots, a_{j'}) \not\in \mathcal{E}(A) \}. \]

(c) Branch nodes. Let \( \vartheta \in \Theta_1 \) and \( \vartheta_2 \in \Theta_1 \) with \( W(\vartheta) = \langle A, S, s \rangle \) and \( W(\vartheta_2) = \langle A_2, S_2, s_2 \rangle \). Note that \( s \) is a leaf in \( S \) while \( s_2 \) is the root of \( S_2 \). Now let \( A_s = (a_0, \ldots, a_w) \) and \( A_{s_2} = (b_0, \ldots, b_w) \), respectively, and let \( \text{dom}(A) \cap \text{dom}(A_2) = \emptyset \).

Let \( \delta \) be a renaming function with \( \delta = \{ a_0 \leftarrow b_0, \ldots, a_w \leftarrow b_w \} \). By applying \( \delta \) to \( \langle A_2, S_2, s_2 \rangle \), we obtain a new triple \( \langle A_2', S_2', s_2' \rangle \) with \( A_2' = A_2\delta \) and \( S_2' = S_2\delta \). In particular, we thus have \( A_{s_2} \delta = (a_0, \ldots, a_w) \). Clearly, \( \langle A_2, s_2 \rangle \equiv_{k}\mathcal{MSO}_{k} \langle A_2', s_2' \rangle \) holds.

For every such pair \( \langle A, S, s \rangle \) and \( \langle A_2', S_2', s_2' \rangle \), we check if the EDBs are inconsistent, i.e., \( \mathcal{E}(A) \cap \mathcal{R}(\vartheta) \not= \mathcal{E}(A_2') \cap \mathcal{R}(\vartheta) \). If this is the case, then we ignore this pair. Otherwise, we construct a new tree decomposition \( S_1 \) by introducing a new leaf node \( s_1 \) and appending both \( s_1 \) and \( s_2 \) as child nodes of \( s \). As the bag of \( s_1 \), we set \( A_{s_1} = A_s = A_2' \). By construction, \( S_1 \) is a normalized tree decomposition of the structure \( A_1 \) with \( \text{dom}(A_1) = \text{dom}(A) \cup \text{dom}(A_2') \) and EDB \( \mathcal{E}(A_1) = \mathcal{E}(A) \cup \mathcal{E}(A_2') \).

As in the cases above, we have to check if there exists a type \( \vartheta_1 \in \Theta_1 \) with \( W(\vartheta_1) = \langle B, T, t \rangle \), s.t. \( \langle A_1, s_1 \rangle \equiv_{k}\mathcal{MSO}_{k} \langle B, t \rangle \). If such a \( \vartheta_1 \) exists, we take it. Otherwise we invent a new token \( \vartheta_1 \), add it to \( \Theta_1 \) and set \( W(\vartheta_1) := \langle A_1, S_1, s_1, s_2 \rangle \). In any case, we add the following rule to the program \( P \):

\[ \vartheta_1(v_1) \leftarrow \text{bag}(v_1, x_0, x_1, \ldots, x_w), \text{child}_1(v_1, v), \text{child}_2(v_2, v), \vartheta(v), \vartheta_2(v_2), \text{bag}(v, x_0, x_1, \ldots, x_w), \text{bag}(v_2, x_0, x_1, \ldots, x_w). \]

Now suppose that \( S_1 \) is constructed from \( S \) and \( S_2 \) by attaching the new node \( s_1 \) as second child of \( s \) and \( s_2 \) as the first child. In this case, the structure \( A_1 \) remains exactly the same as in the case above, since the
order of the child nodes of a node in the tree decomposition is irrelevant. Thus, whenever the above rule is added to the program \( \mathcal{P} \), then also the following rule is added:

\[
\vartheta_1(v_2) \leftarrow \text{bag}(v_2, x_0, x_1, \ldots, x_w), \text{child}_1(v_1, v), \text{child}_2(v_2, v), \vartheta(v), \vartheta_1(v_1),
\]

\[
\text{bag}(v, x_0, x_1, \ldots, x_w), \text{bag}(v_1, x_0, x_1, \ldots, x_w).
\]

3. Element selection.

We consider all pairs of types \( \vartheta_1 \in \Theta^1 \) and \( \vartheta_2 \in \Theta^1 \). Let \( W(\vartheta_1) = \langle A_1, S_1, s_1 \rangle \) and \( W(\vartheta_2) = \langle A_2, S_2, s_2 \rangle \). Moreover, let \( A_{s_1} = (a_0, \ldots, a_w) \) and \( A_{s_2} = (b_0, \ldots, b_w) \), respectively, and let \( \text{dom}(A_1) \cap \text{dom}(A_2) = \emptyset \).

Let \( \delta \) be a renaming function with \( \delta = \{a_0 \leftarrow b_0, \ldots, a_w \leftarrow b_w\} \). By applying \( \delta \) to \( \langle A_2, S_2, s_2 \rangle \), we obtain a new triple \( \langle A'_2, S'_2, s' \rangle \) with \( A'_2 = A_2 \delta \) and \( S'_2 = S_2 \delta \). In particular, we thus have \( A_{s_2} \delta = (a_0, \ldots, a_w) \). Clearly, \( \langle A_2, S_2, s_2 \rangle \equiv_{k}^{\text{MSO}} \langle A'_2, S'_2 \rangle \).

For every such pair \( \langle A_1, S_1, s_1 \rangle \) and \( \langle A'_2, S'_2, s' \rangle \), we check if the EDBs are inconsistent, i.e., \( \mathcal{E}(A_1) \cap \mathcal{R}(\bar{a}) \neq \mathcal{E}(A'_2) \cap \mathcal{R}(\bar{a}) \). If this is the case, then we ignore this pair. Otherwise, we construct a new tree decomposition \( \mathcal{S} \) by identifying \( s_1 \) (the root of \( S_1 \)) with \( s_2 \) (a leaf of \( S_2 \)). By construction, \( \mathcal{S} \) is a normalized tree decomposition of the structure \( \mathcal{A} \) with \( \text{dom}(A) = \text{dom}(A_1) \cup \text{dom}(A'_2) \) and \( \mathcal{E}(A) = \mathcal{E}(A_1) \cup \mathcal{E}(A'_2) \).

Now check for each \( a_i \) in \( A_{s_1} = A_{s_2} \delta \), if \( \mathcal{A} \models \varphi(a_i) \). If this is the case, then we add the following rule to \( \mathcal{P} \):

\[
\varphi(x_i) \leftarrow \vartheta_1(v), \vartheta_2(v), \text{bag}(v, x_0, \ldots, x_w).
\]

We claim that the program \( \mathcal{P} \) with distinguished monadic predicate \( \varphi \) is the desired monadic datalog program, i.e., let \( \mathcal{A} \) be an arbitrary input \( \tau \)-structure with tree decomposition \( \mathcal{S} \) and let \( \mathcal{A}_{\text{id}} \) denote the corresponding \( \tau_{\text{id}} \)-structure. Moreover, let \( a \in \text{dom}(\mathcal{A}) \). Then the following equivalence holds: \( \mathcal{A} \models \varphi(a) \) if and only if \( \mathcal{A}_{\text{id}} \models \varphi(a) \) is in the least fixpoint of \( \mathcal{P} \cup \mathcal{A}_{\text{id}} \).

Note that the intensional predicates in \( \Theta^1 \), \( \Theta^1 \), and \( \{\varphi\} \) are layered in that we can first compute the least fixpoint of the predicates in \( \Theta^1 \), then \( \Theta^1 \), and finally \( \varphi \).

The bottom-up construction of \( \Theta^1 \) guarantees that we indeed construct all possible types of structures \( (\mathcal{B}, t) \) with tree decomposition \( \mathcal{T} \) and root \( t \). This can be easily shown by Lemma 3.5 and an induction on the size of the tree decomposition \( \mathcal{T} \). On the other hand, for every subtree \( S_i \) of \( \mathcal{S} \), the type of the induced substructure \( \mathcal{I}(\mathcal{A}, S_i, s) \) is \( \vartheta \) for some \( \vartheta \in \Theta^1 \) if and only if the atom \( \vartheta(s) \) is in the least fixpoint of \( \mathcal{P} \cup \mathcal{A}_{\text{id}} \).

Again this can be shown by an easy induction argument using Lemma 3.5.

Analogously, we may conclude via Lemma 3.6 that \( \Theta^1 \) contains all possible types of structures \( (\mathcal{B}, t) \) with tree decomposition \( \mathcal{T} \) and some leaf node \( t \). Moreover, for every subtree \( S_i \) of \( \mathcal{S} \), the type of the induced substructure \( \mathcal{I}(\mathcal{A}, S_i, s) \) is \( \vartheta \) for some \( \vartheta \in \Theta^1 \) if and only if the atom \( \vartheta(s) \) is in the least fixpoint of \( \mathcal{P} \cup \mathcal{A}_{\text{id}} \).

The definition of the predicate \( \varphi \) in part 3 is a direct realization of Lemma 3.7. It thus follows that \( \mathcal{A} \models \varphi(a) \) if and only if \( \varphi(a) \) is in the least fixpoint of \( \mathcal{P} \cup \mathcal{A}_{\text{id}} \).

Finally, an inspection of all datalog rules added to \( \mathcal{P} \) by this construction shows that these rules are indeed quasi-guarded, i.e., they all contain an atom \( B \) with an extensional predicate, s.t. all other variables in this rule are functionally dependent on the variables in \( B \). For instance, in the rule added to \( \Theta^1 \) in case of a branch node, the atom \( \text{bag}(v, x_0, \ldots, x_w) \) is the quasi-guard. Indeed, the remaining variables \( v_1 \) and \( v_2 \) in this rule are functionally dependent on \( v \) via the atoms \( \text{child}_1(v_1, v) \) and \( \text{child}_2(v_2, v) \).

Above all, Theorem 4.5 is an expressivity result. However, it can of course be used to derive also a complexity result. Indeed, we can state a slightly extended version of Courcelle’s Theorem as a corollary (which is in turn a special case of Theorem 4.12 in [13]).

**Corollary 4.6** The evaluation problem of unary MSO-queries \( \varphi(x) \) over \( \tau \)-structures \( \mathcal{A} \) with treewidth \( w \) can be solved in time \( O(f(|\varphi(x)|, w) \ast |\mathcal{A}|) \) for some function \( f \).
Proof. Suppose that we are given an MSO-query \( \varphi(x) \) and some treewidth \( w \). By Theorem 4.5, we can construct an equivalent, quasi-guarded datalog program \( P \). The whole construction is independent of the data. Hence, the time for this construction and the size of \( P \) are both bounded by some term \( f(|\varphi(x)|, w) \).

By [3], a tree decomposition \( T \) of \( A \) and, therefore, also the extended structure \( A_{td} \) can be computed in time \( O(|A|) \). Finally, by Theorem 4.4, the quasi-guarded program \( P \) can be evaluated over \( A_{td} \) in time \( O(|P| \cdot |A_{td}|) \), from which the desired overall time bound follows.

Discussion. Clearly, Theorem 4.5 is not only applicable to MSO-definable unary queries but also to 0-ary queries, i.e., MSO-queries defining a decision problem. An inspection of the proof of Theorem 4.5 reveals that several simplifications are possible in this case. Above all, the whole “top-down” construction of \( \Theta \downarrow \) can be omitted. Moreover, the rules with head predicate \( \varphi \) are now much simpler: Let \( \varphi \) be a 0-ary MSO-formula and let \( \Theta \uparrow \) denote the set of types obtained by the “bottom-up” construction in the above proof. Then we define \( \Theta \uparrow_0 = \{ \vartheta | W(\vartheta) = (A, S, s) \text{ and } A \models \varphi \} \). Finally, we add the following set of rules with head predicate \( \varphi \) to our datalog program:

\[
\varphi \leftarrow \text{root}(v), \vartheta_0(v).
\]

for every \( \vartheta_0 \in \Theta \uparrow_0 \). We shall make use of these simplifications in Section 5.1 and 5.2 when we present new algorithms for two decision problems. In contrast, these simplifications are no longer possible when we consider an enumeration problem in Section 5.3. In particular, the “top-down” construction will indeed be required then.

5 Monadic Datalog at Work

We now put monadic datalog to work by constructing several new algorithms. We start off with a simple example, namely the 3-Colorability problem, which will help to illustrate the basic ideas, see Section 5.1. Our ultimate goal is to tackle two more involved problems, namely the PRIMALITY decision problem and the PRIMALITY enumeration problem, see Sections 5.2 and 5.3. All these problems are well-known to be intractable. However, since they are expressible in MSO over appropriate structures, they are fixed-parameter tractable w.r.t. the treewidth. In this section, we show that these problems admit succinct and efficient solutions via datalog.

Before we present our datalog programs, we slightly modify the notion of normalized tree decompositions from Section 2.2. Recall that an element replacement node replaces exactly one element in the bag of the child node by a new element. For our algorithms, it is preferable to split this action into two steps, namely, an element removal node, which removes one domain element from the bag of its child node, and an element introduction node, which introduces one new element. Moreover, it is now preferable to consider the bags as sets of domain elements rather than as tuples. Hence, we may delete permutation nodes from the tree decomposition. Finally, we drop the condition that all bags in a tree decomposition of width \( w \) must have “full size” \( w + 1 \) (by splitting the element replacement into element removal and element introduction, this condition would have required some relaxation anyway). Such a normal form of tree decompositions was also considered in [23]. For instance, recall the tree decomposition \( T' \) from Figure 2. A tree decomposition \( T'' \) compliant with our modified notion of normalized tree decompositions is depicted in Figure 4.

5.1 The 3-Colorability Problem

Suppose that a graph \( (V, E) \) with vertices \( V \) and edges \( E \) is given as a \( \tau \)-structure with \( \tau = \{ e \} \), i.e., \( e \) is the binary edge relation. This graph is 3-colorable, iff there exists a partition of \( V \) into three sets \( R, G, B \), s.t. no two adjacent vertices \( v_1, v_2 \in V \) are in the same set \( R, G, \text{ or } B \). This criterion can be easily expressed by an MSO-sentence, namely
Note that these sets are not sets in the general sense, since their cardinality is restricted by the size $w$ of the bag. In contrast, upper case letters $a$, $b$, $c$, $d$, $e$ (possibly with subscripts) as datalog variables for a single node in $T$ and for a single vertex in $V$, respectively. In contrast, upper case letters $X$, $R$, $G$, and $B$ are used as datalog variables denoting sets of vertices.

Suppose that a graph $(V, E)$ together with a tree decomposition $T$ of width $w$ is given as a $\tau_{td}$-structure with $\tau_{td} = \{ \text{root}, \text{leaf}, \text{child}_1, \text{child}_2, \text{bag} \}$. In Figure 5 we describe a datalog program which takes such a $\tau_{td}$-structure as input and decides if the graph thus represented is 3-colorable.

Some words on the notation used in this program are in order: We are using lower case letters $s$ and $v$ (possibly with subscripts) as datalog variables for a single node in $T$ and for a single vertex in $V$, respectively. In contrast, upper case letters $X$, $R$, $G$, and $B$ are used as datalog variables denoting sets of vertices. Note that these sets are not sets in the general sense, since their cardinality is restricted by the size $w + 1$ of the bag.
the bags, where $w$ is a fixed constant. Hence, these “fixed-size” sets can be simply implemented by means of $k$-tuples with $k \leq (w+1)$ over $\{0,1\}$. For the sake of readability, we are using non-datalog expressions with the set operator $\tilde{\|}$ (disjoint union). For the fixed-size sets under consideration here, one could, of course, easily replace this operator by “proper” datalog expressions of the form $\text{disjoint union}(R, \{v\}, R')$.

It is convenient to introduce the following notation. Let $G = (V, E)$ be the input graph with tree decomposition $T$. For any node $s$ in $T$, we write as usual $T_s$ to denote the subtree of $T$ rooted at $s$. Moreover, we write $V(s)$ and $V(T_s)$ to denote the vertices in the bag of $s$ respectively in any bag in $T_s$.

Our 3-Colorability-program checks if $G$ is 3-colorable via the criterion mentioned above, i.e., there exists a partition of $V$ into three sets $\mathcal{R}, \mathcal{G}, \mathcal{B}$, s.t. no two adjacent vertices $v_1, v_2 \in V$ are in the same set $\mathcal{R}, \mathcal{G}, \mathcal{B}$.

At the heart of this program is the intensional predicate $\text{solve}(s, R, G, B)$ with the following intended meaning: $s$ denotes a node in $T$ and $R, G, B$ are the projections of $\mathcal{R}, \mathcal{G}, \mathcal{B}$ onto $V(s)$. For all values $s, R, G, B$, the ground fact $\text{solve}(s, R, G, B)$ shall be in the least fixpoint of the program plus the input structure, iff the following condition holds:

**PROPERTY A.** There exist extensions $\hat{R}$ of $R$, $\hat{G}$ of $G$, and $\hat{B}$ of $B$ to $V(T_s)$, s.t.

1. $\hat{R}, \hat{G}, \text{ and } \hat{B}$ form a partition of $V(T_s)$ and
2. no two adjacent vertices $v_1, v_2 \in V(T_s)$ are in the same set $\hat{R}, \hat{G}, \text{ or } \hat{B}$.

In other words, $\hat{R}, \hat{G}, \text{ and } \hat{B}$ is a valid 3-coloring of the vertices in $V(T_s)$ and $R, G, B$ are the projections of $\hat{R}, \hat{G}, \text{ and } \hat{B}$ onto $V(s)$.

The main task of the program is the computation of all facts $\text{solve}(s, R, G, B)$ via a bottom-up traversal of the tree decomposition. The other predicates have the following meaning:

- $\text{partition}(s, R, G, B)$ is in the least fixpoint iff $R, G, B$ is a partition of the bag $X$ at node $s$ in the tree decomposition.
- $\text{allowed}(s, X)$ is in the least fixpoint iff $X$ contains no adjacent vertices $v_1, v_2$.

Recall that the cardinality of the sets $X, R, G, B$ occurring as arguments of $\text{partition}$ and $\text{allowed}$ is bounded by the fixed constant $w + 1$. In fact, both the $\text{partition}$ predicate and the $\text{allowed}$ predicate can be treated as extensional predicates by computing all facts $\text{partition}(s, R, G, B)$ and $\text{allowed}(s, X)$ for each node $s$ in $T$ as part of the computation of the tree decomposition. This additional computation also fits into the linear time bound.

The intuition of the rules with the $\text{solve}$-predicate in the head is now clear: At the leaf nodes, the program generates ground facts $\text{solve}(s, R, G, B)$ for all possible partitions of the bag $X$ at $s$, such that none of the sets $R, G, B$ contains two adjacent vertices. The three rules for element introduction nodes distinguish the three cases if the new vertex $v$ is added to $R, G, \text{ or } B$, respectively. Of course, by the $\text{allowed}$-atom in the body of these 3 rules, the attempt to add $v$ to any of the sets $R, G, \text{ or } B$ may fail. The three rules for element removal nodes distinguish the three cases if the removed vertex was in $R, G, \text{ or } B$, respectively. The rule for branch nodes combines $\text{solve}$-facts with identical values of $(R, G, B)$ at the child nodes $s_1$ and $s_2$ to the corresponding $\text{solve}$-fact at $s$.

In summary, the 3-colorability-program has the following properties.

**Theorem 5.1** The datalog program in Figure 5 decides the 3-Colorability problem, i.e., the fact “$\text{success}$” is in the least fixpoint of this program plus the input $\tau_{td}$-structure $A_{td}$ iff $A_{td}$ encodes a 3-colorable graph $(V, E)$. Moreover, for any graph $(V, E)$ with treewidth $w$, the computation of the $\tau_{td}$-structure $A_{td}$ and the evaluation of the program can be done in time $O(f(w) + |(V, E)|)$ for some function $f$.

**Proof.** By the above considerations, it is clear that the predicate $\text{solve}$ indeed has the meaning described by Property A. A formal proof of this fact by structural induction on $T$ is immediate and therefore omitted here. Then the rule with head $\text{success}$ reads as follows: $\text{success}$ is in the least fixpoint, iff $s$ denotes the root of $T$ and there exist extensions $\hat{R}, \hat{G}, \text{ and } \hat{B}$ of $R, G, B$ to $V(T_s)$ (which is identical to $V$ in case of the root node $s$), s.t. $\hat{R}, \hat{G}, \text{ and } \hat{B}$ is a valid 3-coloring of the vertices in $V(T_s) = V$. 

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For the linear time data complexity, the crucial observation is that our program in Figure 5 is essentially a succinct representation of a quasi-guarded monadic datalog program. For instance, in the atom $\text{solve}(s, R, G, B)$, the sets $R, G, B$ are subsets of the bag of $s$. Hence, each combination $R, G, B$ could be represented by 3 subsets $r_1, r_2, r_3$ over $\{0, \ldots, w\}$ referring to indices of elements in the bag of $s$. Recall that $w$ is a fixed constant. Hence, $\text{solve}(s, R, G, B)$ is simply a succinct representation of constantly many monadic predicates of the form $\text{solve}(r_1, r_2, r_3)(s)$. The quasi-guard in each rule can thus be any atom with argument $s$, e.g., $\text{bag}(s, X)$ (possibly extended by a disjoint union with $\{v\}$). Thus, the linear time bound follows immediately from Theorem 4.4.

Discussion. Let us briefly compare the monadic program constructed in the proof of Theorem 4.5 with the 3-Colorability program in Figure 5. Actually, since we are dealing with a decision problem here, we only look at the bottom-up construction in the proof of Theorem 4.5 since the top-down construction is not needed for a 0-ary target formula $\varphi()$. As was already mentioned in the proof of Theorem 5.1, the atoms $\text{solve}(s, R, G, B)$ can be thought of as a succinct representation for atoms of the form $\text{solve}(r_1, r_2, r_3)(s)$.

Now the question naturally arises where the type $\varphi$ of some node $s$ from the proof of Theorem 4.5 is present in the 3-Colorability program. A first tentative answer is that this type essentially corresponds to the set $R(s) = \{(r_1, r_2, r_3) \mid \text{solve}(r_1, r_2, r_3)(s)\}$ is in the least fixpoint. However, there are two significant aspects which distinguish our 3-Colorability program from merely a succinct representation of the type transitions encoded in the monadic datalog program of Theorem 4.5:

1. By Property A, we are only interested in the types of those structures which – in principle – could be extended in bottom-up direction to a structure representing a satisfiable propositional formula. Hence, in contrast to the construction in the proof of Theorem 4.5, our 3-Colorability program does clearly not keep track of all possible types that the substructure induced by some tree decomposition $T_s$ may possibly have.

2. $R(s) = \{(r_1, r_2, r_3) \mid \text{solve}(r_1, r_2, r_3)(s)\}$ is in the least fixpoint does not exactly correspond to the type of $s$. Instead, it only describes the crucial properties of the type. Thus, the 3-Colorability program somehow “aggregates” several types from the proof of Theorem 4.5.

These two properties ensure that the 3-Colorability program is much shorter than the program in the proof of Theorem 4.5 and that the difference between these two programs is not just due to the succinct representation of a monadic program by a non-monadic one. The deeper reason of this improvement is that we take the target MSO formula $\varphi$ (namely, the characterization of 3-Colorability) into account for the entire construction of the datalog program in Figure 5. In contrast, the rules describing the type-transitions in the proof of Theorem 4.5 for a bottom-up traversal of the tree decomposition are fully generic. Only the rules with head predicate $\varphi$ are specific to the actual target MSO formula $\varphi$.

5.2 The Primality Decision Problem

Recall from Section 2.2 that we represent a relational schema $(R, F)$ as a $\tau$-structure with $\tau = \{fd, att, lh, rh\}$. Moreover, recall that, in Section 5, we consider normalized tree decompositions with element removal nodes and element introduction nodes rather than element replacement nodes as in Section 2.2. With our representation of relational schemas $(R, F)$ as finite structures, the domain elements are the attributes and FDs in $(R, F)$. Hence, in total, the former element replacement nodes give rise to four kinds of nodes, namely, attribute removal nodes, FD removal nodes, attribute introduction nodes, and FD introduction nodes. Moreover, we now consider the bags as a pair of sets $(At, Fd)$, where $At$ is a set attributes and $Fd$ is a set of FDs. Again, we may delete permutation nodes from the tree decomposition. Finally, it will greatly simplify the presentation of our datalog program if we require that, whenever an FD $f \in F$ is contained in a bag of the tree decomposition, then the attribute $\text{rhs}(f)$ is as well. In the worst-case, this may double the width of the resulting decomposition.

Suppose that a schema $(R, F)$ together with a tree decomposition $T$ of width $w$ is given as a $\tau_{ad}$-structure with $\tau_{ad} = \{fd, att, lh, rh, root, leaf, child_1, child_2, bag\}$. In Figure 6, we describe a datalog
program, where the input is given as an attribute $a \in R$ and a $\tau_{fd}$-structure, s.t. $a$ occurs in the bag at the root of the tree decomposition.

| Program PRIMALITY |
|-------------------|
| /* leaf node. */ |
| solve(s, Y, FY, $C^o$, $\Delta C$, FC) ← leaf(s), bag(s, At, Fd), $Y \cup C^o = At$, $Y \cap C^o = \emptyset$, outside(FY, Y, At, Fd), $FC \subseteq Fd$, consistent(FC, $C^o$), $\Delta C = \{rhs(f) \mid f \in FC\}$, $\Delta C \subseteq C^o$. |
| /* attribute introduction node. */ |
| solve(s, Y ∪ {b}, FY, $C^o$, $\Delta C$, FC) ← bag(s, At ∪ {b}, Fd), child₁(s, s), bag(s₁, At, Fd), solve(s₁, Y, FY, $C^o$, $\Delta C$, FC). |
| solve(s, Y, FY, $C^o$, $\Delta C$, FC) ← bag(s, At ∪ {f}, Fd), child₁(s, s), bag(s₁, At, Fd), consistent(FC, $C^o$), outside(FY₂, Y, At, Fd), FY = FY₁ ∪ FY₂. |
| /* FD introduction node. */ |
| solve(s, Y, FY, $C^o$, $\Delta C$, FC) ← bag(s, At, Fd ∪ {f}), child₁(s, s), bag(s₁, At, Fd), rh(b, f), b ∈ Y, solve(s₁, Y, FY, $C^o$, $\Delta C$, FC). |
| solve(s, Y, FY, $C^o$, $\Delta C$, FC) ← bag(s, At, Fd ∪ {f}), child₁(s₁, s), bag(s₁, At, Fd), rh(b, f), b ∈ $C^o$, solve(s₁, Y, FY₁, $C^o$, $\Delta C$, FC), consistent({f}, $C^o$), outside(FY₂, Y, At, {f}), FY = FY₁ ∪ FY₂. |
| solve(s, Y, FY, $C^o$, $\Delta C$, FC) ← bag(s, At, Fd ∪ {f}), child₁(s₁, s), bag(s₁, At, Fd), rh(b, f), b ∈ $C^o$, solve(s₁, Y, FY₁, $C^o$, $\Delta C$, FC), outside(FY₂, Y, At, {f}), FY = FY₁ ∪ FY₂. |
| /* attribute removal node. */ |
| solve(s, Y, FY, $C^o$, $\Delta C$, FC) ← bag(s, At, Fd), child₁(s₁, s), bag(s₁, At ∪ {b}, Fd), solve(s₁, Y ∪ {b}, FY, $C^o$, $\Delta C$, FC). |
| solve(s, Y, FY, $C^o$, $\Delta C$, FC) ← bag(s, At, Fd), child₁(s₁, s), bag(s₁, At ∪ {b}, Fd), solve(s₁, Y, FY, $C^o$, $\Delta C$, FC). |
| /* FD removal node. */ |
| solve(s, Y, FY, $C^o$, $\Delta C$, FC) ← bag(s, At, Fd), child₁(s₁, s), bag(s₁, At, Fd ∪ {f}), rh(b, f), b ∈ Y, solve(s₁, Y, FY, $C^o$, $\Delta C$, FC). |
| solve(s, Y, FY, $C^o$, $\Delta C$, FC) ← bag(s, At, Fd), child₁(s₁, s), bag(s₁, At, Fd ∪ {f}), rh(b, f), b ∈ $C^o$, solve(s₁, Y, FY ∪ {f}, $C^o$, $\Delta C$, FC). |
| solve(s, Y, FY, $C^o$, $\Delta C$, FC) ← bag(s, At, Fd), child₁(s₁, s), bag(s₁, At, Fd ∪ {f}), rh(b, f), b ∈ $C^o$, solve(s₁, Y, FY ∪ {f}, $C^o$, $\Delta C$, FC), f ∉ FC. |
| /* branch node. */ |
| solve(s, Y, FY₁ ∪ FY₂, $C^o$, $\Delta C₁$ ∪ $\Delta C₂$, FC) ← bag(s, At, Fd), child₁(s₁, s), bag(s₁, At, Fd), child₁(s₂, s), bag(s₂, At, Fd), solve(s₁, Y, FY₁, $C^o$, $\Delta C₁$, FC), solve(s₂, Y, FY₂, $C^o$, $\Delta C₂$, FC), unique($\Delta C₁$, $\Delta C₂$, FC). |
| /* result (at the root node). */ |
| success ← root(s), bag(s, At, Fd), a ∈ At, solve(s, Y, FY, $C^o$, $\Delta C$, FC), a ∉ Y, FY = \{f ∈ Fd \mid rhs(f) ∉ Y\}, $\Delta C = C^o \setminus \{a\}$. |

Figure 6: Primality Test.

Analogously to Section 5.1, we are using lower case letters $s$, $f$, and $b$ (possibly with subscripts) as datalog variables for a single node in $T$, for a single FD, or for a single attribute in $R$, respectively. Upper case letters are used as datalog variables denoting sets of attributes (in the case of $Y$, $At$, $C^o$, $\Delta C$) or sets of FDs (in the case of $Fd$, $FY$, $FC$). In addition, $C^o$ is considered as an ordered set (indicated by the superscript $o$). When we write $C^o \cup \{b\}$, we mean that $b$ is arbitrarily “inserted” into $C^o$, leaving the order of the remaining elements unchanged. Again, the cardinality of these (ordered) sets is restricted by the size $w + 1$ of the bags, where $w$ is a fixed constant. In addition to $\cup$ (disjoint union) we are now also using the set operators $\cup$, $\cap$, $\subseteq$, and $\in$. For the fixed-size (ordered) sets under consideration here, one could, of course, easily replace these operators by “proper” datalog expressions. Moreover, for the input schema $(R, F)$ with tree decomposition $T$ we use the following notation: We write $FD(s)$ to denote the FDs in the bag of $s$ and $FD(T_s)$ to denote the FDs that occur in any bag in $T_s$. Analogously, we write $Att(s)$ and $Att(T_s)$ as a
short-hand for the attributes occurring in the bag of \( s \) respectively in any bag in \( T_s \).

Our PRIMALITY-program checks the primality of \( a \) by via the criterion used for the MSO-characterization in Example 1.6. We have to search for an attribute set \( Y \subseteq R \), s.t. \( Y \) is closed w.r.t. \( F \) (i.e., \( Y^+ = Y \)), \( a \not\in Y \) and \( (Y \cup \{a\})^+ = R \), i.e., \( Y \cup \{a\} \) is a superkey but \( Y \) is not.

At the heart of our PRIMALITY-program is the intensional predicate \( \text{solve}(s, Y, FC, C, FC) \) with the following intended meaning: \( s \) denotes a node in \( T \). \( Y \) (resp. \( C^o \)) is the projection of \( Y \) (resp. of \( R \setminus Y \)) onto \( \text{Att}(s) \). We consider \( R \setminus Y \) as ordered w.r.t. an appropriate derivation sequence of \( R \) from \( Y \cup \{a\} \), i.e., suppose that \( Y \cup \{a_0\} \rightarrow Y \cup \{a_0, a_1\} \rightarrow Y \cup \{a_0, a_1, a_2\} \rightarrow \ldots \rightarrow Y \cup \{a_0, a_1, \ldots, a_n\} \), s.t. \( a_0 = a \) and \( Y \cup \{a_0, a_1, \ldots, a_n\} = R \). W.l.o.g., the \( a_i \)’s may be assumed to be pairwise distinct. Then for any two \( i \neq j \), we simply set \( A_i \prec A_j \) iff \( i < j \). By the connectedness condition on \( T \), our datalog program ensures that the order on each subset \( C^o \) of \( R \setminus Y \) is consistent with the overall ordering.

The argument \( FY \) of the \( \text{solve} \)-predicate is used to guarantee that \( Y \) is indeed closed. Informally, \( FY \) contains those FDs in \( FD(s) \) for which we have already verified (on the bottom-up traversal of the tree decomposition) that they do not constitute a contradiction with the closedness of \( Y \). In other words, either \( rhs(f) \in Y \) or there exists an attribute in \( lhs(f) \cap \text{Att}(T_s) \) which is not in \( Y \).

The arguments \( \Delta C \) and \( FC \) of the \( \text{solve} \)-predicate are used to ensure that \( (Y \cup \{a\})^+ = R \) indeed holds: The intended meaning of the set \( FC \) is that it contains those FDs in \( FD(s) \) which are used in the above derivation sequence. Moreover, \( \Delta C \) contains those attributes from \( \text{Att}(s) \) for which we have already shown that they can be derived from \( Y \) plus smaller atoms in \( C^o \).

More precisely, for all values \( s, Y, FC, C^o, \Delta C, FC \), the ground fact \( \text{solve}(s, Y, FC, C^o, \Delta C, FC) \) shall be in the least fixpoint of the program plus the input structure, iff the following condition holds:

**Property B.** There exist extensions \( \hat{Y} \) of \( Y \) and \( \hat{C}^o \) of \( C^o \) to \( \text{Att}(T_s) \) and an extension \( FC \) of \( FC \) to \( FD(T_s) \), s.t.

1. \( \hat{Y} \) and \( \hat{C}^o \) form a partition of \( \text{Att}(T_s) \),
2. \( \forall f \in FD(T_s) \setminus FD(s), \text{if} rhs(f) \not\subseteq \hat{Y}, \text{then} lhs(f) \not\subseteq \hat{Y}. \) Moreover, \( FY = \{ f \in FD(s) \mid rhs(f) \not\subseteq \hat{Y} \text{ and } lhs(f) \cap \text{Att}(T_s) \not\subseteq Y \} \).
3. \( \forall f \in FC, f \) is consistent with the order on \( \hat{C}^o \), i.e., \( \forall f \in FC: rhs(f) \in \hat{C}^o \) and \( \forall b \in lhs(f) \cap \hat{C}^o: b < rhs(f) \) holds.
4. \( \Delta C \cup \hat{C}^o \setminus \text{Att}(s) = \{ rhs(f) \mid f \in FC \} \).

The main task of the program is the computation of all facts \( \text{solve}(s, Y, FC, C^o, \Delta C, FC) \) by means of a bottom-up traversal of the tree decomposition. The other predicates have the following meaning:

- **outside** \((FY,Y,At,Fd)\) is in the least fixpoint iff \( FY = \{ f \in Fd \mid rhs(f) \not\subseteq Y \text{ and } lhs(f) \cap At \not\subseteq Y \} \), i.e., for every \( f \in FY \), \( rhs(f) \) is outside \( Y \) but this will never conflict with the closedness of \( Y \) because \( lhs(f) \) contains an attribute from outside \( Y \).

- **consistent** \((FC,C^o)\) is in the least fixpoint iff \( \forall f \in FC \) we have \( rhs(f) \in C^o \) and \( \forall b \in lhs(f) \cap C^o: b < rhs(f) \), i.e., the FDs in \( FC \) are only used to derive greater attributes from smaller ones (plus attributes from \( Y \)).

- The fact unique \((\Delta C_1, \Delta C_2, FC)\) is in the least fixpoint iff the condition \( \Delta C_1 \cap \Delta C_2 = \{ b \mid b = rhs(f) \text{ for some } f \in FC \} \) holds. The unique-predicate is only used in the body of the rule for branch nodes. Its purpose is to avoid that an attribute in \( R \setminus Y \) is derived via two different FDs in the two subtrees at the child nodes of the branch node.

- The 0-ary predicate success indicates if the fixed attribute \( a \) is prime in the schema encoded by the input structure.

The PRIMALITY-program has the following properties.

**Lemma 5.2** The \( \text{solve} \)-predicate has the intended meaning described above, i.e., for all values \( s, Y, FC, C^o, \Delta C, FC \), the ground fact \( \text{solve}(s, Y, FC, C^o, \Delta C, FC) \) is in the least fixpoint of the PRIMALITY-program plus the input structure, iff Property B holds.
Proof Sketch. The lemma can be shown by structural induction on $T$. We restrict ourselves here to outlining the ideas underlying the various rules of the PRIMALITY-program. The induction itself is then obvious and therefore omitted.

(1) leaf nodes. The rule for a leaf node $s$ realizes two “guesses” so to speak: (i) a partition of $At(s)$ into $Y$ and $C^o$ together with an ordering on $C^o$ and (ii) the subset $FC \subseteq Fd(s)$ of FDs which are used in the derivation sequence of $R \setminus \mathcal{Y}$ from $\mathcal{Y} \cup \{a\}$. The remaining variables are thus fully determined: $FY$ is determined via the outside-predicate, while $\Delta C$ is determined via the equality $\Delta C = \{rhs(f) \mid f \in FC\}$. Finally the body of the rule contains the checks consistent($FC, C^o$) and $\Delta C \subseteq C^o$ to make sure that (at least at the leaf node $s$) the “guesses” are allowed.

(2) attribute introduction node. The two rules are used to distinguish 2 cases whether the new attribute $b$ is added to $Y$ or to $C^o$. If $b$ is added to $Y$ then all arguments of the solve-fact at the child node $s_1$ of $s$ remain unchanged at $s$. In contrast, if $b$ is inserted into $C^o$ then the following actions are required:

The atom consistent($FC, C^o \cup \{b\}$) makes sure that the rules in $FC$ are consistent with the ordering of $C^o$, i.e., it must not happen that the new attribute $b$ occurs in $lhs(f)$ for some $f \in FC$, s.t. $b > rhs(f)$ holds.

The new attribute $b$ outside $Y$ may possibly allow us to verify for some additional FDs that they do not contradict the closedness of $\mathcal{Y}$. The atom outside($FY_2, Y, At, Fd$) determines the set $FY_2$ which contains all FDs with $rhs(f) \not\in Y$ but with some attribute from $C^o$ (in particular, the new attribute $b$) in $lhs(f)$.

Recall that we are requiring that, whenever an FD $f \in F$ is contained in a bag of the tree decomposition, then the attribute $rhs(f)$ is as well. Hence, since the attribute $b$ has just been introduced on our bottom-up traversal of the tree decomposition, we can be sure that $b$ does not occur on the right-hand side of any FD in the bag of $s$. Thus, $\Delta C$ is not affected by the transition from $s_1$ to $s$.

(3) FD introduction node. The three rules distinguish, in total, 3 cases: First, does $rhs(f) \in Y$ or $rhs(f) \in C^o$ hold? (Recall that we assume that every bag containing some FD also contains the right-hand side of this FD.) The latter case is then further divided into the subcases if $f$ is used for the derivation of $R \setminus \mathcal{Y}$ or not. The first rule deals with the case $rhs(f) \in Y$. Then all arguments of the solve-fact at the child node $s_1$ of $s$ remain unchanged at $s$.

The second rule addresses the case that $rhs(f) \in C^o$ and $f$ is used for the derivation of $R \setminus \mathcal{Y}$. Then the attribute $rhs(f)$ is added to $\Delta C$. The disjoint union makes sure that this attribute has not yet been derived by another rule with the same right-hand side. The atom consistent($FC, C^o \cup \{b\}$) is used to check the consistency of $f$ with the ordering of $C^o$. The atom outside($FY_2, Y, At, Fd$) is used to check if $f$ may be added to $FY$, i.e., if some attribute in $lhs(f)$ is in $C^o$.

The third rule refers to the case that $rhs(f) \in C^o$ and $f$ is not used for the derivation of $R \setminus \mathcal{Y}$. Again, the atom outside($FY_2, Y, At, Fd$) is used to check if $f$ may be added to $FY$.

(4) attribute removal node. The two rules are used to distinguish 2 cases whether the attribute $b$ was in $Y$ or in $C^o$. If $b$ was in $Y$ then all arguments of the solve-fact at the child node $s_1$ of $s$ remain unchanged at $s$. In contrast, if $b$ was in $C^o$ then we have to check (by pattern matching with the fact solve($s_1, \ldots, \Delta C \cup \{b\}, \ldots$)) that a rule $f$ for deriving $b$ has already been found. Recall that, on our bottom-up traversal of $T$, when we first encounter an attribute $b$, it is either added to $Y$ or $C^o$. If $b$ is added to $C^o$ then we eventually have to determine the FD by which $b$ is derived. Hence, initially, $b$ is in $C^o$ but not in $\Delta C$. However, when $b$ is finally removed from the bag then its derivation must have been verified. The arguments $Y$, $FY$, and $FC$ are of course not affected by this attribute removal.

(5) FD removal node. Similarly to the FD introduction node, we distinguish, in total, 3 cases. If $rhs(f) \in Y$ then all arguments of the solve-fact at the child node $s_1$ of $s$ remain unchanged at $s$. If $rhs(f) \in C^o$ then we further distinguish the subcases if $f$ is used for the derivation of $R \setminus \mathcal{Y}$ or not. The second and third rule refer two these two subcases. The action carried out by these two rules is the same, namely it has to be checked (by pattern matching with the fact solve($s_1, \ldots, FY \cup \{f\}, \ldots$)) that $f$ does not constitute a contradiction with the closedness of $\mathcal{Y}$. In other words, since $rhs(f) \in C^o$, we must have encountered (on our bottom-up traversal of $T$) an attribute in $lhs(f) \not\in \mathcal{Y}$.

(6) branch node. Recall that a branch node $s$ and its two child nodes $s_1$ and $s_2$ have identical bags by our notion of normalized tree decompositions. The argument of the solve-fact at $s$ is then determined from the
arguments at \(s_1\) and \(s_2\) as follows: The arguments \(Y\) and \(C^o\) must have the same value at all three nodes \(s, s_1,\) and \(s_2.\) Likewise, \(FC\) (containing the FDs from the bags at these nodes which are used in the derivation of \(R \setminus Y\)) must be identical. In contrast, \(FY\) and \(\Delta C\) are obtained as the union of the corresponding arguments in the solve-facts at the child nodes \(s_1\) and \(s_2,\) i.e., it suffices to verify at one of the child nodes \(s_1\) or \(s_2\) that some FD does not contradict the closedness of \(Y\) and that some attribute in \(C^o\) is derived by some FD.

Recall that we define an order on the attributes in \(R \setminus Y\) by means of some derivation sequence of \(R \setminus Y\) from \(Y \cup \{a\}\). Hence, we have to make sure that every attribute in \(R \setminus Y\) is derived only once in this derivation sequence. In other words, for every \(b \in R \setminus (Y \cup \{a\}),\) we use exactly one FD \(f\) with \(\text{rhs}(f) = b\) in our derivation sequence. The atom \(\text{unique}(\Delta C_1, \Delta C_2, FC)\) in the rule body ensures that no attribute in \(R \setminus Y\) is derived via two different FDs in the two subtrees at the child nodes of the branch node.

**Theorem 5.3** The datalog program in Figure 6 decides the PRIMALITY problem for a fixed attribute \(a,\) i.e., the fact "success" is in the least fixpoint of this program plus the input \(\tau_{td}\)-structure \(A_{td}\) iff \(A_{td}\) encodes a relational schema \((R,F),\) s.t. \(a\) is part of a key. Moreover, for any schema \((R,F)\) with treewidth \(w,\) the computation of the \(\tau_{td}\)-structure \(A_{td}\) and the evaluation of the program can be done in time \(O(f(w) * |(R,F)|)\) for some function \(f.\)

**Proof.** By Lemma 5.2, the predicate \(\text{solve}\) indeed has the meaning according to Property B. Thus, the rule with head \("success"\) reads as follows: \("success"\) is in the least fixpoint, iff \(s\) denotes the root of \(T, a\) is an attribute in the bag at \(s,\) and \(Y\) is the projection of the desired attribute set \(\mathcal{Y}\) onto \(\text{Att}(s),\) i.e., (1) \(\mathcal{Y}\) is closed (this is ensured by the condition that \(\{f \in Fd \mid \text{rhs}(f) \not\in \mathcal{Y}\} = FY\)), (2) \(a \not\in \mathcal{Y}\) and, finally, (3) all attributes in \(R \setminus (\mathcal{Y} \cup \{a\})\) are indeed determined by \(\mathcal{Y} \cup \{a\}\) (this is ensured by the condition \(\Delta C = C^o \setminus \{a\}\)).

The linear time data complexity is due to the same argument as in the proof of Theorem 5.1. Our program in Figure 6 is essentially a succinct representation of a quasi-guarded monadic datalog program. For instance, in the atom \(\text{solve}(s,Y,FY,C^o,\Delta C,FC),\) the (ordered) sets \(Y, FY, C^o, \Delta C,\) and \(FC\) are subsets of the bag of \(s.\) Hence, each combination \(Y, FY, C^o, \Delta C, FC\) could be represented by 5 subsets resp. tuples \(r_1, \ldots, r_5\) over \(\{0, \ldots, w\}\) referring to indices of elements in the bag of \(s.\) Recall that \(w\) is a fixed constant. Hence, \(\text{solve}(s,Y,FY,C^o,\Delta C,FC),\) is simply a succinct representation of constantly many monadic predicates of the form \(\text{solve}(r_1,\ldots,r_5)(s).\) The quasi-guard in each rule can thus be any atom with argument \(s,\) e.g., \(\text{bag}(s,At,Fd)\) (possibly extended by a disjoint union with \(\{b\}\) or \(\{f\},\) respectively).

Thus, the linear time bound follows immediately from Theorem 4.4.

**5.3 The Primality Enumeration Problem**

In order to extend the Primality algorithm from the previous section to a monadic predicate selecting all prime attributes in a schema, a naive first attempt might look as follows: one can consider the tree decomposition \(T\) as rooted at various nodes, s.t. each \(a \in R\) is contained in the bag of one such root node. Then, for each \(a\) and corresponding tree decomposition \(T,\) we run the algorithm from Figure 6. Obviously, this method has quadratic time complexity w.r.t. the data size. However, in this section, we describe a linear time algorithm.

The idea of this algorithm is to implement a top-down traversal of the tree decomposition in addition to the bottom-up traversal realized by the program in Figure 6. For this purpose, we modify our notion of normalized tree decompositions in the following way: First, any tree decomposition can of course be transformed in such a way that every attribute \(a \in R\) occurs in at least one leaf node of \(T.\) Moreover, for every branch node \(s\) in the tree decomposition, we insert a new node \(u\) as new parent of \(s,\) s.t. \(u\) and \(s\) have identical bags. Hence, together with the two child nodes of \(s,\) each branch node is “surrounded” by three neighboring nodes with identical bags. It is thus guaranteed that a branch node always has two child nodes with identical bags, no matter where \(T\) is rooted. Moreover, this insertion of a new node also implies that the root node of \(T\) is not a branch node.
We propose the following algorithm for computing a monadic predicate \( \text{prime}(\)\), which selects precisely the prime attributes in \((R, F)\). In addition to the predicate \( \text{solve}(\)\), whose meaning was described by Property B in Section 5.2, we also compute a predicate \( \text{solve}↓(\)\), whose meaning is described by replacing every occurrence of \( T_s \) in Property B by \( \overline{T}_s \). As the notation \( \text{solve}↓(\)\) suggests, the computation of \( \text{solve}↓(\)\) can be done via a top-down traversal of \( T \). Note that \( \text{solve}↓(s, . . .) \) for a leaf node \( s \) of \( T \) is exactly the same as if we computed \( \text{solve}(s, . . .) \) for the tree rooted at \( s \). Hence, we can define the predicate \( \text{prime}(\)\) as follows.

**Program Monadic-Primality**

\[
\text{prime}(a) \leftarrow \text{leaf}(s), \text{bag}(s, At, Fd), a \in At, \text{solve}↓(s, Y, F Y, C^o, \Delta C, FC), a \not\in Y, \\
FY = \{ f \in Fd \mid \text{rhs}(f) \not\in Y \}, \Delta C = C^o \setminus \{a\}.
\]

By the intended meaning of \( \text{solve}↓(\)\) and by the properties of the Primality algorithm in Section 5.2, we immediately get the following result.

**Theorem 5.4** The monadic predicate \( \text{prime}(\)\) as defined above selects precisely the prime attributes. Moreover, it can be computed in linear time w.r.t. the size of the input structure.

### 6 Implementation and Results

To test our new datalog programs in terms of their scalability with a large number of attributes and rules, we have implemented the Primality program from Section 5.2 in C++. The experiments were conducted on Linux kernel 2.6.17 with an 1.60GHz Intel Pentium(M) processor and 512 MB of memory. We measured the processing time of the Primality program on different input parameters such as the number of attributes and the number of FDs. The treewidth in all the test cases was 3.

**Test Data Generation.** Due to the lack of available test data, we generated a balanced normalized tree decomposition. Test data sets with increasing input parameters are then generated by expanding the tree in a depth-first style. We have ensured that all different kinds of nodes occur evenly in the tree decomposition.

**Experimental Results.** The outcome of the tests is shown in Table 1 where \( tw \) stands for the treewidth; \#Att, \#FD, and \#tn stand for the number of attributes, FDs, and tree nodes, respectively. The processing time (in ms) obtained with our C++ implementation following the monadic datalog program in Section 5.2 are displayed in the column labelled “MD”. The measurements nicely reflect an essentially linear increase of the processing time with the size of the input. Moreover, there is obviously no big “hidden” constant which would render the linearity useless.

| tw | #Att | #FD | #tn | MD   | MONA |
|----|------|-----|-----|------|------|
| 3  | 3    | 1   | 3   | 0.1  | 650  |
| 3  | 6    | 2   | 12  | 0.2  | 9210 |
| 3  | 9    | 3   | 21  | 0.4  | 17930|
| 3  | 12   | 4   | 34  | 0.5  | –    |
| 3  | 21   | 7   | 69  | 0.8  | –    |
| 3  | 33   | 11  | 105 | 1.0  | –    |
| 3  | 45   | 15  | 141 | 1.2  | –    |
| 3  | 57   | 19  | 193 | 1.6  | –    |
| 3  | 69   | 23  | 229 | 1.8  | –    |
| 3  | 81   | 27  | 265 | 1.9  | –    |
| 3  | 93   | 31  | 301 | 2.2  | –    |

Table 1: Processing Time in ms for PRIMALITY.
In [17], we proved the FPT of several non-monotonic reasoning problems via Courcelle’s Theorem. Moreover, we also carried out some experiments with a prototype implementation using MONA (see [22]) for the MSO-model checking. We have now extended these experiments with MONA to the PRIMALITY problem. The time measurements of these experiments are shown in the last column of Table 1. Due to problems discussed in [17], MONA does not ensure linear data complexity. Hence, all tests below line 3 of the table failed with “out-of-memory” errors. Moreover, also in cases where the exponential data complexity does not yet “hurt”, our datalog approach outperforms the MSO-to-FTA approach by a factor of 1000 or even more.

**Optimizations.** In our implementation, we have realized several optimizations, which are highlighted below.

1. **Succinct representation by non-monadic datalog.** As was mentioned in the proofs of the Theorems 5.1 and 5.3, our datalog programs can be regarded as succinct representations of big monadic datalog programs. If all possible ground instances of our datalog rules had to be materialized, then we would end up with a ground program of the same size as with the equivalent monadic program. However, it turns out that the vast majority of possible instantiations is never computed since they are not “reachable” along the bottom-up computation.

2. **General optimizations and lazy grounding.** In principle, our implementation is based on the general idea of grounding followed by an evaluation of the ground program. This corresponds to the general technique to ensure linear time data complexity, cf. Theorem 4.4. A further improvement is achieved by the natural idea of generating only those ground instances of rules which actually produce new facts.

3. **Problem-specific optimizations of the non-monadic datalog programs.** In the discussion below Theorem 5.1 we have already mentioned that the datalog programs presented in Section 5 incorporate several problem-specific optimizations. The underlying idea of these optimizations is that many transitions which are kept track of by the generic construction in the proof of Theorem 4.5 (and, likewise, in the MSO-to-FTA approach) will not lead to a solution anyway. Hence, they are omitted in our datalog programs right from the beginning.

4. **Language extensions.** As was mentioned in Section 5 we are using language constructs (in particular, for handling sets of attributes and FDs) which are not part of the datalog language. In principle, they could be realized in datalog. Nevertheless, we preferred an efficient implementation of these constructs directly on C++ level. Further language extensions are conceivable and easy to realize.

5. **Further improvements.** We are planning to implement further improvements. For instance, we are currently applying a strict bottom-up intuition as we compute new facts solve\((v, \ldots)\). However, some top-down guidance in the style of magic sets so as not to compute all possible such facts at each level would be desirable. Note that ultimately, at the root, only facts fulfilling certain conditions (like \(a \notin Y\), etc.) are needed in case that an attribute \(a\) is indeed prime.

**7 Conclusion**

In this work, we have proposed a new approach based on monadic datalog to tackle a big class of fixed-parameter tractable problems. Theoretically, we have shown that every MSO-definable unary query over finite structures with bounded treewidth is also definable in monadic datalog. In fact, the resulting program even lies in a particularly efficient fragment of monadic datalog. Practically, we have put this approach to work by applying it to the 3-Colorability problem and the PRIMALITY problem with bounded treewidth. The experimental results thus obtained look very promising. They underline that datalog with its potential for optimizations and its flexibility is clearly worth considering for this class of problems.

Recall that the PRIMALITY problem is closely related to an important problem in the area of artificial intelligence, namely the relevance problem of propositional abduction (i.e., given a system description in form of a propositional clausal theory and observed symptoms, one has to decide if some hypothesis is part of a possible explanation of the symptoms). Indeed, if the clausal theory is restricted to definite Horn clauses and if we are only interested in minimal explanations, then the relevance problem is basically the same as the problem of deciding primality in a subschema \(R' \subseteq R\). Extending our `prime()` program (and, in particular,
the `solve()`-predicate) from Section 5 so as to test primality in a subschema is rather straightforward. On the other hand, extending such a program to abduction with arbitrary clausal theories (which is on the second level of the polynomial hierarchy, see [10]) is much more involved. A monadic datalog program solving the relevance problem also in this general case was presented in [20].

Our datalog program in Section 5 was obtained by an ad hoc construction rather than via a generic transformation from MSO. Nevertheless, we are convinced that the idea of a bottom-up propagation of certain conditions is quite generally applicable. We are therefore planning to tackle many more problems, whose FPT was established via Courcelle’s Theorem, with this new approach. We have already incorporated some optimizations into our implementation. Further improvements are on the way (in particular, further heuristics to prune irrelevant parts of the search space).

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