# ANSWER COUNTING UNDER GUARDED TGDS

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ABSTRACT. We study the complexity of answer counting for ontology-mediated queries and for querying under constraints, considering conjunctive queries and unions thereof (UCQs) as the query language and guarded TGDs as the ontology and constraint language, respectively. Our main result is a classification according to whether answer counting is fixed-parameter tractable (FPT), W[1]-equivalent, #W[1]-equivalent, #W[2]-hard, or #A[2]-equivalent, lifting a recent classification for UCQs without ontologies and constraints due to Dell et al. [DRW19]. The classification pertains to various structural measures of queries, namely treewidth, contract treewidth, starsize, and linked matching number. Our results rest on the assumption that the arity of relation symbols is bounded by a constant and, in the case of ontology-mediated querying, that all symbols from the ontology and query can occur in the data (so-called full data schema). We also study the meta-problems for the mentioned structural measures, that is, to decide whether a given ontology-mediated query or constraint-query specification is equivalent to one for which the structural measure is bounded.

### 1. INTRODUCTION

Tuple-generating dependencies (TGDs) are a prominent formalism for formulating database constraints. A TGD states that if certain facts are true, then certain other facts must be true as well. This can be interpreted in different ways. In *ontology-mediated querying*, TGDs give rise to ontology languages and are used to derive new facts in addition to those that are present in the database. This makes it possible to obtain additional answers if the data is incomplete and also enriches the vocabulary that is available for querying. In a more classical setup that we refer to as *querying under constraints*, TGDs are used as integrity constraints on the database, that is, a TGD expresses the promise that if certain facts are present in the database, then certain other facts are present as well. Integrity constraints are relevant to query optimization as their presence might enable the reformulation of a query into a 'simpler' one. TGDs generalize a wide range of other integrity constraints such as referential integrity constraints (also known as inclusion dependencies), which was the original motivation for introducing them [AHV95].

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When unrestricted TGDs are used as an ontology language, ontology-mediated querying is undecidable even for unary queries that consist of a single atom [CGK13]. This has led to intense research on identifying restricted forms of TGDs that regain decidability, see for instance [BLMS11, CGK13, CGP12, LMTV19] and references therein. In this paper, we consider guardedness as a basic and robust such restriction: a TGD is guarded if some body atom, the guard, contains all body variables [CGK13]. Guarded TGDs are useful also for formalizing integrity constraints. For example, inclusion dependencies are a special case of guarded TGDs.

In what follows, an ontology-mediated query (OMQ) is a triple ( $\mathcal{O}, \mathbf{S}, q$ ) with  $\mathcal{O}$  a set of TGDs (the ontology),  $\mathbf{S}$  a data schema, and Q a union of conjunctive queries (UCQ). Note that  $\mathbf{S}$  contains the relation symbols that can be used in the data while both the ontology and query can also use additional symbols. We use ( $\mathbb{G}, \mathbb{CQ}$ ) to denote the language of OMQs in which the ontology  $\mathcal{O}$  is a set of guarded TGDs and where q is a conjunctive query (CQ), and likewise for ( $\mathbb{G}, \mathbb{UCQ}$ ). For querying under constraints, we consider constraint query specifications (CQSs) of the form ( $\mathcal{T}, \mathbf{S}, q$ ) where  $\mathcal{T}$  is a set of TGDs (the integrity constraints) and q is a query, both over schema  $\mathbf{S}$ . Overloading notation, we use ( $\mathbb{G}, (\mathbb{U})\mathbb{CQ}$ ) also to denote the class of CQSs in which the constraints are guarded TGDs and the queries are (U)CQs; it will always be clear from the context whether ( $\mathbb{G}, (\mathbb{U})\mathbb{CQ}$ ) denotes an OMQ language or a class of CQSs.

While being decidable, both ontology-mediated querying and querying under constraints with guarded TGDs is computationally intractable in combined complexity. Let us make this precise for query evaluation, which is the following problem: given a database D, a query Q, and a candidate answer  $\bar{c}$ , decide whether  $\bar{c}$  is indeed an answer to Q on D. Evaluating OMQs from ( $\mathbb{G}, \mathbb{CQ}$ ) is 2EXPTIME-complete in combined complexity and the same holds for ( $\mathbb{G}, \mathbb{UCQ}$ ) [CGK13]; in both cases, the complexity drops to EXPTIME if the arity of relation symbols is bounded by a constant. Query evaluation for CQSs from ( $\mathbb{G}, \mathbb{CQ}$ ) and ( $\mathbb{G}, \mathbb{UCQ}$ ) is NP-complete.

In this article, we are interested in counting the number of answers to OMQs and to queries posed under integrity constraints, with an emphasis on the limits of efficiency from the viewpoint of parameterized complexity theory. Counting the number of answers is important to inform the user when there are too many answers to compute all of them, and it is supported by almost every data management system. It is also a fundamental operation in data analytics and in decision support where often the count is more important than the actual answers. Despite its relevance, however, the problem has received little attention in ontology-mediated querying and querying under constraints. We refer to [KR15, KK18, BMT20, CCLR20, BMT22] for notable exceptions regarding ontology-mediated querying that, however, study different counting problems than the present paper.

We equate efficiency with fixed-parameter tractability (FPT), the parameter being the size of the OMQ and of the CQS, respectively. Evaluation is W[1]-hard both for ontology-mediated querying in ( $\mathbb{G}$ , ( $\mathbb{U}$ ) $\mathbb{C}\mathbb{Q}$ ) and for querying under constraints in ( $\mathbb{G}$ , ( $\mathbb{U}$ ) $\mathbb{C}\mathbb{Q}$ ) [BDF<sup>+</sup>20]. These lower bounds apply already to Boolean queries where evaluation and counting coincide, and therefore answer counting is in general not fixed-parameter tractable in the mentioned cases unless FPT = W[1]. The main question that we address is: how can we characterize the parameterized complexity of answer counting for classes of OMQs or CQSs  $\mathbb{Q} \subseteq (\mathbb{G}, (\mathbb{U})\mathbb{C}\mathbb{Q})$  and, most importantly, for which such classes  $\mathbb{Q}$  can we count answers in FPT? The classes  $\mathbb{Q}$  will primarily be defined in terms of structural measures of the (U)CQ, but will also take into account the interplay between the ontology/constraints and the (U)CQ. Note that PTIME combined complexity, a (significant) strengthening of FPT, cannot be obtained by structural restrictions on the UCQ in ontology-mediated querying with  $(\mathbb{G}, (\mathbb{U})\mathbb{C}\mathbb{Q})$  because evaluating Boolean OMQs is 2EXPTIME-complete already for unary single-atom queries. For querying under constraints, in contrast, PTIME combined complexity is not excluded up-front and in the case of query evaluation can in fact sometimes be attained in  $(\mathbb{G}, (\mathbb{U})\mathbb{C}\mathbb{Q})$  [BGP16, BFGP20].

A seminal result due to Grohe states that a recursively enumerable class  $\mathbb{Q}$  of CQs can be evaluated in FPT if and only if there is a constant that bounds the treewidths of CQs in Q, modulo equivalence [Gro07]. Grohe considers only Boolean CQs, but it is well-known that the result lifts to the non-Boolean case when the treewidth of a CQ q is taken to mean the treewidth of the Gaifman graph of q after dropping all answer variables, see for instance [BFLP19, BDF<sup>+</sup>20]. The result rests on the assumptions that FPT  $\neq$  W[1] and that the arity of relation symbols is bounded by a constant, which we shall also assume throughout this article. Grohe's result extends to UCQs in the expected way, that is, the characterization for UCQs is in terms of the maximum treewidth of the constituting CQs modulo equivalence, assuming w.l.o.g. that there are no containment relations among the CQs. An adaptation of Grohe's proof was used by Dalmau and Jonsson to show that a class  $\mathbb{O}$  of CQs without quantified variables admits answer counting in FPT if and only if the treewidths of CQs in  $\mathbb{Q}$  is bounded by a constant [DJ04]. In a series of papers by Pichler and Skritek [PS13], Durand and Mengel [DM14, DM15], Chen and Mengel [CM15, CM16], and Dell et al. [DRW19], this was extended to a rather detailed classification of the parameterized complexity of answer counting for classes of CQs and UCQs that may contain both answer variables and quantified variables. The characterization is based on the structural measure of treewidth, which now refers to the entire Gaifman graph including the answer variables. It also refers to the additional measures of contract treewidth, starsize,<sup>1</sup> and linked matching number. It links boundedness of these measures by a constant, modulo equivalence, to the relevant complexities, which turn out to be FPT, W[1]-equivalence, #W[1]-equivalence, #W[2]-hardness, and #A[2]-equivalence. Here, we speak of 'equivalence' rather than of 'completeness' to emphasize that hardness is defined in terms of (parameterized counting) Turing (fpt-)reductions.

The main results of this article are classifications of the complexity of answer counting for classes of ontology-mediated queries from  $(\mathbb{G}, (\mathbb{U})\mathbb{C}\mathbb{Q})$ , assuming that the data schema contains all symbols used in the ontology and query, and for classes of constraint query specifications from  $(\mathbb{G}, (\mathbb{U})\mathbb{C}\mathbb{Q})$ . Our classifications parallel the one for the case without TGDs, involve the same five complexities mentioned above, and link them to the same structural measures. There is, however, a twist. The ontology interacts with all of the mentioned structural measures in the sense that for each measure, there is a class of CQs  $\mathbb{Q}$ and an ontology  $\mathcal{O}$  such that the measure is unbounded for  $\mathbb{Q}$  modulo equivalence while there is a constant k such that each OMQ  $(\mathcal{O}, \mathbf{S}, q), q \in \mathbb{Q}$ , is equivalent to an OMQ  $(\mathcal{O}, \mathbf{S}, q')$ with the measure of q' bounded by k. A similar effect can be observed for querying under constraints. We can thus not expect to link the complexity of a class  $\mathbb{Q}$  of OMQs to the structural measures of the actual queries in the OMQs. Instead, we consider a certain class  $\mathbb{Q}^*$  of CQs that we obtain from the OMQs in  $\mathbb{Q}$  by first rewriting away the existential quantifiers in TGD heads in the ontology, then taking the CQs that occur in the resulting OMQs, combining them conjunctively guided by the inclusion-exclusion principle, next

<sup>&</sup>lt;sup>1</sup>The measure is called dominating starsize in [DRW19] and strict starsize in [CM15]. We only speak of starsize. Note that this is not identical to the original notion of starsize from [DM14, DM15].

chasing them with the ontology (which is a finite operation due to the first step), and then taking the homomorphism core. The structural measures of  $\mathbb{Q}^*$  turn out to determine the complexity of answer counting for the original class of OMQs  $\mathbb{Q}$ . Interestingly, the same is also true for classes of constraint query specifications and thus the characterizations for OMQs and for CQSs coincide. We in fact establish the latter by mutual reduction between answer counting for OMQs and answer counting for CQSs.

We also take a brief look at approximate counting. For CQs without ontologies, significant progress has recently been made by Arenas et al. [ACJR21] who show that a class of CQs  $\mathbb{Q}$ admits a fully polynomial randomized approximation scheme (FPRAS) if and only if there is a constant bound k on the treewidth of the queries in  $\mathbb{Q}$  where, as for exact counting, treewidth refers to the Gaifman graph including answer variables. This result is subject to the assumptions that W[1]  $\neq$  FPT, P = BPP, the arity of relation symbols is bounded by a constant, and for every  $q \in \mathbb{Q}$ , there is a self-join free  $q' \in \mathbb{Q}$  that has the same hypergraph. We observe that it is not hard to derive from this the existence of a fixed-parameter tractable randomized approximation scheme (FPTRAS) for classes of OMQs  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$  that have bounded treewidth modulo equivalence. We leave a matching lower bound as an open problem. It is an interesting contrast that the condition for the existence of an FPTRAS is much less intricate than that for exact counting, in particular bypassing the class of CQs  $\mathbb{Q}^*$ mentioned above.

Inspired by our complexity classifications, we then proceed to study the meta problems to decide whether a given query is equivalent to a query in which some selected structural measures are small, and to construct the latter query if it exists. We do this both for ontology-mediated queries and for queries under constraints, considering all four measures that are featured in the classifications (and sets thereof). We start with querying under constraints where we are able to obtain decidability results in all relevant cases. These results can also be applied to ontology-mediated querying when (i) the data schema contains all symbols used in the ontology and query and (ii) we require that the ontology used in the OMQ cannot be replaced with a different one. For contract treewidth and starsize, we additionally show that it is never necessary to modify the ontology to attain equivalent OMQs with small measures, and we provide decidability results without assumptions (i) and (ii). We also observe that treewidth behaves differently in that modifying the ontology might result in smaller measures. Deciding the meta problem for the measure of treewidth is left open as an interesting and non-trivial open problem.

This article is an extended version of the conference paper [FLP21]. Some proofs are deferred to the appendix. Since we rely profoundly on (refinements of) results due to Chen and Mengel [CM15, CM16], we also provide in the appendix summaries of the proofs of those results.

**Related Work.** The complexity of ontology-mediated querying has been a subject of intense study from various angles, see for example [BO15, BtCLW14, PLC<sup>+</sup>08] and references therein. The parameterized complexity of evaluating ontology-mediated queries has been studied in [BFLP19, BDF<sup>+</sup>20, Fei22]. While [BFLP19] consider description logics such as  $\mathcal{ELI}$  as the ontology language, [BDF<sup>+</sup>20, Fei22] focus on ( $\mathbb{G}, \mathbb{UCQ}$ ). Query evaluation in FPT coincides with bounded treewidth modulo equivalence when the arity of relation symbols is bounded by a constant, unless FPT = W[1] [BDF<sup>+</sup>20]. When there is no such bound, then it coincides with bounded submodular width modulo equality unless the exponential time hypothesis fails[Fei22]. Counting in ontology-mediated querying has been

considered in [KR15, KK18, BMT20, CCLR20, BMT21a, BMT21b]. There, conjunctive queries are equipped with dedicated counting variables and the focus is to decide, given an OMQ  $Q = (\mathcal{O}, \mathbf{S}, q)$ , an **S**-database D and a  $k \geq 0$  whether there is a model of D and  $\mathcal{O}$ such that the homomorphisms from q to that model yield at least/at most k bindings of the counting variables. The ontology languages studied are versions of the description logic DL-Lite, with the exception of [BMT21b] which studies the description logic  $\mathcal{ELI}$ . These can all be viewed as guarded TGDs, up to a certain syntactic normalization in the case of  $\mathcal{ELI}$ .

Query evaluation under constraints that are guarded TGDs has been considered in [BGP16, BFGP20]. A main result is an FPT upper bound for CQs that have bounded generalized hypertreewidth modulo equivalence. These papers also study the meta problem for querying under constraints that are guarded TGDs and for the measure of generalized hypertree width. A topic closely related to the evaluation of queries under constraints is query containment under constraints, see for example [CGL98, JK84, Fig16]. We are not aware that answer counting under integrity constraints has been studied before.

#### 2. Preliminaries

For an integer  $n \ge 1$ , we use [n] to denote the set  $\{1, \ldots, n\}$ . To indicate the cardinality of a set S, we may write #S or |S|.

**Relational Databases.** A schema **S** is a set of relation symbols R with associated arity  $\operatorname{ar}(R) \geq 0$ . We write  $\operatorname{ar}(\mathbf{S})$  for  $\max_{R \in \mathbf{S}} \{\operatorname{ar}(R)\}$ . An **S**-fact is an expression of the form  $R(\overline{c})$ , where  $R \in \mathbf{S}$  and  $\overline{c}$  is an  $\operatorname{ar}(R)$ -tuple of constants. An **S**-instance is a (possibly infinite) set of **S**-facts and an **S**-database is a finite **S**-instance. We write  $\operatorname{adom}(I)$  for the set of constants in an instance I. For a set  $S \subseteq \operatorname{adom}(I)$ , we denote by  $I_{|S}$  the restriction of I to facts that mention only constants from S. A homomorphism from I to an instance J is a function  $h : \operatorname{adom}(I) \to \operatorname{adom}(J)$  such that  $R(h(\overline{c})) \in J$  for every  $R(\overline{c}) \in I$  where  $h(\overline{c})$  means the component-wise application of h. A guarded set in a database D is a set  $S \subseteq \operatorname{adom}(D)$  such that all constants in S jointly occur in a fact in D, possibly together with other constants. With a maximal guarded set, we mean a guarded set that is maximal regarding set inclusion.

We next introduce some operations on instances that are used in the paper. An *induced* subinstance of an **S**-instance I is any **S**-instance I' obtained from I by choosing a  $\Delta \subseteq \operatorname{adom}(I)$ and putting  $I' = \{R(\bar{c}) \in I \mid \bar{c} \in \Delta^{\operatorname{ar}(R)}\}$ . If I and I' are finite, then we speak of an *induced* subdatabase. The disjoint union of two **S**-instances  $I_1$  and  $I_2$  with  $\operatorname{adom}(I_1) \cap \operatorname{adom}(I_2) = \emptyset$ is simply  $I_1 \cup I_2$ . The direct product of two **S**-instances  $I_1$  and  $I_2$  is the **S**-instance I with domain  $\operatorname{adom}(I) = \operatorname{adom}(I_1) \times \operatorname{adom}(I_2)$  defined as

 $I = \{R((a_1, b_1), \dots, (a_n, b_n)) \mid R(a_1, \dots, a_n) \in I_1 \text{ and } R(b_1, \dots, b_n) \in I_2\}.$ 

An instance I' is obtained from an instance I by cloning constants if  $I' \supseteq I$  can be constructed by choosing  $c_1, \ldots, c_n \in \operatorname{adom}(I)$  and positive integers  $m_1, \ldots, m_n$ , reserving fresh constants  $c_1^{i_1}, \ldots, c_n^{i_n}$  with  $1 \le i_\ell \le m_\ell$  for  $1 \le \ell \le n$ , and adding to I each atom  $R(\overline{c}')$  that can be obtained from some  $R(\overline{c}) \in I$  by replacing each occurrence of  $c_i, 1 \le i \le n$ , with  $c_i^j$  for some j with  $1 \le j \le m_i$ .

**CQs and UCQs.** A conjunctive query (CQ)  $q(\bar{x})$  over a schema **S** is a first-order formula of the form  $\exists \bar{y} \varphi(\bar{x}, \bar{y})$  where  $\bar{x}$  and  $\bar{y}$  are disjoint tuples of variables and  $\varphi$  is a conjunction that may contain relational atoms  $R_i(\bar{x}_i)$  with  $R_i \in \mathbf{S}$  and  $\bar{x}_i$  a tuple of variables of length

 $\operatorname{ar}(R_i)$  as well as equality atoms  $x_1 = x_2$ . The variables used in  $\varphi$  must be exactly those in  $\overline{x}$  and  $\overline{y}$ , and only variables from  $\overline{x}$  may appear in equality atoms. We assume that  $\overline{x}$ contains no repeated variables, which is w.l.o.g. due to the presence of equality atoms. With  $\operatorname{var}(q)$ , we denote the set of variables that occur in  $\overline{x}$  or in  $\overline{y}$ . Whenever convenient, we identify a conjunction of atoms with a set of atoms. When we are not interested in order and multiplicity, we treat  $\overline{x}$  as a set of variables. A CQ is equality-free if it contains no equality atoms. Note that we do not admit constants in CQs.<sup>2</sup> We write  $\mathbb{CQ}$  for the class of all CQs.

Every CQ  $q(\bar{x})$  can be seen as a database  $D_q$  in a natural way, namely by dropping the existential quantifier prefix and the equality atoms, and viewing variables as constants. A homomorphism h from a CQ q to an instance I is a homomorphism from  $D_q$  to I such that  $x = y \in q$  implies h(x) = h(y). A tuple  $\bar{c} \in \mathsf{adom}(I)^{|\bar{x}|}$  is an answer to q on I if there is a homomorphism h from q to I with  $h(\bar{x}) = \bar{c}$ .

A union of conjunctive queries (UCQ) over a schema **S** is a first-order formula of the form  $q(\bar{x}) := q_1(\bar{x}) \lor \cdots \lor q_n(\bar{x})$ , where  $n \ge 1$ , and  $q_1(\bar{x}), \ldots, q_n(\bar{x})$  are CQs over **S**. We refer to the variables in  $\bar{x}$  as the answer variables of q and the arity of q is defined as the number of its answer variables. An example for a UCQ with two answer variables  $x_1, x_2$  is  $x_1 = x_2 \lor \exists y R(x_1, y) \land R(x_2, y)$ . A tuple  $\bar{c} \in \operatorname{adom}(I)^{|\bar{x}|}$  is an answer to q on instance I if it is an answer to  $q_i$  on i, for some i with  $1 \le i \le n$ . The evaluation of q on an instance I, denoted q(I), is the set of all answers to q on I. A (U)CQ of arity zero is called Boolean. The only possible answer to a Boolean query is the empty tuple. For a Boolean (U)CQ q, we may write  $I \models q$  if  $q(I) = \{()\}$  and  $I \not\models q$  otherwise. Note that all notions defined for UCQs also apply to CQs, which are simply UCQs with a single disjunct. We write UCQ for the class of all UCQs.

Let  $q_1(\bar{x})$  and  $q_2(\bar{x})$  be two UCQs over the same schema **S**. We say that  $q_1$  is *contained* in  $q_2$ , written  $q_1 \subseteq_{\mathbf{S}} q_2$ , if  $q_1(D) \subseteq q_2(D)$  for every **S**-database *D*. Moreover,  $q_1$  and  $q_2$  are equivalent, written  $q_1 \equiv_{\mathbf{S}} q_2$ , if  $q_1 \subseteq_{\mathbf{S}} q_2$  and  $q_2 \subseteq_{\mathbf{S}} q_1$ .

We next define the important notion of a homomorphism core of a CQ  $q(\bar{x})$ . The potential presence of equality atoms in q brings some subtleties. In particular, it is not guaranteed that there is a homomorphism from q to  $D_q$  that is the identity on  $\bar{x}$ . To address this issue, we resort to the database  $D_q^{\sim}$  obtained from  $D_q$  by identifying any constants/variables  $x_1, x_2$  such that  $x_1 = x_2 \in q$ . For V the set of all variables from  $\bar{x}$  that occur as constants in  $D_q^{\sim}$ , it is easy to see that there is a homomorphism from q to  $D_q^{\sim}$ that is the identity on all variables in V. We say that q is a *core* if every homomorphism h from q to  $D_q^{\sim}$  that is the identity on V is surjective. Every CQ  $q(\bar{x})$  is equivalent to a CQ  $p(\bar{x})$  that is a core and can be obtained from q by dropping atoms. In fact, p is unique up to isomorphism and we call it *the core of* q. For a UCQ q, we use core(q) to denote the disjunction whose disjuncts are the cores of the CQs in q.

For a UCQ q, but also for any other syntactic object q, we use ||q|| to denote the number of symbols needed to write q as a word over a suitable alphabet.

Our main interest is in the complexity of counting the number of answers. Every choice of a query language  $\mathbb{Q}$ , such as  $\mathbb{CQ}$  and  $\mathbb{UCQ}$ , and a class of databases  $\mathbb{D}$  gives rise to the following answer counting problem:

 $<sup>^{2}</sup>$ We believe that, in principle, our results can be adapted to the case with constants. This requires a suitable revision of the structural measures defined in Section 3 as, for example, constants should not contribute to the treewidth of a CQ. Also, the results for CQs without ontologies that we build upon would first have to be extended to include constants.

PROBLEM :	$AnswerCount(\mathbb{Q},\mathbb{D})$
INPUT :	A query $q \in \mathbb{Q}$ over some schema <b>S</b> and an <b>S</b> -database $D \in \mathbb{D}$
OUTPUT :	#q(D)

Our main interest is in the parameterized version of the above problem where we generally assume that the parameter is the size of the input query, see below for more details. When  $\mathbb{D}$  is the class of all databases, we simply write AnswerCount( $\mathbb{Q}$ ).

**TGDs, Guardedness, Fullness** A tuple-generating dependency (TGD) T over  $\mathbf{S}$  is a firstorder sentence of the form  $\forall \bar{x} \forall \bar{y} (\phi(\bar{x}, \bar{y}) \to \exists \bar{z} \psi(\bar{x}, \bar{z}))$  such that  $\exists \bar{y} \phi(\bar{x}, \bar{y})$  and  $\exists \bar{z} \psi(\bar{x}, \bar{z})$ are CQs without equality atoms. As a special case, we also allow  $\phi(\bar{x}, \bar{y})$  to be the empty conjunction, i.e. logical truth, denoted by true. For simplicity, we write T as  $\phi(\bar{x}, \bar{y}) \to \exists \bar{z} \psi(\bar{x}, \bar{z})$ . We call  $\phi$  and  $\psi$  the body and head of T, denoted body(T) and head(T), respectively. An instance I over  $\mathbf{S}$  satisfies T, denoted  $I \models T$ , if  $q_{\phi}(I) \subseteq q_{\psi}(I)$ . It satisfies a set of TGDs S, denoted  $I \models S$ , if  $I \models T$  for each  $T \in S$ . We then also say that I is a model of S. We write  $\mathbb{TGD}$  to denote the class of all TGDs.

A TGD T is guarded if body(T) is true or there exists an atom  $\alpha$  in its body that contains all variables that occur in body(T) [CGK13]. Such an atom  $\alpha$  is a guard of T. While there may be multiple guard atoms in the body of a TGD, we generally assume that one of them is chosen as the actual guard and may thus speak of 'the' guard atom. We write  $\mathbb{G}$  for the class of guarded TGDs. A TGD T is *full* if the tuple  $\overline{z}$  of variables is empty, that is, it uses no existential quantification in the head. We use FULL to denote the class of full TGDs and shall often refer to  $\mathbb{G} \cap \mathbb{FULL}$ , the class of TGDs that are both guarded and full. Note that this class is essentially the class of Datalog programs with guarded rule bodies.

**Ontology-Mediated Queries.** An ontology  $\mathcal{O}$  is a finite set of TGDs. An ontology mediated query (OMQ) takes the form  $Q = (\mathcal{O}, \mathbf{S}, q)$  where  $\mathcal{O}$  is an ontology,  $\mathbf{S}$  is a finite schema called the *data schema*, and q is a UCQ. Both  $\mathcal{O}$  and q can use symbols from  $\mathbf{S}$ , but also additional symbols, and in particular  $\mathcal{O}$  can 'introduce' additional symbols to enrich the vocabulary available for querying. We assume w.l.o.g. that all relation symbols in q that are not from  $\mathbf{S}$  occur also in  $\mathcal{O}$ . In fact, any OMQ violating this condition is trivial in that it never returns any answers. When  $\mathcal{O}$  and q only use symbols from  $\mathbf{S}$ , then we say that the data schema of Q is *full*. The arity of Q is defined as the arity of q. We write  $Q(\bar{x})$  to emphasize that the answer variables of q are  $\bar{x}$  and for brevity often refer to the data schema simply as the schema.

A tuple  $\bar{c} \in \mathsf{adom}(D)^{|\bar{x}|}$  is an *answer* to Q on **S**-database D if  $\bar{c} \in q(I)$  for each model I of  $\mathcal{O}$  with  $I \supseteq D$ . The *evaluation of*  $Q(\bar{x})$  on D, denoted Q(D), is the set of all answers to Q on D.

**Example 2.1.** Consider the OMQ  $(\mathcal{O}, \mathbf{S}, q)$  where  $\mathcal{O}$  consist of the following TGDs:

 $\begin{array}{lll} \mathsf{Book}(x) \to \mathsf{Publication}(x) & \mathsf{Article}(x) \to \mathsf{Publication}(x) \\ \mathsf{Publication}(x) \to \exists y \, \mathsf{hasPublisher}(x,y) & \mathsf{Publication}(x) \to \exists y \, \mathsf{hasAuthor}(x,y) \\ \mathsf{hasPublisher}(x,y) \to \mathsf{Publisher}(y) & \mathsf{hasAuthor}(x,y) \to \mathsf{Author}(y) \\ \mathsf{Publication}(x) \land \mathsf{hasAuthor}(x,y) \land \mathsf{hasPublisher}(x,y) \to \mathsf{SelfPublication}(x), \end{array}$ 

**S** is the set of all relation symbols in  $\mathcal{O}$ , and

 $q(x) = \exists y \operatorname{Author}(x) \land \operatorname{hasAuthor}(y, x) \land \operatorname{SelfPublication}(y).$ 

The conjunctive query q asks to return all authors that have self-published and the ontology  $\mathcal{O}$  adds knowledge about the domain of publications. Now consider the **S**-database D that consists of the following facts:

Book(alice)	hasAuthor(alice, carroll)	has Publisher(alice, macmillan)
Book(finn)	${\sf hasAuthor}({\sf finn},{\sf twain})$	hasPublisher(finn,twain)
Book(beowulf)	SelfPublication(beowulf).	

A straightforward semantic analysis shows that  $\mathsf{twain} \in Q(D)$ , despite the fact that the database D does not explicitly state the fact that finn is a self-publication. While beowulf is a self-publication and we know from the ontology that it has an author, this author is not returned as an answer because their identity is unknown. In fact,  $Q(D) = \{\mathsf{twain}\}$ .

An *OMQ language* is a class of OMQs. For a class of TGDs  $\mathbb{C}$  and a class of UCQs  $\mathbb{Q}$ , we write  $(\mathbb{C}, \mathbb{Q})$  to denote the OMQ language that consists of all OMQs  $(\mathcal{O}, \mathbf{S}, q)$  where  $\mathcal{O}$  is a set of TGDs from  $\mathbb{C}$  and  $q \in \mathbb{Q}$ . For example, we may write  $(\mathbb{G} \cap \mathbb{FULL}, \mathbb{UCQ})$ . We say that an OMQ language  $(\mathbb{C}, \mathbb{Q})$  has *full data schema* if every OMQ in it has.

**The Chase.** We next introduce the well-known chase procedure for making explicit the consequences of a set of TGDs [MMS79, JK84, FKMP05, CGK13]. We first define a single chase step. Let I be an instance over a schema  $\mathbf{S}$  and  $T = \phi(\bar{x}, \bar{y}) \to \exists \bar{z} \, \psi(\bar{x}, \bar{z})$  a TGD over  $\mathbf{S}$ . We say that T is applicable to a tuple  $(\bar{c}, \bar{c}')$  of constants in I if  $\phi(\bar{c}, \bar{c}') \subseteq I$ . In this case, the result of applying T in I at  $(\bar{c}, \bar{c}')$  is the instance  $J = I \cup \psi(\bar{c}, \bar{c}'')$ , where  $\bar{c}''$  is the tuple obtained from  $\bar{z}$  by simultaneously replacing each variable z with a fresh distinct constant that does not occur in I. We describe such a single chase step by writing  $I \xrightarrow{T, (\bar{c}, \bar{c}')} J$ . Let I be an instance and S a finite set of TGDs. A chase sequence for I with S is a sequence of chase steps

$$I_0 \xrightarrow{T_0, (\bar{c}_0, \bar{c}'_0)} I_1 \xrightarrow{T_1, (\bar{c}_1, \bar{c}'_1)} I_2.$$

such that (1)  $I_0 = I$ , (2)  $T_i \in S$  for each  $i \ge 0$ , and (3)  $J \models S$  with  $J = \bigcup_{i\ge 0} I_i$ . The instance J is the (potentially infinite) result of this chase sequence, which always exists. The chase sequence is fair if whenever a TGD  $T \in S$  is applicable to a tuple  $(\bar{c}, \bar{c}')$  in some  $I_i$ , then  $I_j \xrightarrow{T, (\bar{c}, \bar{c}')} I_{j+1}$  is part of the sequence for some  $j \ge i$ . Note that our chase is oblivious, that is, a TGD is triggered whenever its body is satisfied, even if also its head is already satisfied. As a consequence, every fair chase sequence for I with S leads to the same result, up to isomorphism. Thus, we can refer to the result of chasing I with S, denoted  $ch_S(I)$ . The following lemma gives the well-known main properties of the chase.

## Lemma 2.2.

- (1) Let S be a finite set of TGDs and I an instance. Then for every model J of S with  $I \subseteq J$ , there is a homomorphism h from  $ch_S(I)$  to J that is the identity on adom(I).
- (2)  $Q(D) = q(\mathsf{ch}_{\mathcal{O}}(D))$  for every  $OMQ \ Q = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{TGD}, \mathbb{UCQ})$  and  $\mathbf{S}$ -database D.

Point 1 can be proved by constructing h step by step, starting from the identity on adom(I) and following chase rules. Point 2 is an easy consequence of Point 1 and the semantics of OMQs.

We shall often chase with sets S of guarded full TGDs, that is, TGDs from  $\mathbb{G} \cap \mathbb{FULL}$ . In contrast to the case of guarded TGDs, the chase is then clearly finite. Moreover, it can be constructed within the following time bounds. **Lemma 2.3.** Given a database D and finite set S of TGDs from  $\mathbb{G} \cap \mathbb{FULL}$ ,  $ch_S(D)$  can be constructed in time  $f(||S||) \cdot O(||D||^3)$  for some computable function f.

The time bound stated in Lemma 2.3 can be achieved in a straightforward way. To find a homomorphism from a TGD  $\phi(\bar{x}, \bar{y}) \to \psi(\bar{x})$  in S with guard  $R(\bar{x}, \bar{y})$  to D, we can scan Dlinearly to find all facts that  $R(\bar{x}, \bar{y})$  can be mapped to and then verify by additional scans that the remaining atoms in  $\phi$  are also satisfied. This takes time  $||D||^2 \cdot n$ , where n is the number of atoms in  $\phi$ . Because all TGDs are guarded, it is easy to prove by induction on the number of chase rule applications that for every added fact  $R(\bar{b})$ , all constants in  $\bar{b}$  must co-occur in some fact  $T(\bar{c})$  in D where T occurs in S. Consequently, the chase can add at most  $||D|| \cdot k^k \cdot \ell$  fresh facts where k is the maximum arity of relation symbols in S and  $\ell$  is the number of relation symbols that occur on the right-hand side of a TGD in  $\mathcal{O}$ . Note that  $k^k$  is the maximum number of ways to choose a k-tuple of constants from a fact  $T(\bar{c})$  in Dwhere T occurs in S.

For sets S of TGDs from  $\mathbb{G} \cap \mathbb{FULL}$ , we may also chase a CQ  $q(\bar{x})$  with S, denoting the result with  $ch_S(q)$ . What we mean is the (finite) result of chasing database  $D_q$  with S, viewing the result as a CQ with answer variables  $\bar{x}$ , and adding back the equality atoms of q(that are dropped in the construction of  $D_q$ ). We then have the following.

**Lemma 2.4.**  $q(ch_S(D)) = ch_S(q)(ch_S(D))$  for all databases D, CQs q, and finite sets of TGDs S from  $\mathbb{G} \cap \mathbb{FULL}$ .

It is clear that  $\mathsf{ch}_S(q_i)(D) \subseteq q_i(D)$  for every database D because any homomorphism from  $\mathsf{ch}_{\mathcal{O}}(q_i)$  to D' is also a homomorphism from  $q_i$  to D'. The converse containment also holds as every homomorphism from  $q_i$  to  $\mathsf{ch}_S(D)$  is also a homomorphism from  $\mathsf{ch}_{\mathcal{O}}(q_i)$ to  $\mathsf{ch}_S(D)$ . This can be shown by induction, considering all CQs  $q_i = p_1, \ldots, p_\ell = \mathsf{ch}_{\mathcal{O}}(q_i)$ that arise when chasing  $q_i$  with  $\mathcal{O}$ .

**Treewidth.** Treewidth is a widely used notion that measures the degree of tree-likeness of a graph. Let G = (V, E) be an undirected graph. A *tree decomposition* of G is a pair  $\delta = (T_{\delta}, \chi)$ , where  $T_{\delta} = (V_{\delta}, E_{\delta})$  is a tree, and  $\chi$  is a labeling function  $V_{\delta} \to 2^{V}$ , i.e.,  $\chi$ assigns a subset of V to each node of  $T_{\delta}$ , such that:

(1)  $\bigcup_{t \in V_{\delta}} \chi(t) = V$ ,

(2) if  $\{u, v\} \in E$ , then  $u, v \in \chi(t)$  for some  $t \in V_{\delta}$ ,

(3) for each  $v \in V$ , the set of nodes  $\{t \in V_{\delta} \mid v \in \chi(t)\}$  induces a connected subtree of  $T_{\delta}$ . The *width* of  $\delta$  is the number  $\max_{t \in V_{\delta}}\{|\chi(t)|\} - 1$ . If the edge set E of G is non-empty, then

The *whath* of  $\sigma$  is the number  $\max_{t \in V_{\delta}} \{|\chi(t)|\} - 1$ . If the edge set E of G is non-empty, then the *treewidth* of G is the minimum width over all its tree decompositions; otherwise, it is defined to be one. Note that trees have treewidth 1. Each instance I is associated with an undirected graph (without self loops)  $G_I = (V, E)$ , called the *Gaifman graph* of I, defined as follows:  $V = \operatorname{adom}(I)$ , and  $\{a, b\} \in E$  iff there is a fact  $R(\bar{c}) \in I$  that mentions both aand b. The *treewidth* of I is the treewidth of  $G_I$ .

**Parameterized Complexity.** A counting problem over a finite alphabet  $\Lambda$  is a function  $P : \Lambda^* \to \mathbb{N}$  and a parameterized counting problem over  $\Lambda$  is a pair  $(P, \kappa)$ , with P a counting problem over  $\Lambda$  and  $\kappa$  the parameterization of P, a function  $\kappa : \Lambda^* \to \mathbb{N}$  that is computable in PTIME. An example of a parameterized counting problem is #pClique in which P maps (a suitable encoding of) each pair (G, k) with G an undirected graph and  $k \geq 0$  a clique size to the number of k-cliques in G, and where  $\kappa(G, k) = k$ . Another example is #pDomSet where P maps each pair (G, k) to the number of dominating sets of size k, and where again  $\kappa(G, k) = k$ .

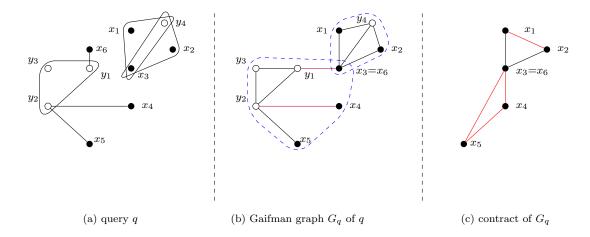


FIGURE 1. An example for Gaifman graphs and their contracts.

A counting problem P is a decision problem if the range of P is  $\{0, 1\}$ , and a parameterized decision problem is defined accordingly. An example of a parameterized decision problem is pClique in which P maps each pair (G, k) to 1 if the undirected graph G contains a k-clique and to 0 otherwise, and where  $\kappa(G, k) = k$ .

A parameterized problem  $(P, \kappa)$  is fixed-parameter tractable (fpt) if there is a computable function  $f : \mathbb{N} \to \mathbb{N}$  such that P(x) can be computed in time  $|x|^{O(1)} \cdot f(\kappa(x))$  for all inputs x. We use FPT to denote the class of all parameterized counting problems that are fixedparameter tractable.

A Turing fpt-reduction from a parameterized counting problem  $(P_1, \kappa_1)$  to a parameterized counting problem  $(P_2, \kappa_2)$  is an algorithm that computes  $P_1$  with oracle access to  $P_2$ , runs within the time bounds of fixed parameter tractability for  $(P_1, \kappa_1)$ , and when started on input x only makes oracle calls with argument y such that  $\kappa_2(y) \leq f(\kappa_1(x))$ , for some computable function f. The reduction is called a *parsimonious fpt-reduction* if only a single oracle call is made at the end of the computation and its output is then returned as the output of the algorithm without any further modification.

A parameterized counting problem  $(P, \kappa)$  is #W[1]-easy if it can be reduced to #pCliqueand it is #W[1]-hard if #pClique reduces to  $(P, \kappa)$ , both in terms of Turing fpt-reductions. W[1]-easiness and -hardness are defined analogously, but using pClique in place of #pClique, and likewise for #W[2] and #pDomSet, and for #A[2] and the parameterized problem of counting the answers to CQs, the parameter being the size of the CQ. For  $C \in \{W[1], \#W[1], \\ \#W[2], \#A[2]\}, (P, \kappa)$  is *C*-equivalent if it is *C*-easy and *C*-hard. Note that we follow [CM15, DRW19] in defining both easiness and hardness in terms of Turing fpt-reductions; stronger notions would rely on parsimonious fpt-reductions [FG04].

# 3. The Classification Without TGDs

In the series of papers [DM14, DM15, CM15, CM16, DRW19], the parameterized complexity of answer counting is studied for classes of CQs and UCQs, resulting in a rather detailed classification. We present it in this section as a reference point and as a basis for establishing our own classifications later on. We start with introducing the various structural measures that play a role in the classification. Let  $q(\bar{x}) = \exists \bar{y} \varphi(\bar{x}, \bar{y})$  be a CQ. The *Gaifman graph* of q, denoted  $G_q$ , is defined as  $G_{D_q^{\sim}}$ . The *treewidth* (*TW*) of  $q(\bar{x})$  is the treewidth of  $G_q$ .

An  $\bar{x}$ -component of  $G_q$  is any undirected graph that can be obtained as follows: (1) take the subgraph of  $G_q$  induced by vertex set  $\bar{y}$ , (2) choose a maximal connected component  $(V_c, E_c)$ , and (3) re-add all edges from  $G_q$  that contain at least one vertex from  $V_c$ . Note that the last step may re-add answer variables as vertices, but no quantified variables. The contract of  $G_q$ , denoted contract $(G_q)$ , is the restriction of  $G_q$  to the answer variables, extended with every edge  $\{x_1, x_2\} \subseteq \bar{x}$  such that  $x_1, x_2$  co-occur in some  $\bar{x}$ -component of  $G_q$ . We shall often be interested in the treewidth of the contract of a CQ q, which we refer to as the contract treewidth (CTW) of q. An example is given in Figure 1. Part (a) shows CQ

$$q(x_1, x_2, x_3, x_4, x_5, x_6) = \exists y_1 \exists y_2 \exists y_3 \exists y_4 T(y_1, y_2, y_3) \land T(x_2, x_3, y_4), T(x_1, y_4, x_3) \land R(x_6, y_1) \land R(x_4, y_2) \land R(y_2, x_5) \land x_3 = x_6$$

where filled nodes indicate answer variables and hollow nodes quantified variables, the triangles represent the ternary relation T, and the edges the binary relation R. Part (b) shows the Gaifman graph  $G_q$  of q, where  $x_3$  and  $x_6$  have been identified. The dashed blue boxes show the  $\bar{x}$ -components and the contract of  $G_q$  is shown in Part (c) with edges that have been added due to the  $\bar{x}$ -components shown in red. Both the treewidth and contract treewidth of q are two.

The starsize (SS) of q is the maximum number of answer variables in any  $\bar{x}$ -component of  $G_q$ . Note that the same notion is called strict starsize in [CM15] and dominating starsize in [DRW19]. It is different from the original notion of starsize from [DM14, DM15]. The starsize of the CQ in Figure 1 is three.

A set of quantified variables S in q is node-well-linked if for every two disjoint sets  $S_1, S_2 \subseteq S$  of the same cardinality, there are  $|S_1|$  vertex disjoint paths in  $G_q$  that connect the vertices in  $S_1$  with the vertices in  $S_2$ . For example, S is node-well-linked if  $G_q|_S$  takes the form of a grid or of a clique. A matching M from the answer variables  $\bar{x}$  to the quantified variables  $\bar{y}$  in the graph  $G_q$  (in the standard sense of graph theory) is linked if the set S of quantified variables that occur in M is node-well-linked. The linked matching number (LMN) of q is the size of the largest linked matching from  $\bar{x}$  to  $\bar{y}$  in  $G_q$ . One should think of the linked matching number as a strengthening of starsize. We do not only demand that many answer variables are interlinked by the same  $\bar{x}$ -component, but additionally require that this component is sufficiently large and highly connected ('linked'). In Part (b) of Figure 1, the purple edges in (b) indicate the maximal matching. The LMN of the CQ in that figure is two.

Figure 2 contains some example CQs with associated measures. For a class of CQs  $\mathbb{C}$ , the contract treewidths of CQs in  $\mathbb{C}$  being bounded by a constant implies that the same is true for starsizes, and bounded starsizes in turn imply bounded linked matching numbers. In fact, the starsize of a CQ q is bounded by the contract treewidth of q plus one and its linked matching number is bounded by its starsize. There are no implications between treewidth and contract treewidth. In Figure 2, Example (a) generalizes to any treewidth while always having contract treewidth 1 and Example (c), which has contract treewidth 3, generalizes to any contract treewidth (and starsize) while always having treewidth 1. We refer to [CM15, DRW19] for additional examples.

It is a fundamental observation that cores of CQs are guaranteed to have minimum measures among all equivalent CQs, as stated by the following lemma [CM15, DRW19].

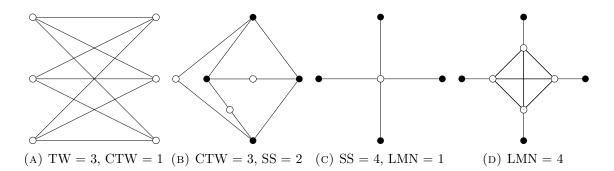


FIGURE 2. Examples for structural measures: Example (a) is the (3,3)-complete bipartite graph, the contract of Example (b) is the 4-clique, Example (c) is a 4-star, and Example (d) is a 4-star with the 4-clique in the centre.

**Lemma 3.1.** If a CQ q is equivalent to a CQ of treewidth k, then core(q) has treewidth at most k. The same is true for contract treewidth, starsize, and linked matching number.

An additional ingredient needed to formulate the classification for UCQs emerges from [CM16]. There, Chen and Mengel associate with every UCQ q a set of CQs  $cl_{CM}(q)$  such that counting the number of answers to q is closely tied to counting the number of answers to the CQs in  $cl_{CM}(q)$ . We now introduce this set, which we refer to as the *Chen-Mengel closure*, in detail.

Two CQs  $q_1(\bar{x}_1)$  and  $q_2(\bar{x}_2)$  over the same schema **S** are *counting equivalent* if  $\#q_1(D) = \#q_2(D)$  for all **S**-databases D. Let  $q(\bar{x}) = p_1 \vee \cdots \vee p_n$ . The starting point for defining  $\mathsf{cl}_{\mathsf{CM}}(q)$  is the observation that, by the inclusion-exclusion principle, every database D satisfies

$$\#q(D) = \sum_{I \subseteq [n]} (-1)^{|I|+1} \cdot \# \big( \bigwedge_{i \in I} p_i(D) \big).$$

We can manipulate this sum as follows: if there are two summands  $c_1 \cdot \#(\bigwedge_{i \in I_1} p_i(D))$  and  $c_2 \cdot \#(\bigwedge_{i \in I_2} p_i(D))$  such that  $\bigwedge_{i \in I_1} p_i$  and  $\bigwedge_{i \in I_2} p_i$  are counting equivalent, then delete both summands and add  $(c_1 + c_2) \cdot \#(\bigwedge_{i \in I_1} p_i(D))$  to the sum. After doing this exhaustively, delete all summands with coefficient zero. The elements of  $\mathsf{cl}_{\mathsf{CM}}(q)$  are all  $\mathsf{CQs} \bigwedge_{i \in I} p_i$  in the original sum that are counting equivalent to some  $\mathsf{CQ} \bigwedge_{i \in J} p_i$  which remains in the sum.<sup>3</sup> Note that the number of  $\mathsf{CQs}$  in  $\mathsf{cl}_{\mathsf{CM}}(q)$  might be exponentially larger than the number of  $\mathsf{CQs}$  in q and that  $\mathsf{cl}_{\mathsf{CM}}(q)$  does not need to contain all  $\mathsf{CQs}$  from the original UCQ q. For a class  $\mathbb{Q}$  of UCQs, we use  $\mathsf{cl}_{\mathsf{CM}}(\mathbb{Q})$  to denote  $\bigcup_{q \in \mathbb{Q}} \mathsf{cl}_{\mathsf{CM}}(q)$ .

**Example 3.2** [CM16]. Consider schema  $\mathbf{S} = \{A, R\}$  with A unary and R binary. Let

$$\begin{aligned} q(x, y, z, t) &= p_1(x, y, z, t) \lor p_2(x, y, z, t) \lor p_3(x, y, z, t) \text{ where} \\ p_1(x, y, z, t) &= R(x, y) \land R(y, z) \land A(x) \land A(y) \land A(z) \land A(t) \\ p_2(x, y, z, t) &= R(z, t) \land R(t, x) \land A(x) \land A(y) \land A(z) \land A(t) \\ p_3(x, y, z, t) &= R(y, z) \land R(z, t) \land A(x) \land A(y) \land A(z) \land A(t) \end{aligned}$$

<sup>&</sup>lt;sup>3</sup>This definition slightly deviates from that of Chen and Mengel, who include no two CQs that are counting equivalent. For all relevant purposes, however, the two definitions are interchangable.

and for  $I \subseteq \{1, 2, 3\}$ , let  $p_I$  be the CQ  $\bigwedge_{i \in I} p_i$ . By inclusion-exclusion, for every **S**-database D we have

$$\begin{aligned} \#q(D) &= & \#p_{\{1\}}(D) + \#p_{\{2\}}(D) + \#p_{\{3\}}(D) \\ &- \#p_{\{1,2\}}(D) - \#p_{\{1,3\}}(D) - \#p_{\{2,3\}}(D) \\ &+ \#p_{\{1,2,3\}}(D) \end{aligned}$$

It is not hard to see that  $p_{\{1\}}$ ,  $p_{\{2\}}$ , and  $p_{\{3\}}$  are pairwise counting equivalent, and so are  $p_{\{1,3\}}$  and  $p_{\{2,3\}}$ . Moreover,  $p_{\{1,2\}}$  and  $p_{\{1,2,3\}}$  are equivalent and thus counting equivalent. Applying the manipulation described above, we thus arrive at the sum

$$#q(D) = 3 \cdot #p_{\{1\}}(D) - 2 \cdot #p_{\{1,3\}}(D).$$

It follows that  $\mathsf{cl}_{\mathsf{CM}}(q) = \{\#p_{\{1\}}, \#p_{\{2\}}, \#p_{\{3\}}, \#p_{\{1,3\}}, \#p_{\{2,3\}}\}$ . Note that the CQs  $p_{\{1,2\}}$  and  $p_{\{1,2,3\}}$  cancelled each other out.

Note that  $\mathsf{cl}_{\mathsf{CM}}(q)$  is defined so that for every **S**-database D, #q(D) can be computed in polynomial time from the counts #q'(D),  $q' \in \mathsf{cl}_{\mathsf{CM}}(q)$ . This, in fact, is the raison d'etre of the Chen-Mengel closure.

We are now ready to state the characterization.

**Theorem 3.3** [CM15, CM16, DRW19]. Let  $\mathbb{Q} \subseteq \mathbb{UCQ}$  be recursively enumerable and have relation symbols of bounded arity, and let  $\mathbb{Q}^* = \{ \mathsf{core}(q) \mid q \in \mathsf{cl}_{\mathsf{CM}}(\mathbb{Q}) \}$ . Then the following holds:

- (1) If the treewidths and the contract treewidths of CQs in  $\mathbb{Q}^*$  are bounded, then AnswerCount( $\mathbb{Q}$ ) is in FPT; it is even in PTIME when  $\mathbb{Q} \subseteq \mathbb{C}\mathbb{Q}$ .
- (2) If the treewidths of CQs in Q<sup>\*</sup> are unbounded and the contract treewidths of CQs in Q<sup>\*</sup> are bounded, then AnswerCount(Q) is W[1]-equivalent.
- (3) If the contract treewidths of CQs in Q<sup>\*</sup> are unbounded and the starsizes of CQs in Q<sup>\*</sup> are bounded, then AnswerCount(Q) is #W[1]-equivalent.
- (4) If the starsizes of CQs in  $\mathbb{Q}^*$  are unbounded, then AnswerCount( $\mathbb{Q}$ ) is #W[2]-hard.
- (5) If the linked matching numbers of CQs in Q<sup>★</sup> are unbounded, then AnswerCount(Q) is #A[2]-equivalent.

We remark that  $cl_{CM}(q) = \{q\}$  when q is a CQ, and thus  $\mathbb{Q}^* = \{core(q) \mid q \in \mathbb{Q}\}$  when  $\mathbb{Q} \subseteq \mathbb{CQ}$  in Theorem 3.3. The assumption that relation symbols have bounded arity is needed only for the lower bounds, but not for the upper bounds.

Note that the classification given by Theorem 3.3 is not complete. It leaves open the possibility that there is a class of (U)CQs  $\mathbb{Q}$  such that  $\mathsf{AnswerCount}(\mathbb{Q})$  is #W[2]-hard, but neither #W[2]-equivalent nor #A[2]-equivalent. It is conjectured in [DRW19] that such a class  $\mathbb{Q}$  indeed exists and in particular that there might be classes  $\mathbb{Q}$  such that  $\mathsf{AnswerCount}(\mathbb{Q})$  is  $\#W_{\mathsf{func}}[2]$ -equivalent. The classification also leaves open whether having unbounded linked matching numbers is a necessary condition for #A[2]-hardness. While a complete classification is certainly desirable we note that, from our perspective, the most relevant aspect is the delineation of the FPT cases from the hard cases, achieved by Points (1)-(3) of the theorem.

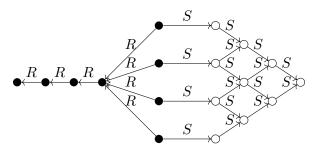


FIGURE 3. CQ  $q_4$  from Example 4.1. Filled circles indicate answer variables.

#### 4. PROBLEMS STUDIED AND MAIN RESULTS

We introduce the problems studied and state the main results of this paper. We start with ontology-mediated querying and then proceed to querying under constraints. Every OMQ language  $\mathbb{Q}$  gives rise to an answer counting problem, defined exactly as in Section 2:

PROBLEM :	$AnswerCount(\mathbb{Q})$
INPUT :	A query $q \in \mathbb{Q}$ over schema <b>S</b> and an <b>S</b> -database D
OUTPUT :	#q(D)

Our first main result is a counterpart of Theorem 3.3 for the OMQ language ( $\mathbb{G}, \mathbb{UCQ}$ ), restricted to OMQs based on the full schema. To illustrate the effect on the complexity of counting of adding an ontology, we first show that the ontology interacts with all of the measures in Theorem 3.3.

**Example 4.1.** Let 
$$\mathcal{O} = \{R(x, y) \to S(x, y)\}$$
 and  $\mathbf{S} = \{R, S\}$ . For all  $n \ge 0$ , let  
 $q_n(x_1, \dots, x_n, z_1, \dots, z_n) = \exists_{1 < i+j < n+2} y_{i,j} \bigwedge_{1 \le i \le n} R(x_i, z_1) \land \bigwedge_{1 \le i < n} R(z_i, z_{i+1}) \land \bigwedge_{i+j=n+1} S(x_i, y_{i,j}) \land \bigwedge_{2 < i+j < n+2} S(y_{i+1,j}, y_{i,j}) \land S(y_{i,j+1}, y_{i,j}).$ 

Then  $q_n$  is a core of treewidth  $\lfloor \frac{n}{2} \rfloor$ , contract treewidth n, starsize n, and linked matching number n. But the OMQ  $(\mathcal{O}, \mathbf{S}, q_n)$  is equivalent to  $(\mathcal{O}, \mathbf{S}, p_n)$  with  $p_n$  obtained from  $q_n$  by dropping all S-atoms. Since  $p_n$  is tree-shaped and has no quantified variables, all measures are at most 1. Figure 3 depicts query  $q_4$ .

Before we state our characterization, we observe as a preliminary that OMQs from  $(\mathbb{G}, \mathbb{UCQ})$  can be rewritten into equivalent ones from  $(\mathbb{G} \cap \mathbb{FULL}, \mathbb{UCQ})$ , that is, existential quantifiers can be removed from rule heads when the actual query is adjusted in a suitable way. This has already been observed in the literature.

**Theorem 4.2** [BDF<sup>+</sup>20]. For every  $OMQ \ Q \in (\mathbb{G}, \mathbb{UCQ})$ , there is an equivalent OMQ from  $(\mathbb{G} \cap \mathbb{FULL}, \mathbb{UCQ})$  that can be effectively computed.

The proof of Theorem 4.2 is constructive, that is, it provides an explicit way of computing, given an OMQ  $Q = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$ , an equivalent OMQ from  $(\mathbb{G} \cap \mathbb{FULL}, \mathbb{UCQ})$ . We denote this OMQ with  $Q^{\exists} = (\mathcal{O}^{\exists}, \mathbf{S}, q^{\exists})$  and call it the  $\exists$ -rewriting of Q. It is worth noting that even if q contains no equality atoms, such atoms might be introduced during the construction of  $q^{\exists}$ . What is more, different CQs in the produced UCQ can comprise different equalities on answer variables, and thus repeated answer variables cannot be used. This is actually the main reason for admitting equality atoms in (U)CQs in this paper. For OMQs  $Q \in (\mathbb{G}, \mathbb{UCQ})$ , we define a set  $\mathsf{cl}_{\mathsf{CM}}(Q)$  of OMQs from  $(\mathbb{G}, \mathbb{CQ})$  in exact analogy with the definition of  $\mathsf{cl}_{\mathsf{CM}}(q)$  for UCQs q, that is, for  $Q = (\mathcal{O}, \mathbf{S}, p_1 \lor \cdots \lor p_n)$ , we use the OMQs  $(\mathcal{O}, \mathbf{S}, p_i)$  in place of the CQs  $p_i$  from the UCQ q in the definition of  $\mathsf{cl}_{\mathsf{CM}}(Q)$ . This requires the use of counting equivalence for OMQs, which is defined in the expected way. For a class  $\mathbb{Q}$  of OMQs, we use  $\mathsf{cl}_{\mathsf{CM}}(\mathbb{Q})$  to denote  $\bigcup_{Q \in \mathbb{Q}} \mathsf{cl}_{\mathsf{CM}}(Q)$ .

For a class  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$ , we now identify a class  $\mathbb{Q}^*$  of CQs by setting

$$\mathbb{Q}^{\star} = \{ \operatorname{core}(\operatorname{ch}_{\mathcal{O}^{\exists}}(p)) \mid \exists Q \in \mathbb{Q} : (\mathcal{O}^{\exists}, \mathbf{S}, p) \in \operatorname{cl}_{\mathsf{CM}}(Q^{\exists}) \}.$$

In other words, the CQs in  $\mathbb{Q}^*$  are obtained by choosing an OMQ from  $\mathbb{Q}$ , replacing it with  $Q^{\exists}$ , then choosing an OMQ ( $\mathcal{O}^{\exists}, \mathbf{S}, p$ ) from  $\mathsf{cl}_{\mathsf{CM}}(Q)$ , chasing p with  $\mathcal{O}^{\exists}$ , and finally taking the core. Our first main result is as follows.

**Theorem 4.3.** Let  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$  be a recursively enumerable class of OMQs with full data schema and relation symbols of bounded arity. Then the following hold:

- If the treewidths and contract treewidths of CQs in Q<sup>\*</sup> are bounded, then AnswerCount(Q) is in FPT.
- (2) If the treewidths of CQs in Q<sup>\*</sup> are unbounded and the contract treewidths of CQs in Q<sup>\*</sup> are bounded, then AnswerCount(Q) is W[1]-equivalent.
- (3) If the contract treewidths of CQs in Q<sup>\*</sup> are unbounded and the starsizes of CQs in Q<sup>\*</sup> are bounded, then AnswerCount(Q) is #W[1]-equivalent.
- (4) If the starsizes of CQs in  $\mathbb{Q}^*$  are unbounded, then AnswerCount( $\mathbb{Q}$ ) is #W[2]-hard.
- (5) If the linked matching numbers of CQs in Q<sup>\*</sup> are unbounded, then AnswerCount(Q) is #A[2]-equivalent.

The upper bounds also hold when the arity of relation symbols is unbounded.

Points (1) to (5) of Theorem 4.3 parallel exactly those of Theorem 3.3, but of course the definition of  $\mathbb{Q}^*$  is a different one. It is through this definition that we capture the potential interaction between the ontology and the structural measures. Note, for example, that the class of OMQs ( $\mathcal{O}, \mathbf{S}, q_n$ ),  $n \geq 1$ , from Example 4.1 would be classified as #A[2]-equivalent if  $\mathsf{core}(\mathsf{ch}_{\mathcal{O}^{\exists}}(p))$  was replaced with p in the definition of  $\mathbb{Q}^*$  while it is in fact in FPT. Also note that the PTIME statement in Point (1) of Theorem 3.3 is absent in Theorem 4.3. In fact, evaluating Boolean OMQs from ( $\mathbb{G}, \mathbb{UCQ}$ ) is 2EXPTIME-complete (EXPTIME-hard when the arity of relation symbols is bounded by a constant) [CGK13] and since for Boolean OMQs evaluation coincides with answer counting, PTIME cannot be attained.

Our second main result concerns querying under integrity constraints that take the form of guarded TGDs. In contrast to OMQs, the constraints are thus not used for deductive reasoning, but instead give rise to a promise regarding the shape of the input database. Following [BDF<sup>+</sup>20], we define a *constraint-query specification* (CQS) to be a triple  $S = (\mathcal{T}, \mathbf{S}, q)$  where  $\mathcal{T}$  is a finite set of TGDs over finite schema  $\mathbf{S}$  and q a UCQ over  $\mathbf{S}$ . We call  $\mathcal{T}$  the set of *integrity constraints*. Overloading notation, we write ( $\mathbb{C}, \mathbb{Q}$ ) for the class of CQSs in which the set of integrity constraints is formulated in the class of TGDs  $\mathbb{C}$ , and the query is coming from the class of QQSs. Every class  $\mathbb{C}$  of CQSs gives rise to the following answer counting problem.

PROBLEM :	$AnswerCount(\mathbb{C})$
INPUT :	A set of TGDs $\mathcal{T}$ , a query $q$ , and an <b>S</b> -database $D$ that satisfies $\mathcal{T}$
	such that $(\mathcal{T}, \mathbf{S}, q) \in \mathbb{C}$ .
OUTPUT :	#q(D)

Our second main result parallels Theorems 3.3 and 4.3. We refrain from explicitly listing all cases again.

**Theorem 4.4.** Let  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$  be a recursively enumerable class of CQSs with relation symbols of bounded arity. Then Statements 1-5 of Theorem 4.3 hold.

Note that the delineation of the considered complexities is identical for ontology-mediated querying and for querying under constraints. In particular, Theorem 4.4 (implicitly) uses exactly the same class of CQs  $\mathbb{Q}^*$  and the same associated measures.

It would be interesting to know whether  $AnswerCount(\mathbb{Q})$  being in FPT coincides with  $AnswerCount(\mathbb{Q})$  being in PTIME for classes of CQSs  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{C}\mathbb{Q})$ . Note that this is the case for evaluation in the presence of constraints that are guarded TGDs [BGP16, BFGP20] and also for answer counting without constraints [CM15]. The proofs of these results, however, break in our setting.

#### 5. Querying Under Integrity Constraints

We derive Theorem 4.4 from Theorem 4.3 by means of reduction, so that in the rest of the paper we may concentrate on the case of ontology-mediated querying. In fact, Theorem 4.4 is a consequence of Theorem 4.3 and the following result.

**Theorem 5.1.** Let  $\mathbb{C} \subseteq (\mathbb{G}, \mathbb{UCQ})$  be a recursively enumerable class of CQSs and let  $\mathbb{C}'$  be  $\mathbb{C}$  viewed as a class of OMQs based on the full schema.<sup>4</sup> Then there is a Turing fpt-reduction from AnswerCount( $\mathbb{C}'$ ) to AnswerCount( $\mathbb{C}$ ) and there is a parsimonious polynomial time reduction from AnswerCount( $\mathbb{C}$ ) to AnswerCount( $\mathbb{C}'$ ).

The reduction from AnswerCount( $\mathbb{C}$ ) to AnswerCount( $\mathbb{C}'$ ) is immediate: given a set of guarded TGDs  $\mathcal{T}$ , a CQ q, and an S-database D that satisfies  $\mathcal{T}$ , we can view ( $\mathcal{T}, \mathbf{S}, q$ ) as an OMQ Q based on the full schema and return #Q(D) as #q(D). It is easy to see that this is correct.

For the converse reduction, we are given a  $Q = (\mathcal{O}, \mathbf{S}, q)$  that is a CQS from  $\mathbb{C}$  viewed as an OMQ and an **S**-database D. It seems a natural idea to simply view Q as a CQS, which it originally was, and replace D with  $ch_{\mathcal{O}}(D)$  so that the promise is satisfied, and to then return  $\#q(ch_{\mathcal{O}}(D))$  as #Q(D). However, there are two obstacles. First,  $ch_{\mathcal{O}}(D)$  need not be finite; and second, chasing adds fresh constants which changes the answer count. We solve the first problem by replacing the infinite chase with a (finite!) database  $D^*$  that extends Dand satisfies  $\mathcal{O}$ . This is based on the following result from [BDF<sup>+</sup>20] which is essentially a consequence of  $\mathbb{G}$  being finitely controllable [BGO10].

**Theorem 5.2** [BDF<sup>+</sup>20]. Given an ontology  $\mathcal{O} \subseteq \mathbb{G}$ , an **S**-database D, and an  $n \ge 1$ , one can effectively construct a finite database  $D^*$  that satisfies the following conditions: (1)  $D^* \models \mathcal{O}$  and  $D \subseteq D^*$ ;

<sup>&</sup>lt;sup>4</sup>Syntactically, a CQS ( $\mathcal{T}$ ,  $\mathbf{S}$ , q) and an OMQ ( $\mathcal{T}$ ,  $\mathbf{S}$ , q) are actually the same thing except that the definition of CQSs is more strict regarding the schema  $\mathbf{S}$ ; as a consequence when viewing a CQS as an OMQ, the latter is based on the full schema.

(2)  $\bar{a} \in q(D^*)$  iff  $\bar{a} \in Q(D)$  for all OMQs  $(\mathcal{O}, \mathbf{S}, q)$  where q has at most n variables and for all tuples  $\bar{a}$  that use only constants in  $\mathsf{adom}(D)$ .

The construction of  $D^*$  takes time  $f(||\mathcal{O}|| + n) \cdot ||D||^{O(1)}$  with f a computable function.

To address the second problem, we correct the count. Note that this cannot be done by introducing fresh unary relation symbols as markers to distinguish the original constants from those introduced by the chase as this would require us to change the query, potentially leaving the class of queries that we are working with. We instead use an approach inspired by [CM15]. The idea is to compute #q(D') on a set of databases D' obtained from  $D^*$ by cloning constants in  $\operatorname{adom}(D) \subseteq \operatorname{adom}(D^*)$ . The results can be arranged in a system of equations whose coefficients form a Vandermonde matrix. Finally, the system can be solved to obtain #q(D). This is formalized by the following lemma where we use  $\operatorname{clones}(D)$ to denote the class of all S-databases that can be obtained from S-database D by cloning constants.

**Lemma 5.3.** There is an algorithm that, given a UCQ  $q(\bar{x})$  over schema **S**, an **S**-database D, and a set  $F \subseteq \operatorname{adom}(D)$ , computes  $\#(q(D) \cap F^{|\bar{x}|})$  in time  $||q||^{O(\operatorname{ar}(S))} \cdot ||D||$  using an oracle for AnswerCount( $\{q\}, \operatorname{clones}(D)$ ).

*Proof.* We first give a brief overview of the algorithm. Assume that the input is a UCQ  $q(\bar{x})$ , a database D, and a set F. The algorithm first constructs databases  $D_1, \ldots, D_{|\bar{x}|+1}$  by starting with D and cloning constants from F. Then, it computes  $\#q(D_j)$  for  $1 \leq j \leq |\bar{x}| + 1$  and, finally, constructs and solves a system of linear equations for which one of the unknowns is the desired value  $\#(q(D) \cap F^{|\bar{x}|})$ . We now make this precise.

For  $1 \leq j < |\bar{x}| + 1$ , database  $D_j$  is constructed from D by cloning each element from F exactly j - 1 times. In particular,  $D_1 = D$ . Observe that

$$|\mathsf{adom}(D_j)| \leq j |\mathsf{adom}(D)|, \quad |D_j| \leq j^{\mathsf{ar}(\mathbf{S})} \cdot |D| \leq ||q||^{\mathsf{ar}(\mathbf{S})} \cdot |D|,$$

and each  $D_i$  can be constructed in time  $||q||^{O(\operatorname{\mathsf{ar}}(S))} \cdot ||D||$ .

Now, for  $0 \leq i \leq |\bar{x}|$  and  $1 \leq j < |\bar{x}| + 1$ , let  $q^i(D_j)$  denote the subset of answers  $\bar{a} \in q(D_j)$  such that exactly *i* positions in  $\bar{a}$  have constants that are in *F* or have been obtained from such constants by cloning. We claim that  $\#q^i(D_j) = j^i \cdot \#q^i(D)$ , that is, having *j* such clones multiplies each answer  $\bar{a} \in q(D)$  having *i* positions of the described kind exactly  $j^i$  times. By the semantics, this is immediate if *q* is a CQ. So assume that  $q(\bar{x}) = p_1(\bar{x}) \vee \cdots \vee p_k(\bar{x})$  where each  $p_i$  is a CQ. By the inclusion exclusion principle,

$$\#q^{i}(D_{j}) = \sum_{S \subseteq \{1,\dots,k\}} (-1)^{|S|-1} \#(\bigwedge_{\ell \in S} p_{\ell})^{i}(D_{j})$$

and likewise for D in place of  $D_j$ . Since  $\#p^i(D_j) = j^i \cdot \#p^i(D)$  for each CQ  $p = \bigwedge_{\ell \in S} p_\ell$  that occurs in the sum, we obtain  $\#q^i(D_j) = j^i \cdot \#q^i(D)$ , as claimed.

Let  $1 \leq j \leq |\bar{x}| + 1$ . Since the sets  $q^i(D_j)$  partition the set  $q(D_j)$ , we have that  $\#q(D_j) = \sum_{i=0}^{|\bar{x}|} \#q^i(D_j)$ . Moreover, since we have shown that  $\#q^i(D_j) = j^i \cdot \#q^i(D)$  we can infer that

$$\#q(D_j) = \sum_{i=0}^{|\bar{x}|} j^i \cdot \#q^i(D).$$

In the above equation, there are  $|\bar{x}| + 1$  unknown values  $\#q^0(D), \ldots, \#q^{|\bar{x}|}(D)$  and one value, i.e.  $\#q(D_i)$ , that can be computed by the oracle.

Taking this equation for  $j = 0, ..., |\bar{x}| + 1$  generates a system of  $|\bar{x}| + 1$  linear equations with  $|\bar{x}| + 1$  variables. The coefficients of the system form a Vandermonde matrix, which implies that the equations are independent and that the system has a unique solution. Thus, we can solve the system in polynomial time, e.g. by Gaussian elimination, to compute the values  $\#q^0(D), \ldots, \#q^{|\bar{x}|}(D)$ .

Clearly  $q^{|\bar{x}|}(D) = q(D) \cap F^{|\bar{x}|}$ , so returning  $\#q^{|\bar{x}|}(D_1)$  yields  $\#(q(D) \cap F^{|\bar{x}|})$ , as desired. It can be verified that, overall, the algorithm runs in the time stated in Lemma 5.3.

Now for the reduction from AnswerCount( $\mathbb{C}'$ ) to AnswerCount( $\mathbb{C}$ ) claimed in Theorem 5.1. Let  $Q(\bar{x}) = (\mathcal{O}, S, q)$  be a CQS from  $\mathbb{C}$  viewed as an OMQ, and let D be an **S**-database. We first construct the database  $D^*$  as per Theorem 5.2 with n being the number of variables in q. We then apply the algorithm asserted by Lemma 5.3 with  $D^*$  in place of D and with  $F := \operatorname{adom}(D)$ . Cloning preserves guarded TGDs and thus we can use the oracle (which can compute #q(D') for any **S**-database D' that satisfies  $\mathcal{O}$ ) for computing AnswerCount( $\{q\}, \operatorname{clones}(D)$ ) as required by Lemma 5.3.

#### 6. Counting Equivalence

For the proofs of both the upper and lower bounds stated in Theorem 4.3, we need a good grasp of counting equivalence. For the lower bounds, the same is true for the related notion of semi-counting equivalence. In this section, we make some fundamental observations regarding these notions.

In the lower bound proofs, we shall often be concerned with classes of databases  $\mathbb{D}_{\mathcal{O}}^{\mathbf{S}} = \{\mathsf{ch}_{\mathcal{O}}(D) \mid D \text{ an } \mathbf{S}\text{-database}\}$  for some ontology  $\mathcal{O}$  from  $\mathbb{G} \cap \mathbb{FULL}$ . Note that since  $\mathcal{O}$  is from  $\mathbb{FULL}$ , each  $\mathsf{ch}_{\mathcal{O}}(D)$  is finite and thus indeed a database. We observe some important properties of the class  $\mathbb{D}_{\mathcal{O}}^{\mathbf{S}}$  that are folklore and easy to see. For a schema  $\mathbf{S}$ , we define the  $\mathbf{S}$ -database  $D_{\mathbf{S}}^{\mathsf{T}}$  by fixing a constant c and setting  $D_{\mathbf{S}}^{\mathsf{T}} = \{R(c,\ldots,c) \mid R \in \mathbf{S}\}$ .

**Lemma 6.1.** For every ontology  $\mathcal{O} \subseteq \mathbb{TGD}$  and schema **S** that contains all symbols in  $\mathcal{O}$ , the class of instances  $\mathbb{D}^{\mathbf{S}}_{\mathcal{O}}$  is closed under direct product and contains  $D^{\mathsf{T}}_{\mathbf{S}}$ . If  $\mathcal{O} \subseteq \mathbb{G}$ , then it is closed under disjoint union and cloning of elements. If  $\mathcal{O} \subseteq \mathbb{G} \cap \mathbb{FULL}$ , then it is closed under induced subdatabases.

For closure under direct products, it suffices to observe that there is a homomorphism from the direct product I of instances  $I_1$  and  $I_2$  to each of the components  $I_1$  and  $I_2$ . Thus, applicability of a TGD in the product implies applicability in both components. Moreover, the result of the applications in the components is then clearly also found in the product, see e.g. [Fag80] for more details. The arguments for the other closure properties are similar, but simpler.

We now make a central observation regarding the relationship between (semi-)counting equivalence over classes of databases  $\mathbb{D}_{\mathcal{O}}^{\mathbf{S}}$  and (semi-)counting equivalence over the class of all databases. But let us first introduce the notion of semi-counting equivalence. Two CQs  $q_1(\bar{x}_1)$  and  $q_2(\bar{x}_2)$  over the same schema **S** are *semi-counting equivalent* if they are counting equivalent over all **S**-databases D such that  $\#q_1(D) > 0$  and  $\#q_2(D) > 0$ . For a CQ q, we use  $\hat{q}$  to denote the CQ obtained from q by dropping all maximal connected subqueries that contain no answer variable.<sup>5</sup>

<sup>&</sup>lt;sup>5</sup>Note that if q is Boolean, then  $\hat{q}$  is the empty CQ. It evaluates to true on every database.

**Lemma 6.2.** Let  $q_1(\bar{x}_1)$  and  $q_2(\bar{x}_2)$  be equality-free CQs over schema **S** and let  $\mathbb{D}$  be a class of **S**-databases that contains  $D_{q_i}$  and  $D_{\hat{q}_i}$  for  $i \in \{1, 2\}$  and is closed under cloning. Then

- (1)  $q_1$  and  $q_2$  are counting equivalent over  $\mathbb{D}$  iff  $q_1$  and  $q_2$  are counting equivalent over the class of all **S**-databases;
- (2) if  $\mathbb{D}$  is closed under disjoint union and contains  $D_{\mathbf{S}}^{\top}$ , then  $q_1$  and  $q_2$  are semi-counting equivalent over  $\mathbb{D}$  iff  $q_1$  and  $q_2$  are semi-counting equivalent over the class of all **S**-databases.

The 'if' directions of Points (1) and (2) of Lemma 6.2 are trivial. The 'only if' directions are a consequence of results on counting equivalence and semi-counting equivalence obtained in [CM16]. We give more details in the appendix.

We next observe that counting equivalence and semi-counting equivalence are decidable over classes of databases  $\mathbb{D}^{\mathbf{S}}_{\mathcal{O}}$ . For the class of all databases, this has been shown in [CM16]. In fact, it is shown there that CQs  $q_1$  and  $q_2$  are counting equivalent iff there is a way to rename their answer variables to make them equivalent in the standard sense, and that they are semi-counting equivalent iff  $\hat{q}_1$  and  $\hat{q}_2$  are counting equivalent. Consequently, both problems are in NP. For a CQ q, let  $\tilde{q}$  denote the CQ obtained from q by removing all equality atoms and identifying any two variables  $x_1, x_2$  with  $x_1 = x_2 \in q$ .

**Proposition 6.3.** Let  $\mathcal{O} \subseteq \mathbb{G} \cap \mathbb{FULL}$  and let **S** be a schema that contains all symbols from  $\mathcal{O}$ . Given  $CQs \ q_1(x_1)$  and  $q_2(x_2)$  over **S**, it is decidable whether  $q_1$  and  $q_2$  are counting equivalent over  $\mathbb{D}^{\mathbf{S}}_{\mathcal{O}}$ . The same holds for semi-counting equivalence.

*Proof.* Let  $q_1(\bar{x}_1)$  and  $q_2(\bar{x}_2)$  be given as the input. Let  $i \in \{1, 2\}$ . It is easy to see that  $q_i(\bar{x}_i)$  is (semi-)counting equivalent to  $\tilde{q}_i(\bar{y}_i)$  over the class of all databases, and consequently also over  $\mathbb{D}_{\mathcal{O}}^{\mathbf{S}}$ . We may thus assume that  $q_1$  and  $q_2$  are equality-free as otherwise we can replace them with  $\tilde{q}_1$  and  $\tilde{q}_2$ . We then construct  $\mathsf{ch}_{\mathcal{O}}(q_1)$  and  $\mathsf{ch}_{\mathcal{O}}(q_2)$ , check whether they are (semi-)counting equivalent over the class of all databases using the decision procedure from [CM16], and return the result.

We have to argue that this is correct. By Lemma 2.4, it suffices to decide whether  $\mathsf{ch}_{\mathcal{O}}(q_1)$  and  $\mathsf{ch}_{\mathcal{O}}(q_2)$  are (semi-)counting equivalent over  $\mathbb{D}_{\mathcal{O}}^{\mathbf{S}}$ , which by Lemma 6.2 is identical to their (semi-)counting equivalence over the class of all databases. Note that the preconditions of Lemma 6.2 are satisfied. In particular,  $q'_i = \mathsf{ch}_{\mathcal{O}}(q_i)$  is equality-free and both  $D_{q'_i}$  and  $D_{\hat{q}'_i}$  are in  $\mathbb{D}_{\mathcal{O}}^{\mathbf{S}}$ .

In the upper bound, it shall be necessary to compute the Chen-Mengel closure of an OMQ  $Q \in (\mathbb{G} \cap \mathbb{FULL}, \mathbb{UCQ})$ . This is possible by simply following the definition of  $\mathsf{cl}_{\mathsf{CM}}(Q)$ , but requires us to decide counting equivalence of OMQs. We show that this is possible.

**Corollary 6.4.** Given  $OMQs Q_1(\bar{x}_1), Q_2(\bar{x}_2) \in (\mathbb{G} \cap \mathbb{FULL}, \mathbb{CQ})$  over the full schema, where  $Q_i = (\mathcal{O}, \mathbf{S}, q_i)$  for  $i \in \{1, 2\}$ , it is decidable whether  $Q_1$  and  $Q_2$  are counting equivalent.

Corollary 6.4 is a direct consequence of Proposition 6.3. In fact, it follows from Point 2 of Lemma 2.2 and the definition of  $\mathbb{D}^{\mathbf{S}}_{\mathcal{O}}$  yields that  $Q_1$  and  $Q_2$  are (semi-)counting equivalent if and only if  $q_1$  and  $q_2$  are (semi-)counting equivalent over  $\mathbb{D}^{\mathbf{S}}_{\mathcal{O}}$ . The latter can be decided using Proposition 6.3.

# 7. Proof of Theorem 4.3

We prove the upper bounds in Theorem 4.3 by Turing fpt-reductions to the corresponding upper bounds in Theorem 3.3, and the lower bounds by Turing fpt-reduction from the corresponding lower bounds in Theorem 3.3. In both cases, the assumption that the arity of relation symbols is bounded is only required for Theorem 3.3, but not for the Turing fpt-reductions that we give. Consequently, any future classifications of  $AnswerCount(\mathbb{C})$  for classes of CQs  $\mathbb{C}$  that does not rely on this assumption also lift to classes of OMQs through our reductions.

7.1. Upper Bounds. We first establish the upper bounds presented in Theorem 4.3. All these bounds are proved in a uniform way, by providing a Turing FPT reduction from AnswerCount( $\mathbb{Q}$ ), for any class  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$  of OMQs, to AnswerCount( $\mathbb{Q}^*$ ). It then remains to use the corresponding upper bounds for classes of CQs from Theorem 3.3. For the reduction, it is not necessary to assume that the arity of relation symbols is bounded by a constant.

Let  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$  be a class of OMQs with the full schema. We need to exhibit an fpt algorithm for AnswerCount( $\mathbb{Q}$ ) that has access to an oracle for AnswerCount( $\mathbb{Q}^*$ ). Let an OMQ  $Q \in \mathbb{Q}$  and an S-database D be given. The algorithm first replaces Q by its  $\exists$ -rewriting  $Q^{\exists} = (\mathcal{O}^{\exists}, \mathbf{S}, q^{\exists})$  as per Theorem 4.2. Equivalence of Q and  $Q^{\exists}$  implies  $\#Q(D) = \#Q^{\exists}(D)$ , and thus it suffices to compute the latter count.

To compute  $\#Q^{\exists}(D)$  within the time requirements of FPT, we first compute the set  $\mathsf{cl}_{\mathsf{CM}}(Q^{\exists})$ , then for every  $Q' \in \mathsf{cl}_{\mathsf{CM}}(Q^{\exists})$  we determine #Q'(D) within the time requirements of FPT, and finally we combine the results to #Q(D) as per the following lemma, which is an immediate consequence of the definition of  $\mathsf{cl}_{\mathsf{CM}}(Q)$ .

**Lemma 7.1.** For each  $Q = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  and  $\mathbf{S}$ -database D, #Q(D) can be computed in polynomial time from the counts #Q'(D),  $Q' \in \mathsf{cl}_{\mathsf{CM}}(Q)$ .

Note that we need to effectively compute  $cl_{CM}(Q^{\exists})$ , which is possible by Corollary 6.4 in the case that the schema is full.

Let  $Q' = (\mathcal{O}^{\exists}, \mathbf{S}, p) \in \mathsf{cl}_{\mathsf{CM}}(Q^{\exists})$ . Since  $\mathcal{O}^{\exists}$  is from  $\mathbb{G} \cap \mathbb{FULL}$ ,  $\mathsf{ch}_{\mathcal{O}^{\exists}}(D)$  can be computed within the time requirements of FPT by Lemma 2.3. To compute #Q'(D), we may thus construct  $\mathsf{ch}_{\mathcal{O}^{\exists}}(D)$  and then compute  $\#p(\mathsf{ch}_{\mathcal{O}^{\exists}}(D))$ . Equivalently, we can compute and use  $\mathsf{core}(\mathsf{ch}_{\mathcal{O}^{\exists}}(p))$  in place of p.

It remains to note that the CQs  $\operatorname{core}(\operatorname{ch}_{\mathcal{O}^{\exists}}(p))$ , for  $(\mathcal{O}^{\exists}, \mathbf{S}, p) \in \operatorname{cl}_{\mathsf{CM}}(Q^{\exists})$ , are exactly the CQs from  $\mathbb{Q}^{\star}$ .

7.2. Lower Bounds: Getting Started. We next turn towards lower bounds in Theorem 4.3, which we all consider in parallel. Let  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$  be a class of OMQs. We provide a Turing fpt-reduction from AnswerCount( $\mathbb{C}$ ) to AnswerCount( $\mathbb{Q}$ ) for a class of CQs  $\mathbb{C}$  such that if  $\mathbb{Q}$  satisfies the preconditions in one of the four lower bounds stated in Theorem 4.3 (in Points (2) to (5), respectively), then  $\mathbb{C}$  satisfies the preconditions from the corresponding point of Theorem 3.3. While the constructed class of CQs  $\mathbb{C}$  is closely related to  $\mathbb{Q}^*$ , it is not identical.

We in fact obtain the desired Turing fpt-reduction by composing three Turing fptreductions. The first reduction consists in transitioning to the ∃-rewritings of the OMQs in the original class. The second reduction enables us to consider OMQs that use CQs rather than UCQs.<sup>6</sup> And in the third reduction, we remove ontologies altogether, that is, we reduce classes of CQs to classes of OMQs. We start with the first reduction, which is essentially an immediate consequence of Theorem 4.2.

**Theorem 7.2.** Let  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$  be recursively enumerable and let  $\mathbb{Q}' \subseteq (\mathbb{G} \cap \mathbb{FULL}, \mathbb{UCQ})$  be the class of  $\exists$ -rewritings of OMQs from  $\mathbb{Q}$ . There is a parsimonious fpt-reduction from AnswerCount( $\mathbb{Q}'$ ) to AnswerCount( $\mathbb{Q}$ ).

*Proof.* Given a  $Q = (\mathcal{O}, \mathbf{S}, q) \in \mathbb{Q}'$  and an **S**-database D, find some  $Q' = (\mathcal{O}', \mathbf{S}, q') \in \mathbb{Q}$  such that Q is an  $\exists$ -rewriting of Q' by recursively enumerating  $\mathbb{Q}$  and exploiting that  $\exists$ -rewritings can be effectively computed as per Theorem 4.2 and OMQ equivalence is decidable in  $(\mathbb{G}, \mathbb{UCQ})$  [BBP18]. Then compute and return #Q'(D).

7.3. Lower Bounds: From UCQs to CQs. The second reduction is given by the following theorem. Recall that for any  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$ , the class  $\mathsf{cl}_{\mathsf{CM}}(\mathbb{Q})$  consists of OMQs from  $(\mathbb{G}, \mathbb{CQ})$ , that is, it only uses CQs but no UCQs.

**Theorem 7.3.** Let  $\mathbb{Q} \subseteq (\mathbb{G} \cap \mathbb{FULL}, \mathbb{UCQ})$  be a recursively enumerable class of OMQs with full schema. Then there is a Turing fpt-reduction from  $AnswerCount(cl_{CM}(\mathbb{Q}))$  to  $AnswerCount(\mathbb{Q})$ .

In [CM16], Chen and Mengel establish Theorem 7.3 in the special case where ontologies are empty. A careful analysis of their proof reveals that it actually establishes something stronger, namely a Turing fpt-reduction from AnswerCount( $cl_{CM}(\mathbb{Q}), \mathbb{D}$ ) to AnswerCount( $\mathbb{Q}, \mathbb{D}$ ) for all classes of UCQs  $\mathbb{Q}$  and all classes of databases  $\mathbb{D}$  that satisfy certain natural properties. This is important for us because it turns out that the class of databases obtained by chasing with an ontology from  $\mathbb{G} \cap \mathbb{FULL}$  satisfies all the relevant properties, and thus Theorem 7.3 is a consequence of Chen and Mengel's constructions. We now make this more precise.

For a class of databases  $\mathbb{D}$  and a CQ q, we use  $\mathsf{cl}_{\mathsf{CM}}^{\mathbb{D}}(q)$  to denote the version of the Chen-Mengel closure that is defined exactly as  $\mathsf{cl}_{\mathsf{CM}}(q)$ , except that all tests of counting equivalence are over the class of databases  $\mathbb{D}$  rather than over the class of all databases.

**Theorem 7.4** [CM16]. Let  $\mathbb{D}$  be a class of databases over some schema **S** such that  $\mathbb{D}$  is closed under disjoint union, direct product, and contains  $D_{\mathbf{S}}^{\top}$ . Then there is an algorithm that

- (1) takes as input a UCQ q, a CQ  $p \in \mathsf{cl}_{\mathsf{CM}}^{\mathbb{D}}(q)$ , and a database  $D \in \mathbb{D}$ , subject to the promise that for all  $p' \in \mathsf{cl}_{\mathsf{CM}}^{\mathbb{D}}(q)$ , there is an equality-free CQ p'' such that  $D_{p''} \in \mathbb{D}$ ,  $D_{\hat{p}''} \in \mathbb{D}$ , and p' and p'' are counting equivalent over  $\mathbb{D}$ ,
- (2) has access to an oracle for AnswerCount({q}, D), to a procedure for enumerating D, and to procedures for deciding counting equivalence and semi-counting equivalence between CQs over D,
- (3) runs in time  $f(||q||) \cdot p(||D||)$  with f a computable function and p a polynomial,
- (4) outputs #p(D).

The difference between access to an oracle and access to procedures in Point (2) of Theorem 7.4 is that the running time of the oracle does not contribute to the running time of the overall algorithm while the running time of the procedures does. When used with

<sup>&</sup>lt;sup>6</sup>It is interesting to note in this context that the construction of  $Q^{\exists}$  may produce a UCQ even if the original OMQ Q uses a CQ.

the class  $\mathbb{D}$  of all databases, Lemma 7.4 is simply the special case of Theorem 7.3 where ontologies are empty. In the appendix, we summarize the proof of Theorem 7.4 given in [CM16], showing that it works not only for the class of all databases as considered in [CM16], but also for all stated classes of databases  $\mathbb{D}$ .

Before we prove that Theorem 7.4 implies Theorem 7.3, we make the following observation on Chen-Mengel closures.

**Lemma 7.5.** Let  $Q = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G} \cap \mathbb{FULL}, \mathbb{UCQ})$  and  $\mathbb{D} = \mathbb{D}^{\mathbf{S}}_{\mathcal{O}}$ . Then  $\mathsf{cl}^{\mathbb{D}}_{\mathsf{CM}}(q) = \{q' \mid (\mathcal{O}, \mathbf{S}, q') \in \mathsf{cl}_{\mathsf{CM}}(Q)\}.$ 

*Proof.* The definitions of  $\mathsf{cl}_{\mathsf{CM}}^{\mathbb{D}}(q)$  and  $\mathsf{cl}_{\mathsf{CM}}(Q)$  exactly parallel each other. In both cases, we build an equation based on the inclusion-exclusion principle, then manipulate it based on certain counting equivalence tests, and then read off  $\mathsf{cl}_{\mathsf{CM}}^{\mathbb{D}}(q)$  resp.  $\mathsf{cl}_{\mathsf{CM}}(Q)$  from the result. The only difference is that the construction of  $\mathsf{cl}_{\mathsf{CM}}(Q)$  uses OMQ  $(\mathcal{O}, \mathbf{S}, p)$  whenever the construction of  $\mathsf{cl}_{\mathsf{CM}}^{\mathbb{D}}(q)$  uses CQ p. In particular, a counting equivalence test between two OMQs  $Q_1 = (\mathcal{O}, \mathbf{S}, q_1)$  and  $Q_2 = (\mathcal{O}, \mathbf{S}, q_2)$  in the former case correspond to a counting equivalence test between  $q_1$  and  $q_2$  over the class of databases  $\mathbb{D} = \mathbb{D}_{\mathcal{O}}^{\mathbf{S}}$  in the latter case. To prove Lemma 7.5, it thus suffices to show that these tests yield the same result. But this follows from the fact that  $Q_i(D) = q_i(\mathsf{ch}_{\mathcal{O}}(D))$  for all **S**-databases D.

We now argue that Theorem 7.4 implies Theorem 7.3. Thus let  $\mathbb{Q} \subseteq (\mathbb{G} \cap \mathbb{FULL}, \mathbb{UCQ})$ be a recursively enumerable class of OMQs with full schema. We need to give an fpt algorithm with an oracle for AnswerCount( $\mathbb{Q}$ ) that, given an OMQ  $Q' = (\mathcal{O}, \mathbf{S}, q') \in \mathsf{cl}_{\mathsf{CM}}(\mathbb{Q})$  and an S-database D, computes #Q'(D). By enumeration, we can find an OMQ  $Q = (\mathcal{O}, \mathbf{S}, q) \in \mathbb{Q}$ such that  $Q' \in \mathsf{cl}_{\mathsf{CM}}(Q)$ . Lemma 7.5 yields  $q' \in \mathsf{cl}_{\mathsf{CM}}^{\mathbb{D}}(q)$  for  $\mathbb{D} = \mathbb{D}_{\mathcal{O}}^{\mathbf{S}}$ . By Lemma 6.1, we may thus invoke the algorithm from Theorem 7.4 with  $\mathbb{D} = \mathbb{D}_{\mathcal{O}}^{\mathbf{S}}$ , the UCQ q, CQ  $q' \in \mathsf{cl}_{\mathsf{CM}}^{\mathbb{D}}(q)$ , and the database  $\mathsf{ch}_{\mathcal{O}}(D)$ . The algorithm returns  $\#q(\mathsf{ch}_{\mathcal{O}}(D)) = \#Q'(D)$ , as desired. Note that  $\mathsf{ch}_{\mathcal{O}}(D)$  is finite because  $\mathcal{O} \subseteq \mathbb{FULL}$  and can be produced within the time requirements of fixed-parameter tractability by Lemma 2.3. Also note that for every  $p' \in \mathsf{cl}_{\mathsf{CM}}^{\mathbb{D}}(q)$ , we may use  $\mathsf{ch}_{\mathcal{O}}(\tilde{p}')$  as the equality-free CQ p'' required by Point (1) of Theorem 7.4. In fact,  $\tilde{p}'$  is counting equivalent to p', even over the class of all databases, and  $\mathsf{ch}_{\mathcal{O}}(\tilde{p}')$  is equivalent to  $\tilde{p}'$ over  $\mathbb{D} = \mathbb{D}_{\mathcal{O}}^{\mathbf{S}}$  by Lemma 2.4.

We still need to argue that the oracle and procedures from Point (2) of Theorem 7.4 are indeed available. As the oracle for  $\mathsf{AnswerCount}(\{q\}, \mathbb{D}^{\mathbf{S}}_{\mathcal{O}})$ , we can use an oracle for  $\mathsf{AnswerCount}(\{Q\})$ : by definition of  $\mathbb{D}^{\mathbf{S}}_{\mathcal{O}}$ , any  $D \in \mathbb{D}^{\mathbf{S}}_{\mathcal{O}}$  satisfies q(D) = Q(D). And as an oracle for  $\mathsf{AnswerCount}(\{Q\})$ , in turn, we can clearly use the strictly more general oracle for  $\mathsf{AnswerCount}(\mathbb{Q})$  that we have at our disposal in the Turing fpt-reduction that we are building. The procedure for enumerating  $\mathbb{D}^{\mathbf{S}}_{\mathcal{O}}$  required by Point (2) is also easy to provide. We can just enumerate all **S**-databases, chase with  $\mathcal{O}$ , and filter out duplicates. Finally, the procedures for deciding counting equivalence and semi-counting equivalence of CQs over  $\mathbb{D}^{\mathbf{S}}_{\mathcal{O}}$ are provided by Proposition 6.3.

7.4. Lower Bounds: Removing Ontologies. We next give the reduction that removes ontologies.

**Theorem 7.6.** Let  $\mathbb{Q} \subseteq (\mathbb{G} \cap \mathbb{FULL}, \mathbb{CQ})$  be a recursively enumerable class of OMQs with full schema. There is a class  $\mathbb{C} \subseteq \mathbb{CQ}$  that only contains cores and such that:

(1) there is a Turing fpt-reduction from  $AnswerCount(\mathbb{C})$  to  $AnswerCount(\mathbb{Q})$ ;

# (2) for every $OMQ \ Q = (\mathcal{O}, \mathbf{S}, q) \in \mathbb{Q}$ , we find a $CQ \ p \in \mathbb{C}$ such that p and $core(ch_{\mathcal{O}}(q))$ have the same Gaifman graph.

Before we prove Theorem 7.6, we first show how we can make use of the three Turing fptreductions stated as Theorems 7.2, 7.3, and 7.6, to obtain the lower bounds in Theorem 4.3 from those in Theorem 3.3. Let us consider, for example, the W[1] lower bound from Point (2) of Theorem 4.3. Take a class  $\mathbb{Q}_0 \subseteq (\mathbb{G}, \mathbb{UCQ})$  of OMQs such that the treewidths of CQs in

$$\mathbb{Q}_0^{\star} = \{ \operatorname{core}(\operatorname{ch}_{\mathcal{O}^{\exists}}(p)) \mid \exists Q \in \mathbb{Q}_0 : (\mathcal{O}^{\exists}, \mathbf{S}, p) \in \operatorname{cl}_{\mathsf{CM}}(Q^{\exists}) \}$$

are unbounded. Theorems 7.2 and 7.3 give a Turing fpt-reduction from  $\mathsf{AnswerCount}(\mathbb{Q})$  to  $\mathsf{AnswerCount}(\mathbb{Q}_0)$  where

$$\mathbb{Q} = \{ Q' \mid \exists Q \in \mathbb{C}_0 : Q' \in \mathsf{cl}_{\mathsf{CM}}(Q^{\exists}) \}.$$

By assumption, the treewidths of the CQs  $\operatorname{core}(\operatorname{ch}_{\mathcal{O}}(q))$ ,  $(\mathcal{O}, \mathbf{S}, q) \in \mathbb{Q}$ , are unbounded. Let  $\mathbb{C}$  be the class of CQs whose existence is asserted by Theorem 7.6. By Point (2) of that theorem, the treewidths of the CQs in  $\mathbb{C}$  are unbounded and thus  $\operatorname{AnswerCount}(\mathbb{C})$  is W[1]-hard by Point (2) of Theorem 3.3. Composing the Turing fpt-reduction from  $\operatorname{AnswerCount}(\mathbb{C})$  to  $\operatorname{AnswerCount}(\mathbb{Q})$  given by Point (1) of Theorem 7.6 with the reduction from  $\operatorname{AnswerCount}(\mathbb{Q})$  to  $\operatorname{AnswerCount}(\mathbb{Q}_0)$ , we obtain a Turing fpt-reduction from  $\operatorname{AnswerCount}(\mathbb{C})$  to  $\operatorname{AnswerCount}(\mathbb{Q}_0)$  and thus the latter is W[1]-hard. The other lower bounds can be proved analogously.

We now turn to the proof of Theorem 7.6 which in turn uses three consecutive fptreductions. The first reduction is easy and ensures that all involved CQs (inside OMQs) are equality-free. The second reduction allows us, informally spoken, to mark every variable in a CQ (inside an OMQ) by a unary relation symbol that uniquely identifies it. In the third reduction, we make use of these markings to remove the ontology. For the first reduction, recall that CQ  $\tilde{q}$  is obtained from CQ q by removing all equality atoms and identifying any two variables  $x_1, x_2$  with  $x_1 = x_2 \in q$ .

**Lemma 7.7.** Let  $\mathbb{Q} \subseteq (\mathbb{G} \cap \mathbb{FULL}, \mathbb{CQ})$  be a recursively enumerable class of OMQs with full schema and let  $\mathbb{Q}^{\sim} = \{(\mathcal{O}, \mathbf{S}, \tilde{q}) \mid (\mathcal{O}, \mathbf{S}, q) \in \mathbb{Q}.$  Then there is a Turing fpt-reduction from AnswerCount( $\mathbb{Q}^{\sim}$ ) to AnswerCount( $\mathbb{Q}$ ).

*Proof.* Given a  $Q = (\mathcal{O}, \mathbf{S}, q) \in \mathbb{Q}^{\sim}$  and an **S**-database D, find a  $Q' = (\mathcal{O}, \mathbf{S}, p) \in \mathbb{Q}$  such that  $q = \tilde{p}$  by recursively enumerating  $\mathbb{Q}$ . Then compute and return #Q'(D). By construction of  $q = \tilde{p}$ , it is clear that q and p are counting equivalent. Consequently,  $\#Q'(D) = \#p(\mathsf{ch}_{\mathcal{O}}(D)) = \#q(\mathsf{ch}_{\mathcal{O}}(D)) = \#Q(D)$ .

We next give the second reduction. The marking of a CQ q over schema **S** is the CQ  $q^m$  obtained from q by adding an atom  $R_x(x)$  for each  $x \in var(q)$  where  $R_x$  is a fresh unary relation symbol. Note that  $q^m$  is over schema **S**<sup>m</sup> obtained from **S** by adding all the fresh unary symbols. The core-chased marking of an OMQ  $Q = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G} \cap \mathbb{FULL}, \mathbb{CQ})$  is the OMQ  $Q^m = (\mathcal{O}, \mathbf{S}^m, \operatorname{core}(\operatorname{ch}_{\mathcal{O}}(q))^m) \in (\mathbb{G} \cap \mathbb{FULL}, \mathbb{CQ})$ . This can be lifted to classes of OMQs  $\mathbb{Q}$  as expected, that is,  $\mathbb{Q}^m = \{Q^m \mid Q \in \mathbb{Q}\}$ .

**Lemma 7.8.** Let  $\mathbb{Q} \subseteq (\mathbb{G} \cap \mathbb{FULL}, \mathbb{CQ})$  be a recursively enumerable class of equality-free OMQs with full schema. Then there is a Turing fpt-reduction from AnswerCount( $\mathbb{Q}^m$ ) to AnswerCount( $\mathbb{Q}$ ).

To prove Lemma 7.8, we again adapt a reduction by Chen and Mengel that addresses the case of CQs without ontologies, but that can be lifted to relevant classes of databases similarly to Theorem 7.4.

**Theorem 7.9** [CM15]. Let  $\mathbb{D}$  be a class of databases over schema  $\mathbf{S}^m$  that is closed under direct products, cloning, and induced subdatabases. Then there is an algorithm that

- takes as input an equality-free  $CQ \ q$  such that  $q^m$  is over schema  $\mathbf{S}^m$  and a database  $D \in \mathbb{D}$ , subject to the promise that q is a core and  $D_{q^m} \in \mathbb{D}$ ,
- has access to an oracle for AnswerCount( $\{q\}, \mathbb{D}$ ),<sup>7</sup>
- runs in time  $f(||q||) \cdot p(||D||)$ , f a computable function and p a polynomial, and
- outputs  $\#q^m(D)$ .

When used with the class  $\mathbb{D}$  of all databases, Lemma 7.9 is simply the special case of Lemma 7.8 where ontologies are empty. In the appendix, we give an overview of the proof of Lemma 7.9 in [CM15], also showing that it extends to classes of databases  $\mathbb{D}$  that satisfy the stated properties.

We now use Lemma 7.9 to prove Lemma 7.8. Let  $\mathbb{Q} \subseteq (\mathbb{G} \cap \mathbb{FULL}, \mathbb{C}\mathbb{Q})$  be a recursively enumerable class of equality-free OMQs with full schema. We give an fpt algorithm that uses AnswerCount( $\mathbb{Q}$ ) as an oracle and, given an OMQ  $Q^m(\bar{x}) = (\mathcal{O}, \mathbf{S}^m, \operatorname{core}(\operatorname{ch}_{\mathcal{O}}(q))^m) \in \mathbb{Q}^m$ and an  $\mathbf{S}^m$ -database D, computes  $\#Q^m(D)$ .

First, the algorithm enumerates  $\mathbb{Q}$  to find an OMQ  $Q(\bar{x})$  such that  $Q^m$  is the core-chased marking of Q, that is,  $Q = (\mathcal{O}, \mathbf{S}, q)$ . It then starts the algorithm from Lemma 7.9 for the class of databases

$$\mathbb{D}_{\mathcal{O}}^{\mathbf{S}^m} = \{ \mathsf{ch}_{\mathcal{O}}(D') \mid D' \text{ an } \mathbf{S}^m \text{-database} \},\$$

and with the CQ  $\operatorname{core}(\operatorname{ch}_{\mathcal{O}}(q))$  and the database  $\operatorname{ch}_{\mathcal{O}}(D)$  as the input. The algorithm outputs  $\#\operatorname{core}(\operatorname{ch}_{\mathcal{O}}(q))^m(\operatorname{ch}_{\mathcal{O}}(D)) = \#Q^m(D)$ , as required.

We should argue that the preconditions of Lemma 7.9 are satisfied. By Lemma 6.1,  $\mathbb{D}_{\mathcal{O}}^{\mathbf{S}^m}$  is closed under direct products and cloning. Since the ontologies in  $\mathbb{Q}$  are from  $\mathbb{FULL}$ ,  $\mathbb{D}_{\mathcal{O}}^{\mathbf{S}^m}$  is also closed under induced subdatabases. Moreover, class  $\mathbb{D}_{\mathcal{O}}^{\mathbf{S}^m}$  contains  $D_{\mathsf{core}(\mathsf{ch}_{\mathcal{O}}(q))^m}$  since  $\mathsf{core}(\mathsf{ch}_{\mathcal{O}}(q))^m = \mathsf{ch}_{\mathcal{O}}(\mathsf{core}(\mathsf{ch}_{\mathcal{O}}(q))^m)$  and the schema is full. As the oracle for  $\mathsf{AnswerCount}(\{\mathsf{core}(\mathsf{ch}_{\mathcal{O}}(q))\}, \mathbb{D}_{\mathcal{O}}^{\mathbf{S}^m})$  needed by the algorithm, we can use the oracle for  $\mathsf{AnswerCount}(\mathbb{Q})$  that we have available, as follows.

Given a database  $D \in \mathbb{D}_{\mathcal{O}}^{\mathbf{S}^m}$ , we first construct database  $D|_{\mathbf{S}}$  by dropping all atoms that use a symbol from  $\mathbf{S}^m \setminus \mathbf{S}$  and then ask the oracle for  $\mathsf{AnswerCount}(\mathbb{Q})$  to return  $\#Q(D|_{\mathbf{S}})$ . We argue that this is the same as the required  $\#\mathsf{core}(\mathsf{ch}_{\mathcal{O}}(q))(D)$ . In fact,

$$\#Q(D|_{\mathbf{S}}) = \#q(\mathsf{ch}_{\mathcal{O}}(D|_{\mathbf{S}})) = \#q(D|_{\mathbf{S}}) = \#q(D) = \#\mathsf{core}(\mathsf{ch}_{\mathcal{O}}(q))(D).$$

The first equality is due to the universality of the chase. For the second equality, recall that  $D \in \mathbb{D}_{\mathcal{O}}^{\mathbf{S}^m}$  and is thus of the form  $D = \mathsf{ch}_{\mathcal{O}}(D')$  with D' an  $\mathbf{S}^m$ -database. Since  $\mathcal{O}$  does not use the symbols from  $\mathbf{S}^m \setminus \mathbf{S}$ , this implies the second equality. The third equality holds because q does not use the symbols from  $\mathbf{S}^m \setminus \mathbf{S}$ . And the final equality holds because  $D = \mathsf{ch}_{\mathcal{O}}(D')$  and thus any homomorphism from q to D is also a homomorphism from  $\mathsf{ch}_{\mathcal{O}}(q)$  to D. Moreover, taking the core produces an equivalent CQ.

Now for the third fpt-reduction that we use in the proof of Theorem 7.4. It facilitates that with the presence of markings it is possible to remove ontologies, in the following sense.

<sup>&</sup>lt;sup>7</sup>Note that since  $\mathbf{S} \subseteq \mathbf{S}^m$ , q may be viewed as a CQ over schema  $\mathbf{S}^m$ .

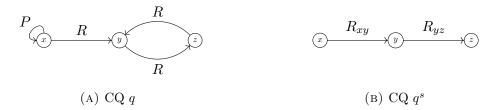


FIGURE 4. A CQ q and its self-join free counterpart  $q^s$ .

**Lemma 7.10.** Let  $\mathbb{Q} \subseteq (\mathbb{G} \cap \mathbb{FULL}, \mathbb{CQ})$  be a recursively enumerable class of equality-free OMQs with full schema and  $\mathbb{Q}^m$  their core-chased markings. There exists a class  $\mathbb{C} \subseteq \mathbb{CQ}$  of cores with the arities of relation symbols identical to those in  $\mathbb{Q}$  such that:

- (1) there is a Turing fpt-reduction from  $AnswerCount(\mathbb{C})$  to  $AnswerCount(\mathbb{Q}^m)$ ;
- (2)  $\mathbb{C}$  is based on the same Gaifman graphs as  $\mathbb{Q}^m$ :  $\{G_q \mid q \in \mathbb{C}\} = \{G_q \mid (\mathcal{O}, \mathbf{S}, q) \in \mathbb{Q}^m\}.$

We provide a proof of Lemma 7.10 below. Before, however, we show how Theorem 7.6 follows from Lemmas 7.8 and 7.10.

Proof of Theorem 7.6. Let  $\mathbb{Q} \subseteq (\mathbb{G} \cap \mathbb{FULL}, \mathbb{CQ})$  be a recursively enumerable class of OMQs with full schema. From Lemma 7.10, we obtain a class  $\mathbb{C}$  of CQs that are cores and are based on the same Gaifman graphs as  $\mathbb{Q}^m$ . This is the class whose existence is postulated by Theorem 7.6. We argue that Points (1) and (2) of that theorem are satisfied. The Turing fpt-reduction required by Point (1) is the composition of the reductions asserted by Lemmas 7.10, 7.8, and 7.7. Point (2) is a consequence of the facts that  $\mathbb{C}$  is based on the same Gaifman graphs as  $\mathbb{Q}^m$  and neither does marking a CQ affect its Gaifman graph nor does the transition from a CQ q to  $\tilde{q}$ . To see the latter, recall that the same variable identifications that take place when constructing  $\tilde{q}$  from q are also part of the definition of the Gaifman graph  $D_q$  of q.

Now for the announced proof of Lemma 7.10, a key ingredient to the proof of Theorem 4.3.

Proof of Lemma 7.10. To prove the lemma, we define the required class of CQs  $\mathbb{C}$  and describe an fpt algorithm that takes as an input a query  $q \in \mathbb{C}$  over schema **S** and an **S**-database D, has access to an oracle for AnswerCount( $\mathbb{Q}^m$ ), and outputs #q(D). Every  $Q = (\mathcal{O}, \mathbf{S}, q) \in \mathbb{Q}$  gives rise to a CQ  $q^s$  in  $\mathbb{C}$  that is formulated in a schema different from **S** (whence the superscript 's'). To define  $q^s$ , fix a total order on  $\operatorname{var}(q)$ . For every guarded set S in  $D_q$ , let  $\overline{S}$  be the tuple that contains the variables in S in the fixed order. Now  $q^s$  contains, for every maximal guarded set S in  $D_q$ , the atom  $R_S(\overline{S})$  where  $R_S$  is a fresh relation symbol of arity |S|. Note that  $q^s$  is self-join free, that is, it contains no two distinct atoms that use the same relation symbol. It is thus a core. Moreover, the Gaifman graph of  $q^s$  is identical to that of  $q^m$  since the maximal guarded sets of  $D_{q^m}$  are exactly those of  $D_{q^s}$ . An example of a transformation from q to  $q^s$  can be found in Figure 4. This defines the class of CQs  $\mathbb{C}$ .

We now describe the algorithm. Let a CQ  $q^s \in \mathbb{C}$  over schema  $\mathbf{S}^s$  and an  $\mathbf{S}^s$ -database  $D^s$  be given as input. To compute  $\#q^s(D^s)$ , we first enumerate  $\mathbb{Q}$  to find an OMQ  $Q = (\mathcal{O}, \mathbf{S}, q)$  such that  $q^s$  can be obtained from q as described above.

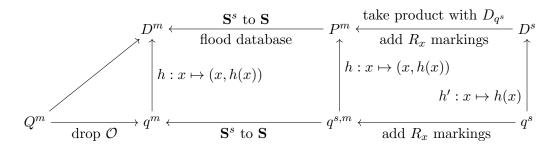


FIGURE 5. Proof strategy of Lemma 7.10.

Construct the  $\mathbf{S}^s$ -database  $P = D_{q^s} \times D^s$  and then from P the  $\mathbf{S}^m$ -database

 $D^{m} = \{R(\bar{a}) \mid \bar{a} \text{ tuple over some guarded set } S \text{ in } P \text{ and } R \in \mathbf{S} \text{ of arity } |\bar{a}|\} \cup \{R_{x}((x,a)) \mid x \in \mathsf{var}(q^{m}) \text{ and } (x,a) \in \mathsf{adom}(P)\}$ 

where a tuple is over set S if it contains only constants from S, in any order and possibly with repetitions. Intuitively, the first line 'floods' the database with facts without creating fresh guarded sets, by adding all possible facts that use a relation symbol from **S** and only constants from some guarded set in P. As a consequence and since  $\mathcal{O}$  is a set of guarded TGDs,  $D^m = ch_{\mathcal{O}}(D^m)$ . The relations  $R_x$  used in the second line are the marking relations from **S**<sup>m</sup>.

Clearly, the databases P and  $D^m$  can be constructed within the time requirements of FPT and we can use the oracle to compute  $\#Q(D^m)$ . Let  $q^{s,m}$  be obtained from  $q^s$  by adding  $R_x(x)$  for every  $x \in \mathsf{var}(q^s)$  and let  $P^m$  be obtained from P by adding  $R_x(x, a)$  for every  $a \in \mathsf{adom}(D^s)$ . To end the proof, it suffices to show that

$$#Q(D^m) = #q^m(D^m) = #q^{s,m}(P^m) = #q^s(D^s).$$

The above equalities, as well as the construction of the involved databases and queries, are illustrated in Figure 5. The figure also shows some homomorphisms used in the remaining proof.

The first equality is immediate since  $D^m = ch_{\mathcal{O}}(D^m)$ . For the third equality, let  $\bar{x} = x_1 \cdots x_n$  be the answer variables in  $q^s$  and for any  $\bar{a} = a_1 \cdots a_n \in adom(D^s)^n$ , let  $\bar{x} \times \bar{a}$  denote the tuple  $(x_1, a_1) \cdots (x_n, a_n) \in adom(P)^n$ . Then  $q^{s,m}(P^m) = \{\bar{x} \times \bar{a} \mid \bar{a} \in q(D^s)\}$ . In fact, if h is a homomorphism from  $q^{s,m}$  to  $P^m$  and  $x \in var(q^{s,m})$ , then  $h(x) \in \{x\} \times adom(P^m)$  due to the use of the marking relation  $R_x$  in  $q^{s,m}$  and in  $P^m$ . Moreover, every such homomorphism h gives rise to a homomorphism h' from  $q^s$  to  $D^s$  by setting h'(x) = c if h(x) = (x, c), for all  $x \in var(q^s)$ . Conversely, every homomorphism h from  $q^s$  to  $D^s$  gives rise to a homomorphism h' from  $q^s$ .

It thus remains to deal with the second equality by showing that  $q^m(D^m) = q^{s,m}(P^m)$ . It is enough to observe that any function  $h: var(q^m) \to adom(D^m)$  is a homomorphism from  $q^m$  to  $D^m$  if and only if it is a homomorphism from  $q^{s,m}$  to  $P^m$ .

For the "if" direction, let h be a homomorphism from  $q^{s,m}$  to  $P^m$ . First let  $R(\bar{y})$  be an atom in  $q^m$  with  $R \in \mathbf{S}$ . There is a maximal guarded set S of  $D_{q^m}$  that contains all variables in  $\bar{y}$ . Then  $R_S(\bar{S})$  is an atom in  $q^s$  and thus  $R_S(h(\bar{S})) \in P$ . By construction of  $D^m$  and since  $\bar{y}$  is a tuple over S, this yields  $R(h(\bar{y})) \in D^m$ , as required. Now let  $R_x(x)$  be an atom in  $q^m$ . Then  $R_x(x)$  is also an atom in  $q^{s,m}$  and thus  $h(x) \in \{x\} \times \operatorname{adom}(D^s)$  due to the definition of  $P^m$ . But then  $R_x(h(x)) \in D^m$  by definition of  $D^m$ .

Vol. 19:3

Vol. 19:3

For the "only if" direction, let h be a homomorphism from  $q^m$  to  $D^m$ . First consider atoms  $R_S(\overline{S})$  in  $q^{s,m}$ . Then  $q^m$  contains an atom  $R(\overline{y})$  where  $\overline{y}$  contains exactly the variables in S and thus  $R(h(\overline{y})) \in D^m$ . By construction of  $D^m$ ,  $h(\overline{y})$  is thus a tuple over some guarded set in P, that is, P contains an atom  $Q(\overline{a})$  where  $\overline{a}$  contains all constants from  $h(\overline{y})$ . In the following, we show that  $Q(\overline{a})$  must in fact be  $R_S(h(\overline{S}))$ , as required.

Let  $\bar{a} = (z_1, c_1), \ldots, (z_n, c_n)$  and  $\bar{z} = z_1, \ldots, z_n$ . By construction of P as  $D_{q^s} \times D^s$ ,  $Q(\bar{a}) \in P$  implies that  $q^s$  contains an atom  $Q(\bar{z})$ . It suffices to show that  $\bar{z}$  contains all variables from S: since the construction of  $q^s$  uses as S only maximal guarded sets, the only such atom in  $q^s$  is  $R_S(\overline{S})$ . By construction of P, we must thus have  $Q(\bar{a}) = R_S(h(\overline{S}))$ .

Let V be the variables in  $\bar{z}$ . Since  $Q(\bar{z}) \in q^s$ , V is a guarded set in  $q^s$ . Now note that we must have  $h(y) \in \{y\} \times \operatorname{adom}(D^s)$  for every variable y in  $\bar{y}$  due to the use of the relation symbol  $R_y$  in  $q^m$  and  $D^m$ . Since  $\bar{a}$  contains all constants from  $h(\bar{y})$ , every variable from  $\bar{y}$ occurs in V. Moreover, these are exactly the variables in S and thus  $S \subseteq V$ .

#### 8. Approximation and FPTRASES

In many applications of answer counting, it suffices to produce a good approximation of the exact count. For CQs without ontologies, significant progress on approximate answer counting has recently been made by Arenas et al. [ACJR21], see also [FGRZ21] for follow-up work. We observe some important consequences for approximately counting the number of answers to ontology-mediated queries.

A randomized approximation scheme for a counting problem  $P : \Lambda^* \to \mathbb{N}$  is a randomized algorithm that takes as input a word  $w \in \Lambda^*$  and an approximation factor  $\epsilon \in (0, 1)$  and outputs a value  $v \in \mathbb{N}$  such that

$$\Pr(|P(w) - v| \le \epsilon \cdot P(w)) \ge \frac{3}{4}.$$

A fixed-parameter tractable randomized approximation scheme (FPTRAS) for a parameterized counting problem  $(P, \kappa)$  over alphabet  $\Lambda$  is a randomized approximation scheme for the counting problem P with running time at most  $f(\kappa(w)) \cdot p(|w|, \frac{1}{\epsilon})$  for some computable function f and polynomial p. The results proved in [ACJR21] imply the following. An OMQ  $Q \in (\mathbb{G}, \mathbb{UCQ})$  has semantic treewidth at most  $k \geq 1$  if there is an OMQ  $Q' \in (\mathbb{G}, \mathbb{UCQ})$ such that  $Q \equiv Q'$  and Q' has treewidth at most k.

**Theorem 8.1.** Let  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$ . If  $\mathbb{Q}$  has bounded semantic treewidth, then there is an *FPTRAS* for AnswerCount( $\mathbb{Q}$ ).

Proof. Let  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$  and let  $k \geq 1$  be an upper bound on the semantic treewidth of OMQs from  $\mathbb{Q}$ . The FPTRAS for  $\mathbb{Q}$  works as follows. Assume that an OMQ  $Q(\bar{x}) = (\mathcal{O}, \mathbf{S}, q) \in \mathbb{Q}$ , an **S**-database D, and an  $\epsilon \in (0, 1)$  are given as input. We enumerate  $(\mathbb{G}, \mathbb{UCQ})$  until we find an OMQ  $Q'(\bar{x}) = (\mathcal{O}', \mathbf{S}, q')$  such that  $Q' \equiv Q$  and Q' is of treewidth at most k. By Theorem 5.2, we can compute in time  $f(||Q'||) \cdot p(||D||)$  a database  $D^* \supseteq D$ such that  $Q'(D) = q'(D^*) \cap \operatorname{adom}(D)^{|\bar{x}|}$ . To get rid of the intersection with  $\operatorname{adom}(D)$ , let  $\widehat{Q}'(\bar{x}) = (\mathcal{O}', \widehat{\mathbf{S}}, \widehat{q}')$  be obtained from  $Q'(\bar{x})$  by setting  $\widehat{\mathbf{S}} = \mathbf{S} \cup \{A\}$  where A is a fresh unary relation and constructing  $\widehat{q}'$  from q' by adding A(x) for every variable x in  $\bar{x}$ . Note that the treewidth of  $\widehat{Q}'$  is still at most k. Let  $\widehat{D}^*$  be obtained from  $D^*$  by adding A(c) for all  $c \in \operatorname{adom}(D)$ , that is, A marks the constants that are already in D, but not those that have been freshly introduced when constructing  $D^*$ . It is clear that  $Q'(D) = \widehat{q}'(\widehat{D}^*)$ . Now, let  $\mathbb{UCQ}_k$  be the class of UCQs that have treewidth at most k. By Propoposition 3.5 of [ACJR21], there is an FPRAS for AnswerCount( $\mathbb{UCQ}_k$ ), where an FPRAS is defined like an FPTRAS except that the running time may be at most  $p(|w|, \frac{1}{\epsilon})$ . We use this FPRAS to compute an approximation of  $\#\hat{q}'(\hat{D}^*)$  and return the result. Overall, this yields the desired FPTRAS for  $\mathbb{Q}$ .

It is interesting to note the contrast between Theorem 8.1 and Point 1 of Theorem 4.3: the latter refers to the treewidth and contract treewidth of the class of CQs  $\mathbb{Q}^*$ , which is defined in a non-trivial way, while Theorem 8.1 simply speaks about the semantic treewidth of the OMQs in  $\mathbb{Q}$  and is thus in line with the characterizations of efficient OMQ *evaluation* given in [BFLP19, BDF<sup>+</sup>20]. In fact, the classes of OMQs covered by Theorem 8.1 are precisely those subclasses of ( $\mathbb{G}$ ,  $\mathbb{UCQ}$ ) for which evaluation is in FPT [BDF<sup>+</sup>20], paralleling the situation for CQs without ontologies. Informally, exact counting and approximate counting differ in how the CQs inside a UCQ interact (and we cannot avoid UCQs when we eliminate existential quantifiers from ontologies). In exact counting, the Chen-Mengel closure captures this interaction, demonstrating that answer counting for a UCQ may enable answer counting for CQs whose structural measures are higher than that of any CQ in the UCQ. In approximate counting, such effects do not seem to play a role. Also note that Theorem 8.1 does not rely on the data schema to be full, unlike the upper bounds in Theorem 4.3.

It may well be the case that a matching lower bound can be proved for Theorem 8.1 under the assumptions that  $W[1] \neq FPT$  and B = BPP, that is, if  $\mathbb{Q} \subseteq (\mathbb{G}, \mathbb{UCQ})$  does not have bounded semantic treewidth, then there is no FPTRAS for AnswerCount( $\mathbb{Q}$ ) unless one of the mentioned assumptions fails. This was proved in [ACJR21] for classes  $\mathbb{Q}$  of CQs (without ontologies) under the additional assumption that for every  $q \in \mathbb{Q}$ , there is a self-join free  $q' \in \mathbb{Q}$  that has the same hypergraph as q. It is currently only known that this assumption can be dropped when all OMQs in  $\mathbb{Q}$  are Boolean and when none of the OMQs in  $\mathbb{Q}$  contains quantified variables. We conjecture that it is possible to lift these restricted cases from pure CQs to OMQs from ( $\mathbb{G}, \mathbb{UCQ}$ ), building on results from [BDF<sup>+</sup>20]. The general case, however, remains open.

#### 9. The Meta Problems—Equivalent Queries with Small Measures

Theorems 4.3 and 4.4 show that low values for the structural measures of treewidth, contract treewidth, starsize, and linked matching number are central to efficient answer counting. This suggests the importance of the meta problem to decide whether a given query is equivalent to one in which some selected structural measures are small, and to construct the latter query if it exists. We present some results on this topic both for ontology-mediated querying and for querying under constraints. These results and their proofs also shed some more light on the interplay between the ontology and the structural measures.

9.1. Querying Under Constraints. We start with querying under constraints, considering all measures in parallel. In fact, we even consider sets of measures since some of the statements in Theorems 4.3 and 4.4 refer to multiple measures and it is not a priori clear whether the fact that each measure from a certain set of measures can be made small in an equivalent query implies that the same is true for all measures from the set simultaneously.

Our approach is as follows. For a given CQS  $(\mathcal{T}, \mathbf{S}, q)$ , we construct a certain CQ q' that approximates q from below under the constraints in  $\mathcal{T}$  and that has small measures. Similar

approximations have been considered for instance in [BLR14], without constraints. We then show that if there is any CQ q'' that has small measures and is equivalent to q under the constraints in  $\mathcal{T}$ , then q' is equivalent to q. In this way, we are able to simultaneously solve the decision and computation version of the meta problem at hand. With 'approximation from below', we mean that the answers to q' are contained in those to q on all **S**-databases. This should not be confused with computing an approximation of the *number* of answers to a given query as considered in Section 8.

A set of measures is a subset  $M \subseteq \{\text{TW}, \text{CTW}, \text{SS}, \text{LMN}\}$  with the obvious meaning. For a set of measures M and  $k \ge 1$ , we say that a UCQ q is an  $M_k$ -query if for every CQ in q, every measure from M is at most k. If  $\mathcal{T}$  is a finite set of TGDs from  $(\mathbb{G}, \mathbb{UCQ})$  over schema  $\mathbf{S}$  and  $q_1(\bar{x}), q_2(\bar{x})$  are UCQs over  $\mathbf{S}$ , then we say that  $q_1$  is contained in  $q_2$  under  $\mathcal{T}$ , written  $q_1 \subseteq_{\mathcal{T}} q_2$ , if  $q_1(D) \subseteq q_2(D)$  for every  $\mathbf{S}$ -database D that is a model of  $\mathcal{T}$ , and likewise for equivalence and  $q_1 \equiv_{\mathcal{T}} q_2$ .

**Definition 9.1.** Let  $(\mathcal{T}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  be a CQS, M a set of measures, and  $k \geq 1$ . An  $M_k$ -approximation of q under  $\mathcal{T}$  is a UCQ q' such that

(1)  $q' \subseteq_{\mathcal{T}} q$ ,

(2) q' is an  $M_k$ -query, and

(3) for each UCQ q'' that satisfies Conditions 1 and 2,  $q'' \subseteq_{\mathcal{T}} q'$ .

It might be useful for the reader to reconsider Example 4.1, which for every  $n \ge 0$  gives an OMQ  $(\mathcal{O}, \mathbf{S}, q_n)$  with full schema such that has high measures, but is equivalent to an OMQ  $(\mathcal{O}, \mathbf{S}, p_n)$  with low measures. The equivalence also holds true if the OMQs are viewed as CQSs, that is,  $q_n \equiv_{\mathcal{O}} p_n$ . If we choose for example  $M = \{TW, CTW\}$  and k = 1, then it can be seen that every  $M_k$ -approximation of  $q_n$  must contain a CQ that is equivalent to  $p_n$ .

We next identify a simple way to construct  $M_k$ -approximations. Let  $(\mathcal{T}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$ be a CQS, M a set of measures, and  $k \geq 1$ . Moreover, let  $\ell$  be the maximum number of variables in any CQ in q and fix a set  $\mathcal{V}$  of exactly  $\ell \cdot \operatorname{ar}(\mathbf{S})$  variables. Assuming that  $\mathcal{T}$ is understood from the context, we define  $q_k^M$  to be the UCQ that contains as a disjunct any CQ p such that  $p \subseteq_{\mathcal{T}} q$ , p is an  $M_k$ -query, and p uses only variables from  $\mathcal{V}$ . As containment between UCQs under constraints from  $\mathbb{G}$  is decidable [BBP18], given  $(\mathcal{T}, \mathbf{S}, q)$ we can effectively compute  $q_k^M$ . We show next that  $q_k^M$  is an  $M_k$ -approximation of q under  $\mathcal{T}$ .

**Lemma 9.2.** Let  $(\mathcal{T}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  be a CQS, M a set of measures, and  $k \geq 1$ . Then  $q_k^M$  is an  $M_k$ -approximation of q under  $\mathcal{T}$ .

*Proof.* By construction,  $q_k^M$  satisfies Points 1 and 2 from Definition 9.1. We show that it satisfies also Point 3. Let  $q''(\bar{x})$  be a UCQ such that  $q'' \subseteq_{\mathcal{T}} q$  and q'' is an  $M_k$ -query. Further, let p be a CQ in q''. We have to show that  $q_k^M$  contains a CQ p' with  $p \subseteq_{\mathcal{T}} p'$ .

We apply Theorem 5.2 to the ontology  $\mathcal{O} = \mathcal{T}$ , the database  $D = D_p$ , and the integer n, defined to be the maximum number of variables of CQs in q. This yields a database  $D_p^*$  which has the properties that  $D_p^* \models \mathcal{T}$ ,  $D_p \subseteq D_p^*$ , and thus  $\bar{x} \in p(D_p^*)$ . From  $q'' \subseteq_{\mathcal{T}} q$ , it follows that  $\bar{x} \in q(D_p^*)$ , and thus there must be CQ  $q_i$  in q such that  $\bar{x} \in q_i(D_p^*)$ . From Point 2 of Theorem 5.2 and  $|\operatorname{var}(q_i)| \leq \ell$ , it follows that  $\bar{x} \in Q(D_p)$  for the OMQ  $Q = (\mathcal{T}, \mathbf{S}, q_i)$ . Consequently,  $q_i$  maps into  $\operatorname{ch}_{\mathcal{T}}(D_p)$  via some homomorphism h that is the identity on  $\bar{x}$ . We intend to use h for identifying the desired CQ p' in  $q_k^M$  such that  $p \subseteq_{\mathcal{T}} p'$ . We need some preliminaries that we keep on an intuitive level here and flesh out in the appendix. Since  $\mathcal{T}$  is a set of guarded TGDs,  $ch_{\mathcal{T}}(D_p)$  is of a certain regular shape. Informally, it looks like  $D_p$  with a tree-like structure attached to every guarded set X in  $D_p$ .<sup>8</sup> Note that the constants in  $D_p$  are exactly the variables in p. We refer to all other constants in  $ch_{\mathcal{T}}(D_p)$  as *nulls*. Formally we first identify with every fact  $R(\bar{c}) \in ch_{\mathcal{T}}(D_p)$  such that  $\bar{c}$ contains at least one null a unique 'source' fact  $src(R(\bar{b})) \in D_p$  that played the role of the guard when the tree-like structure that  $R(\bar{c})$  is in was generated by the chase and then use src to identify the tree-like structures in  $ch_{\mathcal{T}}(D_p)$ .

Start with setting  $\operatorname{src}(R(\bar{c})) = R(\bar{c})$  for all  $R(\bar{c}) \in D_p$ . Next assume that  $R(\bar{c}) \in \operatorname{ch}_{\mathcal{T}}(D_p)$ was introduced by a chase step that applies a TGD  $T \in \mathcal{T}$  at a tuple  $(\bar{d}, \bar{d}')$ , and let R'be the relation symbol in the guard atom in  $\operatorname{body}(T)$ . Then we set  $\operatorname{src}(R(\bar{c})) = R'(\bar{d}, \bar{d}')$  if  $\bar{d} \cup \bar{d}' \subseteq \operatorname{adom}(D_p)$  and  $\operatorname{src}(R(\bar{c})) = \operatorname{src}(R'(\bar{d}, \bar{d}'))$  otherwise. For any guarded set X of  $D_p$ , define  $\operatorname{ch}_{\mathcal{T}}(D_p)|_X^{\downarrow}$  to contain those facts  $R(\bar{c}) \in \operatorname{ch}_{\mathcal{T}}(D_p)$  such that the constants in  $\operatorname{src}(R(\bar{c}))$ are exactly those in X.

In the appendix, we show the following:

- (A) for every guarded set X in  $D_p$ , there is a homomorphism from  $\mathsf{ch}_{\mathcal{T}}(D_p)|_X^{\downarrow}$  to  $\mathsf{ch}_{\mathcal{T}}(\mathsf{ch}_{\mathcal{T}}(D_p)|_X)$  that is the identity on all constants in X;
- (B) if  $c \in \operatorname{adom}(\operatorname{ch}_{\mathcal{T}}(D_p))$  is a null and  $R_1(\bar{c}_1), R_2(\bar{c}_2) \in \operatorname{ch}_{\mathcal{T}}(D_p)$  such that c occurs in both  $c_1$  and  $c_2$ , then  $\operatorname{src}(R_1(\bar{c}_1)) = \operatorname{src}(R_2(\bar{c}_2))$ .

Informally, Condition (A) may be viewed as a locality property of the chase an Condition (B) says that, as expected, attached tree-like structures do not share any variables.

As announced, we now construct the CQ p' in  $q_k^M$ . All atoms in p' are facts from  $ch_{\mathcal{T}}(p)|_{\mathsf{var}(p)}$ , viewed as atoms. To control the number of variables in p', however, we do not include all such atoms, but only a selection of them. Consider each atom  $R(\bar{y})$  in  $q_i$  and distinguish the following cases:

- if  $h(\bar{y})$  contains only variables, then add  $R(h(\bar{y}))$  to p';
- if  $h(\bar{y})$  contains a null, then consider the atom  $S(\bar{z}) = \operatorname{src}(R(h(\bar{y}))) \in D_p$  and let X be the set of variables in  $\bar{z}$ ; add all facts in  $\operatorname{ch}_{\mathcal{T}}(p)|_X$  as atoms to p'.

The answer variables of p' are exactly those of p. All these variables must be present since h is the identity on  $\bar{x}$ . It follows from the construction of p' that the identity is a homomorphism from p' to  $ch_{\mathcal{T}}(p)$ . Thus  $p \subseteq_{\mathcal{T}} p'$  and it remains to show that, up to renaming the variables so that they are from the set  $\mathcal{V}$  fixed for the construction of  $q_k^M$ , p' is a CQ in  $q_k^M$ . This is a consequence of the following properties:

#### (1) p' is an $M_k$ -query.

By definition of p', all guarded sets in p' are also guarded sets in  $ch_{\mathcal{T}}(D_p)$ . Moreover, those guarded sets contain no nulls and are thus also guarded sets in p. Consequently, the Gaifman graph of p' is a subgraph of the Gaifman graph of p, and all measures are monotone regarding subgraphs.

(2)  $p' \subseteq_{\mathcal{T}} q_i$ .

It suffices to construct a homomorphism h' from  $q_i$  to  $ch_{\mathcal{T}}(D_{p'})$ . This can be done as follows. For each  $x \in var(q_i)$  with h(x) a variable, put h'(x) = h(x). It remains to deal with all  $x \in var(q_i)$  with h(x) a null.

With any such x, we associate a unique atom  $\Gamma(x) = \operatorname{src}(R_1(h(\bar{x}_1))) \in D_p$ , identifying the tree-like structure in  $\operatorname{ch}_{\mathcal{T}}(D_p)$  that h(x) is in. Take any atom  $R(\bar{y}) \in q_i$  such that  $\bar{y}$  contains

<sup>&</sup>lt;sup>8</sup>More precisely, a structure of treewidth  $\ell$ , where  $\ell$  is the maximum number of variables in the head of a TGD from  $\mathcal{T}$ .

x. It follows from (B) above that  $\operatorname{src}(R(h(\bar{y})))$  is the same, no matter which such atom  $R(\bar{y}) \in q_i$  we take. We may thus associate with x the unique atom  $\Gamma(x) = \operatorname{src}(R(h(\bar{y}))) \in D_p$ .

Now consider any maximal set X of variables  $x \in \operatorname{var}(q_i)$  such that h(x) is a null and  $x_1, x_2 \in X$  implies  $\Gamma(x_1) = \Gamma(x_2)$ . Then h is a homomorphism from  $q_1|_X$  to  $\operatorname{ch}_{\mathcal{T}}(D_p)|_X^{\downarrow}$ . By (A) above, there is a homomorphism  $h_X$  from  $\operatorname{ch}_{\mathcal{T}}(D_p)|_X^{\downarrow}$  to  $\operatorname{ch}_{\mathcal{T}}(\operatorname{ch}_{\mathcal{T}}(D_p)|_X)$  that is the identity on all constants in X. Moreover, the construction of p' yields  $\operatorname{ch}_{\mathcal{T}}(D_p)|_X \subseteq p'$ . We may thus view  $h_X$  as a homomorphism from  $\operatorname{ch}_{\mathcal{T}}(D_p)|_X^{\downarrow}$  to  $\operatorname{ch}_{\mathcal{T}}(p')$ . Set  $h'(x) = h_X \circ h(x)$  for all  $x \in X$ .

It can be verified that the constructed h' is indeed a homomorphism from  $q_i$  to  $ch_{\mathcal{T}}(D_{p'})$ . (3)  $|adom(p')| \le \ell \cdot ar(\mathbf{S})$ .

A straightforward analysis of the construction of p' shows that it introduces into p' the following variables, implying the statement:

- for every  $x \in q_i$  with h(x) a variable, the variable h(x),
- for every  $x \in q_i$  with h(x) a null, the variables that occur in  $\Gamma(x)$ , where  $\Gamma$  is as above.

In fact, assume that an atom  $R(\bar{y})$  is treated in the construction of p' and let  $\bar{y} = y_1, \ldots, y_k$ . If Case 1 of the construction applies, then the variables  $h(y_1), \ldots, h(y_k)$  are introduced. For Case 2 of the construction, we reuse the function  $\Gamma$  defined in the proof of the previous property. If this case applies, then by definition  $\Gamma(x)$  is identical for every variable x in  $\bar{y}$ with h(x) a null, subsequently just referred to as  $\Gamma$ . This  $\Gamma$  contains h(x) for all variables xin  $\bar{y}$  with h(x) a variable, and  $\Gamma$  is precisely the set of variables introduced in this step.  $\Box$ 

Let  $(\mathcal{T}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  be a CQS. By definition of  $M_k$ -approximations, it is clear that if there exists a UCQ q' such that  $q' \equiv_{\mathcal{T}} q$  and q' is an  $M_k$ -query, then any  $M_k$ -approximation  $q^*$  of q under  $\mathcal{T}$  also satisfies  $q^* \equiv_{\mathcal{T}} q$ . The following is thus an immediate consequence of Lemma 9.2 and the fact that containment between UCQs under constraints from  $\mathbb{G}$  is decidable.

**Theorem 9.3.** Let M be a set of measures. Given a  $CQS(\mathcal{T}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  and  $k \geq 1$ , it is decidable whether q is equivalent under  $\mathcal{T}$  to a UCQ q' that is an  $M_k$ -query. Moreover, if this is the case, then such a q' can be effectively computed.

A particularly relevant case is  $M = \{\text{TW}, \text{CTW}\}\)$ , as it is linked to fixed-parameter tractability. From the above results, we obtain that answer counting in FPT is possible for CQSs that are *semantically* of bounded treewidth and contract treewidth, provided that only CQs are admitted as the actual query. Let us make this more precise. Fix  $k \ge 1$ and let  $\mathbb{C}_k$  be the class of CQSs  $(\mathcal{T}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{CQ})$  such that  $q \equiv_{\mathcal{T}} q'$  for some UCQ q' of treewidth and contract treewidth at most k. Then AnswerCount $(\mathbb{C}_k)$  is in FPT: given a CQS  $(\mathcal{T}, \mathbf{S}, q) \in \mathbb{C}_k$  and an **S**-database D, we may compute, as per Theorem 9.3, a UCQ q' that is an  $M_k$ -query and satisfies  $q \equiv_{\mathcal{T}} q'$ . Since q is a CQ, it is easy to see that there must be a single disjunct  $q^*$  of q such that  $q \equiv_{\mathcal{T}} q^*$ . We can effectively identify  $q^*$  and use Point 1 of Theorem 3.3 as a blackbox to count answers to  $q^*$  on D. The same is probably not true when we define  $\mathbb{C}_k$  as a subclass of  $(\mathbb{G}, \mathbb{UCQ})$  rather than  $(\mathbb{G}, \mathbb{CQ})$ . Then, we have to count the answers to q' on D rather than to a single CQ  $q^*$  in q', but for UCQs of bounded treewidth and contract treewidth, Point 1 of Theorem 3.3 does not always guarantee answer counting in FPT because of the use of the Chen-Mengel closure in that theorem. 9.2. Ontology-Mediated Queries. We now turn to ontology-mediated queries, starting with the definition of their approximations. We say that OMQ  $Q_1(\bar{x}) = (\mathcal{O}_1, \mathbf{S}, q_1)$  is contained in OMQ  $Q_2(\bar{x}) = (\mathcal{O}_2, \mathbf{S}, q_2)$ , written  $Q_1 \subseteq Q_2$ , if  $Q_1(D) \subseteq Q_2(D)$  for every S-database D.  $Q_1$  and  $Q_2$  are equivalent, written  $Q_1 \equiv Q_2$ , if  $Q_1 \subseteq Q_2$  and  $Q_2 \subseteq Q_1$ . We say that an OMQ  $Q = (\mathcal{O}, \mathbf{S}, q)$  is an  $M_k$ -query if q is.

**Definition 9.4.** Let  $Q = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  be an OMQ, M a set of measures, and  $k \geq 1$ . An  $M_k$ -approximation of Q is an OMQ  $Q' = (\mathcal{O}', \mathbf{S}, q') \in (\mathbb{G}, \mathbb{UCQ})$  such that

- (1)  $Q' \subseteq Q$ ,
- (2) Q' is an  $M_k$ -query, and

(3) for each  $Q'' = (\mathcal{O}'', \mathbf{S}, q'') \in (\mathbb{G}, \mathbb{UCQ})$  that satisfies Conditions 1 and 2,  $Q'' \subseteq Q'$ .

We say that Q' is an  $M_k$ -approximation of Q while preserving the ontology if it is an  $M_k$ -approximation and  $\mathcal{O}' = \mathcal{O}$ .

We next observe that  $M_k$ -approximations of OMQs  $(\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  based on the full schema and while preserving the ontology are closely related to the approximations studied in the previous section in the context of CQSs.

**Lemma 9.5.** Let  $Q(\bar{x}) = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  be an OMQ based on the full schema, M a set of measures, and  $k \geq 1$ . Then an OMQ  $Q'(\bar{x}) = (\mathcal{O}, \mathbf{S}, q') \in (\mathbb{G}, \mathbb{UCQ})$  is an  $M_k$ -approximation of Q while preserving the ontology iff q' is an  $M_k$ -approximation of q under  $\mathcal{O}$ .

*Proof.* "if". Assume that q' is an  $M_k$ -approximation of q under  $\mathcal{O}$ . To show that  $Q'(\bar{x}) = (\mathcal{O}, \mathbf{S}, q)$  is an  $M_k$ -approximation of Q, we have to show that Points (1) to (3) from Definition 9.4 hold. Point (2) is obvious.

(1)  $Q' \subseteq Q$ .

Let D be an S-database. Further, let  $D^*$  be the database from Theorem 5.2 invoked with  $\mathcal{O}$ , D, and  $n = \max\{|var(q)|, |var(q')|\}$ . Then

$$Q'(D) = q'(D^{\star}) \cap \operatorname{adom}(D)^{|\overline{x}|} \subseteq q(D^{\star}) \cap \operatorname{adom}(D)^{|\overline{x}|} = Q(D).$$

The containment in the center holds since q' is an  $M_k$ -approximation of q under  $\mathcal{O}$ .

(3)  $P \subseteq Q'$  for all  $P(\bar{x}) = (\mathcal{O}, \mathbf{S}, p) \in (\mathbb{G}, \mathbb{UCQ})$  such that  $P \subseteq Q$  and p is an  $M_k$ -query.

We first observe that  $p \subseteq_{\mathcal{O}} q$ . Thus let D be an **S**-database that satisfies all TGDs from  $\mathcal{O}$ . Then P(D) = p(D) and Q(D) = q(D), thus  $P \subseteq Q$  implies  $p(D) \subseteq q(D)$ .

We now show that  $P \subseteq Q'$ , as required. Let  $D^*$  be the database from Theorem 5.2 invoked with  $\mathcal{O}$ , D, and  $n = \max\{|\mathsf{var}(q')|, |\mathsf{var}(p)|\}$ . Then

$$P(D) = p(D^{\star}) \cap \operatorname{adom}(D)^{|\bar{x}|} \subseteq q'(D^{\star}) \cap \operatorname{adom}(D)^{|\bar{x}|} = Q'(D).$$

The containment in the center holds since  $p \subseteq_{\mathcal{O}} q$  and q' is an  $M_k$ -approximation of q under  $\mathcal{O}$ .

"only if". Assume that  $Q'(\bar{x}) = (\mathcal{O}, \mathbf{S}, q')$  is an  $M_k$ -approximation of Q while preserving the ontology. To show that q' is an  $M_k$ -approximation of q under  $\mathcal{O}$ , we have to show that Points (1) to (3) from Definition 9.1 are satisfied. Again, Point 2 is obvious. (1)  $q' \subseteq_{\mathcal{O}} q$ .

Follows from the fact that  $q'(D) = Q'(D) \subseteq Q(D) = q(D)$  for all **S**-databases D that satisfy  $\mathcal{O}$ . The containment holds since Q' is an  $M_k$ -approximation of Q.

(2)  $p \subseteq_{\mathcal{O}} q'$  for all UCQs p such that  $p \subseteq_{\mathcal{O}} q$  and p is an  $M_k$ -query.

We first observe that  $P \subseteq Q'$  where  $P = (\mathcal{O}, \mathbf{S}, p)$ . In fact, let D be an **S**-database. Now take the database  $D^*$  from Theorem 5.2 invoked with  $\mathcal{O}$ , D, and  $n = \max\{|\mathsf{var}(q')|, |\mathsf{var}(p)|\}$ . Then

$$P(D) = p(D^*) \cap \operatorname{adom}(D)^{|\bar{x}|} \subseteq q'(D^*) \cap \operatorname{adom}(D)^{|\bar{x}|} = Q'(D).$$

Now,  $p \subseteq_{\mathcal{O}} q'$  is a consequence of  $P \subseteq Q'$  and the fact that P(D) = p(D) and Q(D) = q(D) for all **S**-databases D that satisfy  $\mathcal{O}$ .

Lemma 9.5 allows us to compute approximations of OMQs using the construction given in Section 9.1. As in the CQS case, it is easy to see that a given OMQ  $Q = (\mathcal{O}, \mathbf{S}, q)$  is equivalent to an OMQ  $Q' = (\mathcal{O}, \mathbf{S}, q')$  that is an  $M_k$ -query if and only if the  $M_k$ -approximation of Q is an  $M_k$ -query. We thus obtain the following.

**Theorem 9.6.** Let M be a set of measures. Given an  $OMQ \ Q = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$ based on the full schema and  $k \geq 1$ , it is decidable whether Q is equivalent to an OMQ $Q' = (\mathcal{O}, \mathbf{S}, q') \in (\mathbb{G}, \mathbb{UCQ})$  that is an  $M_k$ -query. Moreover, if this is the case, then such a Q' can be effectively computed.

While Theorem 9.6 requires the schema to be full and the ontology to be preserved, we now turn to approximations of OMQs that need neither preserve the ontology nor assume the full schema. We focus on contract treewidth and starsize and leave treewidth and dominating starsize as open problems. To simplify notation, instead of  $\{\text{CTW}\}_k$ -approximations we speak of  $\text{CTW}_k$ -approximations, and likewise for  $\text{SS}_k$ -approximations.

A collapsing of a CQ  $q(\bar{x})$  is a CQ  $p(\bar{x})$  that can be obtained from q by identifying variables and adding equality atoms (on answer variables). When an answer variable x is identified with a non-answer variable y, the resulting variable is x; the identification of two answer variables is not allowed. The  $CTW_k$ -approximation of an OMQ  $Q = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$ , for  $k \geq 1$ , is the OMQ  $Q_k^{\text{CTW}} = (\mathcal{O}, \mathbf{S}, q_k^{\text{CTW}})$  where  $q_k^{\text{CTW}}$  is the UCQ that contains as CQs all collapsings of q that have contract treewidth at most k. The  $SS_k$ -approximation of Q is defined accordingly, and denoted with  $Q_k^{\text{SS}}$ .

**Theorem 9.7.** Let  $(\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  be an OMQ and  $k \geq 1$ . Then  $Q_k^{CTW}$  is a  $CTW_k$ -approximation of Q. Moreover, if  $k \geq \operatorname{ar}(\mathbf{S})$ , then  $Q_k^{SS}$  is an  $SS_k$ -approximation of Q.

The proof of Theorem 9.7 is non-trivial and relies on careful manipulations of databases that are tailored towards the structural measure under consideration. Details are given below. The theorem gives rise to decidability results that, in contrast to Theorem 9.6, neither require the ontology to be preserved nor the schema to be full.

**Corollary 9.8.** Given an  $OMQ \ Q = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  and  $k \ge 1$ , it is decidable whether Q is equivalent to an  $OMQ \ Q' \in (\mathbb{G}, \mathbb{UCQ})$  of contract treewidth at most k. Moreover, if this is the case, then such a Q' can be effectively computed. The same is true for starsize in place of contract treewidth.

Note that, although we are concerned here with approximations that are not required to preserve the ontology, Theorem 9.7 implies that for  $CTW_k$ -approximations and  $SS_k$ approximations, it is never necessary to use an ontology different from the one in the original OMQ. Before proving Theorem 9.7, we observe that treewidth behaves differently in this respect, and thus a counterpart of Theorem 9.7 for treewidth cannot be expected. This is even true when the schema is full.



FIGURE 6. Queries  $q_2$  and  $p_2$  from Example 9.10.

**Example 9.9.** For  $n \ge 3$ , let  $Q_n() = (\emptyset, \mathbf{S}_n, q_n \lor p_n)$  where  $\mathbf{S}_n = \{W, R_1, \ldots, R_n\}$  with W of arity n and each  $R_i$  binary and where

$$q_n = \exists x_1 \cdots \exists x_n W(x_1, \dots, x_n) \text{ and } p_n = \exists x_1 \cdots \exists x_n \exists y R_1(x_1, y), \dots, R_n(x_n, y).$$

Then  $Q'_n() = (\mathcal{O}_n, \mathbf{S}_n, p_n)$  with  $\mathcal{O}_n = \{W(\bar{x}) \to p_n(\bar{x})\}$  is a TW<sub>1</sub>-approximation of  $Q_n$ . In fact, it is equivalent to  $Q_n$ . However,  $Q_n$  has no TW<sub>k</sub>-approximation  $Q^*$  based on the same (empty) ontology for any k < n-1 since  $Q_n \not\subseteq Q^*$  for any  $Q^* = (\emptyset, \mathbf{S}_n, q^*)$  such that  $q^*$  is of treewidth k < n-1. In fact, any  $Q^*$  of treewidth k < n-1 does not return any answers on the database  $\{W(a_1, \ldots, a_n)\}$ .

One might criticize that in Example 9.9, the arity of relation symbols grows unboundedly. The next example shows that this is not necessary. It does, however, use a data schema that is not full.

**Example 9.10.** Let  $\mathbf{S} = \{W, R\}$  with W of arity 3 and R of arity 2. For  $n \ge 0$ , let  $Q_n() = (\emptyset, \mathbf{S}, q_n)$  where

$$q_n = \exists z_1 \exists z_2 \exists z_3 \exists x_1 \cdots \exists x_n \bigwedge_{1 \leq i, j < n; i \neq j} R(x_i, x_j) \land \bigwedge_{1 \leq i, j < n; j \in \{1, 2, 3\}} R(x_i, z_j) \land W(z_1, z_2, z_3).$$

Then,  $G_{q_n}$  is the (n + 3)-clique and thus the treewidth of  $q_n$  is n + 2. Since  $q_n$  is a core, there is no OMQ based on the empty ontology that is equivalent to  $Q_n()$  and in which the actual query has treewidth less than n + 2.

For  $n \ge 0$ , let  $P_n() = (\mathcal{O}, \mathbf{S}, p_n)$  where

$$p_n = \exists y \exists z_1 \exists z_2 \exists z_3 \exists x_1 \cdots \exists x_n \bigwedge_{1 \le i, j < n; i \ne j} R(x_i, x_j) \land \bigwedge_{1 \le i, j < n; j \in \{1, 2, 3\}} R(x_i, z_j) \land \bigwedge_{1 \le i \le 3} S(z_i, y)$$

and

$$\mathcal{O} = W(z_1, z_2, z_3) \to \exists y \bigwedge_{1 \le i \le 3} S(z_i, y).$$

Then  $p_n$  has treewidth n+1 and  $P_n$  is equivalent to  $Q_n$ . Consequently,  $P_n$  is a TW<sub>n+1</sub>-approximation of  $Q_n$ . For the case n = 2, the involved CQs are displayed in Figure 6.

We now turn to the proof of Theorem 9.7. Here, we present only the statement about starsize made in Theorem 9.7, restated as Lemma 9.11 below. The statement about contract treewidth is proved in the appendix. The proof follows a similar strategy as for starsize, but is a bit more involved.

A pointed **S**-database is a pair  $(D, \bar{c})$  with D an **S**-database and  $\bar{c}$  a tuple of constants from  $\mathsf{adom}(D)$ . The contract treewidth and starsize of  $(D, \bar{c})$  are that of D viewed as a conjunctive query with constants from  $\bar{c}$  playing the role of answer variables. **Lemma 9.11.** Let  $(\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  be an OMQ and  $k \geq \operatorname{ar}(\mathbf{S})$ . Then  $Q_k^{SS}$  is an  $SS_k$ -approximation of Q.

*Proof.* Let  $Q(\bar{x}) = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$ . By construction of  $Q_k^{SS} = (\mathcal{O}, \mathbf{S}, q_k^{SS})$ , it is clear that Points 1 and 2 of the definition of  $SS_k$ -approximations are satisfied. It remains to establish Point 3.

Let  $P(\bar{x}) = (\mathcal{O}', \mathbf{S}, p) \in (\mathbb{G}, \mathbb{UCQ})$  such that  $P \subseteq Q$  with p of starsize at most k. We have to show that  $P \subseteq Q_k^{SS}$ , i.e.,  $\bar{c} \in P(D)$  implies  $\bar{c} \in Q_k^{SS}(D)$  for all **S**-databases D. Thus let D be an **S**-database and let  $\bar{c} \in P(D)$ . Since  $P \subseteq Q$ , we have  $\bar{c} \in Q(D)$ . We construct a pointed **S**-database  $(D', \bar{c})$  such that

- (1)  $\bar{c} \in P(D')$ ,
- (2) the starsize of  $(D', \bar{c})$  at most k, and

(3) there is a homomorphism from D' to D that is the identity on  $\bar{c}$ .

In the following, we consider sets S of constants that occur in  $\bar{c}$ , with  $|S| \leq k$ . Let S denote the set of all such sets S. For every  $S \in S$ , let  $D_S$  denote the database obtained from D by renaming every constant  $c \notin S$  to  $c^S$ . We then define

$$D' = \bigcup_{S \in \mathcal{S}} D_S.$$

By definition,  $(D', \bar{c})$  has no  $\bar{c}$ -component with more than k constants from  $\bar{c}$ , and thus Point 2 is satisfied. Point 3 is clear by construction of  $(D', \bar{c})$ . We need to show that Point 1 also holds.

Since  $\bar{c} \in P(D)$ , there is a homomorphism h from some CQ  $p'(\bar{x})$  in p to  $ch_{\mathcal{O}'}(D)$ . We construct a homomorphism h' from p' to  $ch_{\mathcal{O}'}(D)$ , which shows  $\bar{c} \in P(D')$  as desired.

For every  $S \in S$ , there is a homomorphism (even isomorphism)  $h_S$  from D to  $D_S$  that is the identity on S. This homomorphism can be extended to a homomorphism from  $ch_{\mathcal{O}'}(D)$  to  $ch_{\mathcal{O}'}(D_S)$  by following the chase steps used to construct  $ch_{\mathcal{O}'}(D)$ . Moreover,  $ch_{\mathcal{O}'}(D_S) \subseteq ch_{\mathcal{O}'}(D')$ , and thus we can view  $h_S$  as a homomorphism from  $ch_{\mathcal{O}}(D)$  to  $ch_{\mathcal{O}}(D)$  to  $ch_{\mathcal{O}}(D')$  that is the identity on S.

Now for the construction of h'. For all answer variables x in p', we set h'(x) = h(x). Note that this yields  $h'(\bar{x}) = \bar{c}$ . For every quantified variable y, let S be the set of answer variables that are part of the unique  $\bar{x}$ -component that contains y. Then set  $h'(y) = h_S \circ h(y)$ . This is well-defined since p has starsize at most k, and thus  $|S| \leq k$  implying  $S \in S$ .

We argue that h' is indeed a homomorphism. For every atom  $R(\bar{z}) \in p'$ , we have  $R(h(\bar{z})) \in ch_{\mathcal{O}'}(D)$ . First assume that the variables in  $\bar{z}$  are all answer variables. Let S be the set of all constants in  $h(\bar{z})$ . We have  $|S| \leq k$  since  $k \geq ar(S)$ . Since  $h'(\bar{z}) = h(\bar{z})$  and  $h_S$  is the identity on S,  $R(h(\bar{z})) \in ch_{\mathcal{O}'}(D)$  implies  $R(h'(\bar{z})) \in ch_{\mathcal{O}'}(D')$ , as required. Now assume that  $\bar{z}$  contains at least one quantified variable. Then all variables in  $\bar{z}$  belong to the same  $\bar{x}$ -component of p'. Let S be the set of constants h(x) such that x is an answer variable in this  $\bar{x}$ -component. Then  $h'(\bar{z}) = h_S \circ h(\bar{z})$  and we are done. We have thus established Point 1 above.

From  $P \subseteq Q$  and  $\bar{c} \in P(D')$ , we obtain  $\bar{c} \in Q(D')$ . Thus, for some CQ q' in q, there is a homomorphism g from q' to  $ch_{\mathcal{O}}(D')$  such that  $g(\bar{x}) = \bar{c}$ . Let  $\hat{q}$  denote the collapsing of q' that is obtained by identifying  $y_1$  and  $y_2$  whenever  $g(y_1) = g(y_2)$  with at least one of  $y_1, y_2$  a quantified variable and adding  $x_1 = x_2$  whenever  $g(x_1) = g(x_2)$  and  $x_1, x_2$  are both answer variables. Then g is also a homomorphism from  $\hat{q}$  to  $ch_{\mathcal{O}}(D')$ . By Point 3, there is a homomorphism  $h_D$  from D' to D, which can be extended to a homomorphism from  $\mathsf{ch}_{\mathcal{O}}(D')$  to  $\mathsf{ch}_{\mathcal{O}}(D)$ . The composition  $h_D \circ g$  is a homomorphism from  $\widehat{q}$  to  $\mathsf{ch}_{\mathcal{O}}(D)$ , and thus  $\overline{c} \in Q_k^{SS}(D)$ . To finish the proof, it thus remains to show that  $\widehat{q}$  is a CQ in  $q_k^{SS}$ .

Assume to the contrary of what is to be shown that the starsize of  $\hat{q}(\bar{x})$  is at least  $\ell = \max\{k, \operatorname{ar}(\mathbf{S})\} + 1$ . Then, there is an  $\bar{x}$ -component S of  $\hat{q}$  with at least  $\ell$  distinct answer variables, say  $x_1, x_2, \ldots, x_{\ell}$  such that  $\hat{q}$  does not contain atoms  $x_i = x_j$  for  $1 \leq i < j \leq \ell$ . Let y be a quantified variable in S. By definition of  $\bar{x}$ -components,  $G_{\hat{q}}$  contains (simple) paths  $P_i$  between y and  $x_i$ , for  $1 \leq i \leq \ell$ . Together with the homomorphism g, each path  $P_i$  gives rise to a path  $P'_i$  in  $G_{\operatorname{ch}_{\mathcal{O}}(D')}$  between a = h(y) and  $c_i = h(x_i)$ , for  $1 \leq i \leq \ell$ . By definition of  $\hat{q}$ ,  $g(z_1) = g(z_2)$  implies that  $z_1 = z_2$  or  $z_1, z_2$  are both answer variables and  $\hat{q}$  contains an equality atom  $z_1 = z_2$ . It follows:

- (a) the constants  $c_1, \ldots, c_\ell$  and a are all different;
- (b) a is different from all constants in  $\bar{c}$ ;
- (c) path  $P'_i$  contains no constants from  $\bar{c}$  as inner nodes.

First assume that  $a \in \operatorname{adom}(D')$ . An easy analysis of the chase shows that, due to the existence of the path  $P'_i$  and since all TGDs in  $\mathcal{O}$  are guarded, for every  $1 \leq i \leq \ell$  there is a path  $P''_i$  in  $G_{D'}$  between  $c_i$  and a such that  $P''_i$  uses no constants introduced by the chase. In fact, we can obtain  $P''_i$  from  $P'_i$  by dropping all constants that have been introduced by the chase. It then follows from (a) to (c) that the starsize of  $(D', \bar{c})$  is at least  $\ell$ , a contradiction.

Now assume that  $a \notin \operatorname{adom}(D')$ . Let  $b_i$  be the last constant on the path  $P'_i$  that is in  $\operatorname{adom}(D')$  when traveling the path from  $c_i$  to a. Thus, the subpath of  $P'_i$  that connects (the last occurrence of)  $b_i$  with a uses only constants introduced by the chase as inner nodes. Another easy analysis of the chase reveals that since all paths  $P'_1, \ldots, P'_\ell$  end at the same constant a, there must be a fact in D' that contains all of  $b_1, \ldots, b_\ell$ . Note that  $\{c_1, \ldots, c_\ell\} \subseteq \{b_1, \ldots, b_\ell\}$  is impossible since  $\operatorname{ar}(\mathbf{S}) < \ell$ . It thus follows from (c) that some  $b_i$  is not in  $\bar{c}$ . Consequently, there is a path  $P''_i$  in  $G_{D'}$  that connects  $c_i$  and  $b_i$  and uses no constants from  $\bar{c}$  as inner nodes, for  $1 \leq i \leq \ell$ . We may again obtain  $P''_i$  by dropping constants introduced by the chase. This implies that the starsize of  $(D', \bar{c})$  is at least  $\ell$ , a contradiction.

#### 10. Conclusions

We have provided a complexity classification for counting the number of answers to UCQs in the presence of TGDs that applies both to ontology-mediated querying and to querying under constraints. The classification also applies to ontology-mediated querying with the OMQ language ( $\mathcal{ELIH}$ , UCQ) where  $\mathcal{ELIH}$  is a well-known description logic [BHLS17]. In fact, this is immediate if the ontologies in OMQs are in a certain well-known normal form that avoids nesting of concepts [BHLS17]. In the general case, it suffices to observe that all our proofs extended from guarded TGDs to frontier-guarded TGDs [BLMS11] with bodies of bounded treewidth, a strict generalization of  $\mathcal{ELIH}$ . In contrast, a complexity classification for OMQs based on frontier-guarded TGDs with unrestricted bodies is an interesting problem for future work.

There are several other interesting questions that remain open. In querying under constraints that are guarded TGDs, does answer counting in FPT coincide with answer counting in PTIME? Do our results extend to ontology-mediated querying when the data schema is not required to be full? What happens when we drop the restriction that relation symbols are of bounded arity? What about OMQs and CQSs based on other decidable classes of TGDs? And how can we decide the meta problems for the important structural measure of treewidth when the ontology needs not be preserved, with full data schema or even with unrestricted data schema?

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# APPENDIX A. PRELIMINARY NOTES

The main purpose of Sections B, C, and D of the appendix is to provide proof sketches for the results that we take over from Chen and Mengel, that is, Lemma 6.2, Theorem 7.4, and Lemma 7.9, respectively. These results are implicit in [CM15, CM16]. They are stated there explicitly only for the class of all databases, while we need them for classes of databases that satisfy certain properties, made precise in the mentioned lemmas and theorem. In Sections B, C, and D, we summarize the proofs given in [CM15, CM16] so that the reader can convince themselves that all results indeed hold in the form stated in the current paper. We use our own terminology and language in the proof sketches, so the presentation is somewhat different from the one given in Lemma 7.9 where, for example, relational structures are used in place of conjunctive queries.

### APPENDIX B. ADDITIONAL DETAILS FOR SECTION 6

In this section we describe constructions from [CM16] that relate to the notions of counting equivalence and semi-counting equivalence. In particular, we provide the proof of Lemma 6.2.

**Lemma 6.2.** Let  $q_1(\bar{x}_1)$  and  $q_2(\bar{x}_2)$  be equality-free CQs over schema **S** and let  $\mathbb{D}$  be a class of **S**-databases that contains  $D_{q_i}$  and  $D_{\hat{q}_i}$  for  $i \in \{1, 2\}$  and is closed under cloning. Then

- (1)  $q_1$  and  $q_2$  are counting equivalent over  $\mathbb{D}$  iff  $q_1$  and  $q_2$  are counting equivalent over the class of all **S**-databases;
- (2) if  $\mathbb{D}$  is closed under disjoint union and contains  $D_{\mathbf{S}}^{\top}$ , then  $q_1$  and  $q_2$  are semi-counting equivalent over  $\mathbb{D}$  iff  $q_1$  and  $q_2$  are semi-counting equivalent over the class of all **S**-databases.

We start with two simple, yet crucial, observations about counting: one regarding products and one regarding cloning. Those observation will often be used implicitly in the following three sections of the appendix.

**Lemma B.1** (product rule). Let  $q(\bar{x})$  be a CQ over schema **S** and D, D' be **S**-databases. Then,  $\#q(D \times D') = \#q(D) \cdot \#q(D')$ .

The proof is folklore.

We need one more definition before we formulate the statement regarding cloning. Let D be an **S**-database and  $q(\bar{x})$  be a CQ over schema **S**. For a number  $i \geq 0$  and a set  $T \subseteq \mathsf{adom}(D)$ , by  $\hom_{i,T}(q, D, \bar{x})$  we denote the set of all functions  $h: \bar{x} \to \mathsf{adom}(D)$  that extend to a homomorphism from q to D such that h maps exactly i variables from  $\bar{x}$  to T.

**Lemma B.2.** Let D be an S-database, let  $i \ge 0, j > 0$  be natural numbers, and  $T \subseteq \operatorname{adom}(D)$  be a subset of the active domain of D. Let  $q(\bar{x})$  be an equality-free CQ over schema S.

If  $D_j$  is a database obtained from D by cloning every element from T exactly j-1 times and  $T_j \subseteq \operatorname{adom}(D_j)$  is the set of all those clones, then  $|\hom_{i,T_j}(q, D_j, \bar{x})| = j^i |\hom_{i,T}(q, D, \bar{x})|$ .

As before, the proof is straightforward. Nevertheless, observe that in the above statement it is crucial that the answer variables are independent and do not repeat in the tuple  $\bar{x}$ .

For the notion of counting equivalence, we inspect the strongly related notion of being renaming equivalent. Let  $q_1(\bar{x}_1), q_2(\bar{x}_2)$  be CQs over some schema **S**. We say that  $q_1$  and  $q_2$ are *renaming equivalent* if there are two surjections  $h_1: \bar{x}_1 \to \bar{x}_2$  and  $h_2: \bar{x}_2 \to \bar{x}_1$  that can be extended to homomorphisms  $h_1: q_1 \to D_{q_2}$  and  $h_2: q_2 \to D_{q_1}$ . **Lemma B.3** (counting equivalence). Let  $q_1(\bar{x}_1), q_2(\bar{x}_2)$  be equality-free CQs over schema **S**. Let  $\mathbb{D}$  be a class of databases such that

- $D_{q_1}, D_{q_2} \in \mathbb{D}$  and
- $\mathbb{D}$  is closed under cloning.

Then  $q_1$  and  $q_2$  are renaming equivalent or there is a  $D \in \mathbb{D}$  such that  $\#q_1(D) \neq \#q_2(D)$ .

*Proof.* We start by observing that if  $|\bar{x}_1| \neq |\bar{x}_2|$  then there is a database  $D \in \mathbb{D}$  such that  $\#q_1(D) \neq q_2(D)$ .

Assume that  $|\bar{x}_1| \neq |\bar{x}_2|$ . If  $\#q_1(D_{q_1}) \neq \#q_2(D_{q_1})$  then we take  $D = D_{q_1}$  and we are done. Hence, assume otherwise, i.e.  $\#q_1(D_{q_1}) = \#q_2(D_{q_1})$ . Let D be  $D_{q_1}$  with every element cloned once, in particular  $|\mathsf{adom}(D)| = 2|\mathsf{adom}(D_{q_1})|$ . Clearly,  $D \in \mathbb{D}$ . Therefore, if we show that  $\#q_1(D) \neq \#q_2(D)$  then we will prove the observation.

Since  $q_1$  is equality free we have  $\#q_1(D_{q_1}) > 0$ . Moreover, the following holds:

$$\#q_1(D) = 2^{|\bar{x}_1|} \#q_1(D_{q_1}) = 2^{|\bar{x}_1|} \#q_2(D_{q_1}) \neq 2^{|\bar{x}_2|} \#q_2(D_{q_1}) = \#q_2(D).$$

The first equality is a consequence of Lemma B.2, so is the last one. The middle equality follows from the fact that  $|x_1| \neq |x_2|$  and the assumption that  $\#q_1(D_{q_1}) = \#q_2(D_{q_1})$ . Indeed, since  $\#q_1(D_{q_1}) > 0$ , we have  $\#q_2(D_{q_1}) > 0$ . Thus,  $2^{|\bar{x}_1|} \#q_2(D_{q_1}) \neq 2^{|\bar{x}_2|} \#q_2(D_{q_1})$  is equivalent to  $|x_1| \neq |x_2|$ . Hence, we infer that  $\#q_1(D) \neq \#q_2(D)$ , which ends the proof of the observation.

Now, we show that if  $\#q_1(D) = \#q_2(D)$  for all databases  $D \in \mathbb{D}$  then  $q_1$  and  $q_2$  are renaming equivalent. Since  $\#q_1(D) = \#q_2(D)$  for all databases  $D \in \mathbb{D}$ , the above observation yields  $|\bar{x}_1| = |\bar{x}_2|$ . Hence, possibly after some renaming, we can assume that  $\bar{x}_1 = \bar{x}_2$ , drop the subscript, and simply write  $\bar{x}$ .

Let  $q(\bar{x})$  be a CQ over schema **S**, let D be an **S**-database such that  $\bar{x} \subseteq \mathsf{adom}(D)$ . By  $\mathsf{hom}(q, D, \bar{x})$  we denote all mappings from  $\bar{x}$  to  $\mathsf{adom}(D)$  that can be extended to homomorphisms from q to D. Similarly, by  $\mathsf{surj}(q, D, \bar{x})$  we denote all surjections from  $\bar{x}$  to  $\bar{x}$  that lie in  $\mathsf{hom}(q, D, \bar{x})$ . Notice that if  $|\mathsf{surj}(q_1, D_{q_2}, \bar{x})| > 0$  and  $|\mathsf{surj}(q_2, D_{q_1}, \bar{x})| > 0$  then, by definition,  $q_1$  and  $q_2$  are renaming equivalent.

For  $T \subseteq \bar{x}$  let  $\hom_T(q, D, \bar{x})$  denote the set of mappings  $h \in \hom(q, D, \bar{x})$  such that  $h(\bar{x}) \subseteq T$ . By an inclusion-exclusion argument we get

$$|\operatorname{surj}(q,D,\bar{x})| = \sum_{T \subseteq \bar{x}} (-1)^{|\bar{x}| - |T|} |\operatorname{hom}_T(q,D,\bar{x})|.$$

We now show how to compute  $\hom_T(q, D, \bar{x})$  for all  $T \subseteq \bar{x}$ . For  $i \ge 0$ , let  $\hom_{i,T}(q, D, \bar{x})$ be the set of mappings  $h \in \hom(q, D, \bar{x})$  such that h maps exactly i variables from  $\bar{x}$  into T. In particular,  $\hom_T(q, D, \bar{x}) = \hom_{|\bar{x}|,T}(q, D, \bar{x})$ . For  $j \ge 1$  and  $T \subseteq \operatorname{adom}(D)$ , let  $D_{j,T}$  be a database obtained from D by cloning all elements from T exactly j-1 times, i.e. for every  $a \in T$  the database  $D_{j,T}$  has exactly j clones of a. In particular,  $D_{1,T} = D$ .

By Lemma B.2, for every  $T \subseteq \bar{x}$  and every j > 0, we have

$$\#q(D_{j,T}) = |\mathsf{hom}(q, D_{j,T}, \bar{x})| = \sum_{i=0}^{|\bar{x}|} i^j |\mathsf{hom}_{i,T}(q, D, \bar{x})|.$$

Since the above equation holds for every  $j \ge 1$ , by taking first  $|\bar{x}|+1$  equations we construct a system of linear equations where  $|\mathsf{hom}_{i,T}(q, D, \bar{x})|$  are the unknowns, the coefficients  $i^j$  form a Vandermonde matrix, and  $\#q(D_{j,T})$  are the constant terms. Notice that the matrix does not depend on q nor D. Since the matrix has full rank, the values  $|\mathsf{hom}_{i,T}(q, D, \bar{x})|$  are uniquely determined by, and can be effectively computed from, the constant terms  $\#q(D_{j,T})$ . In particular, the value  $|\mathsf{hom}_T(q, D, \bar{x})| = |\mathsf{hom}_{|\bar{x}|,T}(q, D, \bar{x})|$  is uniquely determined by the constant terms, and, in consequence, so is the value  $|\mathsf{surj}(q, D, \bar{x})|$ .

If we apply the above system of equations to CQ  $q_1$  and database  $D_{q_2}$  we can conclude that  $|\operatorname{surj}(q_1, D_{q_2}, \bar{x})|$  is uniquely determined by the values  $\#q_1(D)$  for databases D from a certain set  $S \subseteq \mathbb{D}$ . Similarly,  $|\operatorname{surj}(q_2, D_{q_2}, \bar{x})|$  is uniquely determined the same equations with the values  $\#q_1(D)$  replaced by  $\#q_2(D)$ .

Now, since the equations' coefficients do not depend on the query nor on the database and since we have  $\#q_1(D) = \#q_2(D)$  for all  $D \in \mathbb{D}$ , we can infer that  $|\operatorname{surj}(q_1, D_{q_2}, \bar{x})| = |\operatorname{surj}(q_2, D_{q_2}, \bar{x})|$ . Hence,  $|\operatorname{surj}(q_1, D_{q_2}, \bar{x})| > 0$  as the identity function clearly belongs to  $\operatorname{surj}(q_2, D_{q_2}, \bar{x})$ .

A similar reasoning shows that  $|surj(q_2, D_{q_1}, \bar{x})| > 0$  and ends the proof.

The notion of renaming equivalence is also connected to semi-counting equivalence.

**Lemma B.4** (semi-counting equivalence). Let  $q_1(\bar{x}_1), q_2(\bar{x}_2)$  be equality-free CQs over schema **S**. Let  $\mathbb{D}$  be a class of databases such that

• 
$$D_{\mathbf{S}}^{\top}, D_{\hat{a}_1}, D_{\hat{a}_2} \in \mathbb{D},$$

and D is closed under cloning and disjoint union.

Either  $\hat{q}_1$ ,  $\hat{q}_2$  are renaming equivalent or there is, and can be computed, a database  $D \in \mathbb{D}$  such that  $|q_1(D)| \neq |q_2(D)|$  and for every CQ q over schema **S** we have that |q(D)| > 0.

*Proof.* We will show that if  $\hat{q}_1$ ,  $\hat{q}_2$  are not renaming equivalent then there is a database  $D \in \mathbb{D}$  such that  $\#q_1(D) \neq \#q_2(D)$  and such that for every CQ q over schema **S** we have that #q(D) > 0.

Since  $\hat{q}_1$ ,  $\hat{q}_2$  are not renaming equivalent then, by the previous lemma, we can find a database  $D' \in \mathbb{D}$  such that  $\#\hat{q}_1(D') \neq \#\hat{q}_2(D')$ .

Consider the function  $f_1 : k \mapsto \#q_1(D' + kD_{\mathbf{S}}^{\top})$  defined for  $k \ge 1$ , where  $D' + kD_{\mathbf{S}}^{\top}$  is the disjoint union of D' and k copies of  $D_{\mathbf{S}}^{\top}$ . After some elementary transformations on  $\#q_1(D' + kD_{\mathbf{S}}^{\top})$  we can infer that  $f_1$  is a polynomial in k whose constant term, i.e. term of degree 0, is  $\#\hat{q}_1(D')$ . Similarly, the function  $f_2 : k \mapsto \#q_2(D' + kD_{\mathbf{S}}^{\top})$  is a polynomial whose constant term is  $\#\hat{q}_2(D')$ . For the details please refer to the proof of Theorem 5.9 in [CM16].

If the counts of  $q_1$  and  $q_2$  would agree on all databases from  $\mathbb{D}$  then for all  $k \ge 1$  we would have that  $f_1(k)=f_2(k)$ . Moreover, since  $f_1, f_2$  are polynomials, this would imply that  $f_1$  and  $f_2$  are equal, i.e. they have the same degree and their corresponding coefficients coincide. In particular, this would imply that  $\#\hat{q}_1(D')=\#\hat{q}_2(D')$ . But this is impossible, as D' was chosen so that  $\#\hat{q}_1(D') \neq \#\hat{q}_2(D')$ . Therefore, there is  $k' \ge 1$  such that  $f_1(k') \neq f_2(k')$ .

What remains is to check that  $D = D' + k'D_{\mathbf{S}}^{\perp}$  is as required. First, by definition  $D \in \mathbb{D}$ . Moreover, since k' > 0, for every CQ q over schema **S** we have that #q(D) > 0. Finally, we observe that  $\#q_1(D) = f_1(k') \neq f_2(k') = \#q_2(D)$ .

From Lemma B.3 and Lemma B.4 we obtain the following.

**Lemma B.5.** Let  $q_1, q_2$  be CQs over some schema **S**. The following holds:

- $q_1$  and  $q_2$  are counting equivalent if and only if they are renaming equivalent;
- $q_1$  and  $q_2$  are semi-counting equivalent if and only if  $\hat{q}_1$  and  $\hat{q}_2$  are renaming equivalent.

*Proof.* For the first bullet we argue as follows. If  $q_1$  and  $q_2$  are not renaming equivalent then they are not counting equivalent. Indeed, by Lemma B.3 there is a database Dsuch that  $\#q_1(D) \neq \#q_2(D)$ . On the other hand, if  $q_1$  and  $q_2$  are renaming equivalent then the surjections promised by the definition of renaming equivalence provide for every **S**-database D surjections  $g_1^D: q_1(D) \rightarrow q_2(D)$  and  $g_2^D: q_2(D) \rightarrow q_1(D)$ . Clearly, these are then even bijections. This shows that  $\#q_1(D) = \#q_2(D)$  for every **S**-database D and, thus, shows that  $q_1$  and  $q_2$  are counting equivalent.

For the second bullet we observe that if  $\hat{q}_1$  and  $\hat{q}_2$  are not renaming equivalent then by Lemma B.4 there is a database D such that  $\#q_1(D) > 0$ ,  $\#q_2(D) > 0$ , and  $\#q_1(D) \neq \#q_2(D)$ . Thus,  $q_1$  and  $q_2$  are not semi-counting equivalent. On the other hand, if  $\hat{q}_1$  and  $\hat{q}_2$  are renaming equivalent then they are counting equivalent and for every database such that  $\#q_1(D) > 0$  and  $\#q_2(D) > 0$  we have that  $\#q_1(D) = \#\hat{q}_1(D) = \#\hat{q}_1(D) = \#q_2(D)$ . Thus,  $q_1$  and  $q_2$  are semi-counting equivalent. The middle equality follows from counting equivalence, the other follow from the fact that maximal Boolean connected components either force the answer set to be empty or do not change the size of the answer set.

As a consequence, we get the following.

**Lemma B.6** (equivalence relations). Counting equivalence and semi-counting equivalence are equivalence relations.

We can finally prove the first missing lemma.

Proof of Lemma 6.2. For Point 1, if  $q_1$  and  $q_2$  are counting equivalent, then they are counting equivalent over class  $\mathbb{D}$ . On the other hand, if they are not counting equivalent then, by Lemma B.5, they are not renaming equivalent. Thus, by Lemma B.3 there is a database  $D \in \mathbb{D}$  such that  $\#q_1(D) \neq \#q_2(D)$ . This implies that  $q_1$  and  $q_2$  are not counting equivalent over  $\mathbb{D}$ . Therefore,  $q_1$  and  $q_2$  are counting equivalent if and only if they are counting equivalent over  $\mathbb{D}$ .

For Point 2, if  $q_1$  and  $q_2$  are semi-counting equivalent, then they are clearly semi-counting equivalent over class  $\mathbb{D}$ . On the other hand, if they are not semi-counting equivalent, then by Lemma B.5  $\hat{q}_1$  and  $\hat{q}_2$  are not renaming equivalent. Thus, by Lemma B.4 there is a database  $D \in \mathbb{D}$  such that  $\#q_1(D) > 0$ ,  $\#q_2(D) > 0$ , and  $\#q_1(D) \neq \#q_2(D)$ . Hence,  $q_1$  and  $q_2$  are not semi-counting equivalent over  $\mathbb{D}$ . Therefore,  $q_1$  and  $q_2$  are semi-counting equivalent if and only if they are semi-counting equivalent over  $\mathbb{D}$ .

## APPENDIX C. ADDITIONAL DETAILS FOR SECTION 7.3

This section is dedicated to the results from [CM16] that culminate in the algorithm promised in the statement below.

**Theorem 7.4** [CM16]. Let  $\mathbb{D}$  be a class of databases over some schema **S** such that  $\mathbb{D}$  is closed under disjoint union, direct product, and contains  $D_{\mathbf{S}}^{\top}$ . Then there is an algorithm that

(1) takes as input a UCQ q, a CQ  $p \in \mathsf{cl}^{\mathbb{D}}_{\mathsf{CM}}(q)$ , and a database  $D \in \mathbb{D}$ ,

subject to the promise that for all  $p' \in \mathsf{cl}_{\mathsf{CM}}^{\mathbb{D}}(q)$ , there is an equality-free CQ p'' such that  $D_{p''} \in \mathbb{D}$ ,  $D_{\hat{p}''} \in \mathbb{D}$ , and p' and p'' are counting equivalent over  $\mathbb{D}$ ,

- (2) has access to an oracle for AnswerCount({q}, D), to a procedure for enumerating D, and to procedures for deciding counting equivalence and semi-counting equivalence between CQs over D,
- (3) runs in time  $f(||q||) \cdot p(||D||)$  with f a computable function and p a polynomial,
- (4) outputs #p(D).

As mentioned before, the statements are provided in our notation and are enough for our purposes. For the original statements please refer to [CM16].

We start by proving a stronger version of Lemma B.4. We show that given a set of pairwise not semi-counting equivalent CQs, we can always find a database that distinguishes those queries.

**Lemma C.1** (inequivalence witness; Lemma 5.12 from [CM16]). Let  $q_1(\bar{x}_1), q_2(\bar{x}_2), \ldots, q_n(\bar{x}_n), n > 0$ , be equality-free CQs over schema **S** such that for all  $1 \le i \le n$  we have that  $|\bar{x}_i| > 0$ . Let  $\mathbb{D}$  be a class of databases, such that

- $D_{\mathbf{S}}^{\top} \in \mathbb{D},$
- $D_{q_i}, D_{\hat{q}_i} \in \mathbb{D}$ , for  $1 \le i \le n$ ,

• and  $\mathbb{D}$  is closed under direct product, disjoint union, and cloning.

Then there is, and can be computed, a database  $D \in \mathbb{D}$  such that

- for all  $1 \le i \le n \ \#q_i(D) > 0$ ,
- and for all  $1 \le i, j \le n$  if  $q_i, q_j$  are not semi-counting equivalent then  $\#q_i(D) \ne \#q_j(D)$ .

*Proof.* We construct the database inductively. By requirement, the constructed database D will satisfy that #q(D) > 0 for every CQ  $q(\bar{x})$  over schema **S**. Therefore, for every pair of semi-counting equivalent CQs q, q' we will necessarily have that #q(D) = #q'(D). This allows us to assume without loss of generality that the CQs  $q_i$  used in the construction are pairwise not semi-counting equivalent.

For the base case, i.e. n=1, take database  $D_{\mathbf{S}}^{\top}$ . Now, let us assume that n > 0 and we have already created the database  $D_n$  for the queries  $q_1, \ldots, q_n$ . For the inductive step, we show how to construct database  $D_{n+1}$  for the queries  $q_1, \ldots, q_n, q_{n+1}$ .

Without loss of generality, we can assume that  $0 < \#q_1(D_n) < \#q_2(D_n) < \cdots < \#q_n(D_n)$ . Now, if  $\#q_{n+1}(D_n) \neq \#q_i(D_n)$  for all  $1 \leq i \leq n$  then we are done and we take  $D_{n+1} = D_n$ . Otherwise, let us assume that there is  $1 \leq i \leq n$  such that  $\#q_{n+1}(D_n) = \#q_i(D_n)$ .

By Lemma B.4 there is a database  $D' \in \mathbb{D}$  such that  $\#q_{n+1}(D') \neq \#q_i(D')$  and for every CQ q over schema **S** we have that #q(D') > 0. We can assume that  $\#q_{n+1}(D') > \#q_i(D')$ . If the equality is reversed we simply swap  $q_{n+1}$  with  $q_i$  before proceeding.

Now, we can show that there is l > 0 such that for the database  $D = D' \times (D_n)^l$ , where  $(D_n)^l$  is the direct product of l copies of  $D_n$ , we have

$$0 < \#q_1(D) < \dots < \#q_i(D) < \#q_{n+1}(D) < \#q_{i+1}(D) < \dots < \#q_n(D).$$

By the product rule, see Lemma B.1, the inequality  $\#q_i(D) < \#q_{n+1}(D)$  holds trivially for all l > 0. For the remaining inequalities, observe that for any two CQs p, p' over schema **S** and ant two **S**-databases B, C such that 0 < #p(B) < #p'(B) and #p(C), #p'(C) > 0 we have that  $1 < \frac{\#p'(B)}{\#p(B)}$ . Thus, there is l > 0 such that  $\frac{\#p(C)}{\#p'(C)} < (\frac{\#p'(B)}{\#p(B)})^l$ . For such l we have that  $\#p(C) \#p(B)^l < \#p'(C) \#p'(B)^l$  and, finally,  $\#p(C \times B^l) < \#p'(C \times B^l)$ .

Clearly, #q(D) > 0 for every CQ  $q(\bar{x})$  over schema **S**. Moreover, since D is a product of databases from  $\mathbb{D}$  we have that  $D \in \mathbb{D}$ . Thus, taking  $D_{n+1} = D$  ends the inductive step and the whole construction.

The witness produced in the above statement will not distinguish two CQs in  $\mathsf{cl}_{\mathsf{CM}}^{\mathbb{C}}(q)$ that are semi-counting equivalent, but not counting equivalent. The below lemma shows that this is not necessarily a problem.

**Lemma C.2** (Lemma 5.18 in [CM16]: extracting counts from semi-counting equivalence classes). Let  $p_1, \ldots, p_n$  be a set of semi-counting equivalent equality-free CQs that are pairwise not counting equivalent and let  $c_1, \ldots, c_n$  be a set of non-zero integers. Let  $\mathbb{D}$  be a class of databases such that

- D<sub>pi</sub> ∈ D, for 1 ≤ i ≤ n,
  and D is closed under direct product.

There is an fpt algorithm that performs the following: given a database  $D \in \mathbb{D}$  and a  $CQ \ q \in \{p_1, \ldots, p_n\}$  the algorithm computes #q(D); the algorithm may make calls to an oracle  $\mathcal{A}$  that provides  $\sum_i c_i \cdot \# p_i(D')$  upon being given a database  $D' \in \mathbb{D}$ .

*Proof.* Let  $S = \{p_1, \ldots, p_n\}$ . We start with the observation that for all non-empty subsets  $S' \subseteq S$  there are, and can be computed, a CQ  $q_{S'} \in S'$  and a database  $D_{S'}$  such that

 $(\diamond) \ \#q_{S'}(D') > 0$  and for all  $q \in S' \setminus \{q_{S'}\}$  we have that  $\#q(D_{S'}) = 0$ .

Indeed, let  $q_1(\bar{x}_1), q_2(\bar{x}_2) \in S'$  be two different CQs. Since  $q_1, q_2$  are semi-counting equivalent, the CQs  $\hat{q}_1, \hat{q}_2$  are renaming equivalent by Lemma B.5. Hence, there are two surjections  $h_1: \bar{x}_1 \to \bar{x}_2$  and  $h_2: \bar{x}_2 \to \bar{x}_1$  that can be extended to homomorphisms  $h_1: \hat{q}_1 \to D_{\hat{q}_2}$  and  $h_2: \hat{q}_2 \to D_{\hat{q}_1}$ . Therefore, if there would be homomorphisms  $g_1: q_1 \to D_{q_2}$ and  $g_2: q_2 \to D_{q_1}$  then we could extend the surjections  $h_1$  and  $h_2$  to homomorphisms  $h_1: q_1 \to D_{q_2}$  and  $h_2: q_2 \to D_{q_1}$ , respectively. This would imply that  $q_1$  and  $q_2$  are renaming equivalent and, by Lemma B.5, counting equivalent. Since they are not counting equivalent, one of the homomorphisms  $g_1$  or  $g_2$  does not exist.

Let  $q_{S'}$  be a minimal element in S' with respect to the partial order defined as  $q \leq q'$  if there is a homomorphism from q' to  $D_q$ . Let  $D_{S'} = D_{q_{S'}}$ . It is easy to check that the pair  $(q_{S'}, D_{S'})$  satisfies the requirements in  $(\diamond)$ . Let get-min(S') be the algorithm that given a set  $S' \subseteq \{p_1, \ldots, p_n\}$  returns the pair  $(q_{S'}, D_{S'})$ .

Finally we can describe the desired algorithm. For  $T \subseteq \{p_1, \ldots, p_n\}$ , let  $\mathcal{A}_T$  be an oracle that takes a database  $D \in \mathbb{D}$  and returns the value  $\sum_{p_i \in T} c_i \cdot \# p_i(D)$ . Then, the algorithm promised by the lemma, let us call it  $compute-count(T, q, A_T, D)$ , takes a set of CQs T, a CQ  $q \in T$ , an oracle  $\mathcal{A}_T(\cdot)$ , a database  $D \in \mathbb{D}$ , and outputs the value #q(D). The algorithm works as follows.

First, the algorithm finds the pair  $(p_i, D_i) = get - min(T)$ . If  $p_i = q$  then it returns  $\frac{\mathcal{A}_T(D \times D_i)}{c_i \cdot \# p_i(D_i)}$ . Otherwise, it returns the result of the recursive call  $compute-count(T', q, \mathcal{A}_{T'}, D)$ where  $T' = T \setminus \{p_i\}$  and  $\mathcal{A}_{T'}$  is an fpt algorithm that given database  $D' \in \mathbb{D}$  returns  $\mathcal{A}_{T'}(D') = \mathcal{A}_T(D') - \frac{\mathcal{A}_T(D \times D_i)}{\#q(D_i)} = \sum_{p_j \in T'} c_j \cdot \#p_j(D').$  The algorithm clearly belongs to FPT. To infer that it returns the desired value, we observe that

$$\frac{\mathcal{A}_T(D \times D_i)}{\#p_i(D_i)} = \frac{1}{\#p_i(D_i)} \cdot \sum_{p_j \in T} c_j \cdot \#p_j(D \times D_i) \\
= \frac{1}{\#p_i(D_i)} \cdot \sum_{p_j \in T} c_j \cdot \#p_j(D) \cdot \#p_j(D_i) \\
= \frac{1}{\#p_i(D_i)} \cdot c_i \cdot \#p_i(D) \#p_i(D_i) = c_i \cdot \#p_i(D).$$

The first equality follows from definition of  $\mathcal{A}_T$ , the second is the product rule, the third from the fact that by construction of  $D_i$ , for all  $p_j \in T$  we have that  $\#p_j(D_i) = 0$  if and only if  $p_i \neq p_i$ . The last equality is trivial. 

**Lemma C.3** (reduction from CQs to UCQs, the all free case in [CM16]). Let  $q(\bar{x})$  be an UCQ over schema **S** and  $|\bar{x}| > 0$ ; let  $p_1(\bar{x}_1), \ldots, p_n(\bar{x}_n)$  be a set of equality-free CQs such that  $|\bar{x}_i| > 0$  for  $0 < i \le n$ ; and let  $c_1, \ldots, c_n$  be a sequence of non-zero integers. Let  $\mathbb{D}$  be a class of databases such that

- $D_{\mathbf{S}}^{\top} \in \mathbb{D}$ ,
- $D_{p_i}, D_{\hat{p}_i} \in \mathbb{D}$ , for  $1 \le i \le n$ ,
- and D is closed under disjoint union, direct product, and cloning.

If  $p_1, \ldots, p_n$  are pairwise not counting equivalent and for every database  $D \in \mathbb{D}$  we have that  $(\dagger) \#q(D) = \sum_i c_i \cdot \#p_i(D)$ , then there is an algorithm that

- takes as an input a database  $D \in \mathbb{D}$  and a  $CQ \ p \in \{p_1, \ldots, p_n\}$ ;
- has an access to an oracle for AnswerCount({q}, D);
- works in time f(K)·poly(||D||), where f is some computable function and K is the combined size of p<sub>1</sub>,..., p<sub>n</sub>, c<sub>1</sub>,..., c<sub>n</sub>, and q;
- and outputs #p(D).

*Proof.* Let  $D_{\circ}$  be an **S**-database as in Lemma C.1. Let  $\varphi_1, \ldots, \varphi_k$  be the set of equivalence classes of the semi-counting equivalence. Then, for every  $1 \leq i \leq k$  for  $q, q' \in \varphi_i$  we have that  $\#q(D_{\circ}) = \#q'(D_{\circ})$ . Let  $d_i$  denote the value  $\#q(D_{\circ})$  for some  $q \in \varphi_i$ . For an **S**-database  $D \in \mathbb{D}$ , let  $\varphi_j(D) = \sum_{p_i \in \varphi_i} c_i \cdot \#p_i(D)$ .

Then, for  $l \ge 0$  we have the following.

$$#q(D \times D_{\circ}^{l}) = \sum_{1 \le i \le n} c_{i} \cdot #p_{i}(D \times D_{\circ}^{l}) = \sum_{1 \le i \le n} c_{i} \cdot #p_{i}(D)(#p_{i}(D_{\circ}))^{l} = \sum_{1 \le j \le k} \varphi_{j}(D) \cdot d_{j}^{l}$$

First equality holds because of (†), the second equality holds by product rule, see Lemma B.1, and the final equality holds by definitions of  $\varphi_i(D)$  and  $d_i$ .

Invoking the above equation for integers l = 1, 2, ..., k we obtain a system of linear equations where  $\varphi_j(D)$  are the unknowns,  $(d_j)^l$  form the matrix of coefficients, and  $\#q(D \times D_o^l)$  are the constant terms. Since the matrix is a Vandermonde matrix, this system of equations has an unique solution and gives an fpt algorithm  $\mathcal{A}(\varphi_j, D)$  with access to an oracle for  $\mathsf{AnswerCount}(\{q\}, \mathbb{D})$  that given one of the equivalence classes  $\varphi_j$  and a database  $D \in \mathbb{D}$  computes the values  $\varphi_j(D) = \sum_{p_i \in \varphi_j} c_i \cdot \#p_i(D)$ .

Let  $\varphi$  be the equivalence class containing CQ p. The fpt algorithm promised in the lemma works by invoking the algorithm from Lemma C.2 with the set of queries  $\varphi$  and the oracle being the algorithm  $\mathcal{A}(\varphi, \cdot)$ .

We can now prove the blackbox Theorem 7.4.

Proof of Theorem 7.4. Let  $\{p_1, \ldots, p_n\} \subseteq \mathsf{cl}_{\mathsf{CM}}^{\mathbb{D}}(q)$  be a maximal set of pairwise not semicounting equivalent CQs such that  $p_1 = p$ . Let  $c_1, \ldots, c_n$  be the sequence of non-zero integers such that for every **S**-database  $D' \in \mathbb{D}$  we have that  $\#q(D') = \sum_{i=1}^{n} c_i \#p_i(D')$ . By the definition of the Chen-Mengel closure, we know that such set of CQs exists and that this sequence of integers is well defined. Now, for every  $p_i$  we enumerate  $\mathbb{D}$  to find the promised databases  $D_{p''_i}$  and thus the equality-free CQs  $p''_i$ . We can do this, as we have access to a procedure that decides counting equality over  $\mathbb{D}$ . Since for all  $1 \leq i \leq n$  we have that  $p_i$  and  $p''_i$  are counting equivalent over  $\mathbb{D}$ , the equality  $\#q(D') = \sum_{i=1}^n c_i \#p''_i(D')$  hold for every database  $D' \in \mathbb{D}$ . Before we proceed, we observe that by the definition of UCQs, either UCQ q is Boolean and so is every CQ in  $\mathsf{cl}^{\mathbb{D}}_{\mathsf{CM}}(q)$  or q has at least one answer variable and so does every CQ in  $\mathsf{cl}^{\mathbb{D}}_{\mathsf{CM}}(q)$ . Hence, either all CQs  $p''_1, \ldots, p''_n$  are Boolean or none is.

If q has a non-empty set of answer variables then we simply apply Lemma C.3. Otherwise, q is Boolean and so is every query in  $\{p''_1, \ldots, p''_n\}$ . Hence all those CQs are semi-counting equivalent and we can apply Lemma C.2 directly.

### APPENDIX D. ADDITIONAL DETAILS FOR SECTION 7.4

For the sake of completeness, this section provides the construction from [CM15] that allows us to remove markings from the query. In particular, we provide the algorithm promised by the below statement.

**Theorem 7.9** [CM15]. Let  $\mathbb{D}$  be a class of databases over schema  $\mathbf{S}^m$  that is closed under direct products, cloning, and induced subdatabases. Then there is an algorithm that

- takes as input an equality-free  $CQ \ q$  such that  $q^m$  is over schema  $\mathbf{S}^m$  and a database  $D \in \mathbb{D}$ , subject to the promise that q is a core and  $D_{q^m} \in \mathbb{D}$ ,
- has access to an oracle for AnswerCount( $\{q\}, \mathbb{D}$ ),<sup>9</sup>
- runs in time  $f(||q||) \cdot p(||D||)$ , f a computable function and p a polynomial, and
- outputs  $\#q^m(D)$ .

*Proof.* We need to exhibit an fpt algorithm that given a CQ  $q(\bar{x})$  and an  $\mathbf{S}^m$ -database D computes  $\#q^m(D)$ . The algorithm may ask the oracle for the values #q(D') for  $D' \in \mathbb{D}$ . Let V be the set of variables in  $\bar{x}$ .

Let  $D^{\times}$  be the product of  $D_{q^m}$  and D, thus in particular  $\operatorname{adom}(D^{\times}) = \operatorname{adom}(D_{q^m}) \times \operatorname{adom}(D)$ . Let  $D^{\circ} \subseteq D^{\times}$  be the subdatabase induced by the set  $\{(x, a) \in \operatorname{adom}(D^{\times}) \mid x \in \operatorname{var}(q) \text{ and } R_x(a) \in D\}$ . Clearly,  $D^{\circ} \in \mathbb{D}$ .

Let  $\mathcal{H}$  be the set of functions  $g: V \to \mathsf{adom}(D^\circ)$  such that g can be extended to a homomorphism  $g: q \to D^\circ$  such that for all  $x \in V$ , g(x) = (y, b) implies x = y. Moreover, let  $\mathcal{H}'$ be the set of functions  $g: V \to \mathsf{adom}(D^\circ)$  such that g can be extended to a homomorphism  $g: q \to D^\circ$  and satisfy  $\{x \in V \mid \exists b: (x, b) \in g(V)\} = V$ , that is, all variables from V occurs in the first component of some element hit by g. Finally, let  $\mathcal{I}$  be the set of mappings  $g: V \to V$  that can be extended to an automorphism  $g: q \to q$ .

Claim 1. There is a bijection between  $q^m(D)$  and  $\mathcal{H}$ . Claim 2.  $|\mathcal{H}'| = |\mathcal{I}| \cdot |\mathcal{H}|$ .

Claim 1 follows from the fact that we simulate markings by enforcing that for all functions  $q \in \mathcal{H}$  and all answer variables x we have g(x) = (x, b) for some  $b \in \mathsf{adom}(D^\circ)$ . Claim 2 is shown by arguing that every function in  $\mathcal{H}'$  can be obtained as the composition of a function from  $\mathcal{H}$  with a permutation of answer variables from  $\mathcal{I}$ . The precise proofs of the above claims can be found in [CM15].

For  $T \subseteq V$ , let  $\mathcal{H}_T$  be the set of functions  $g: V \to \mathsf{adom}(D^\circ)$  that can be extended to a homomorphism  $g: q \to D^\circ$  and satisfy  $\{y \in V \mid \exists x \in V : g(x) = (y, b)\} \subseteq T$ , that is, g maps

<sup>&</sup>lt;sup>9</sup>Note that since  $\mathbf{S} \subseteq \mathbf{S}^m$ , q may be viewed as a CQ over schema  $\mathbf{S}^m$ .

all variables from V to elements that have a variable from T in its first component. By an inclusion-exclusion argument, we get the equation

$$|\mathcal{H}'| = \sum_{T \subseteq V} (-1)^{|V \setminus T|} |\mathcal{H}_T|$$

The above equation used together with Claims 1 and 2 gives the following.

Claim 3.  $\#q^m(D) = \frac{1}{|\mathcal{I}|} \cdot \sum_{T \subseteq V} (-1)^{|V \setminus T|} |\mathcal{H}_T|.$ 

Since  $|\mathcal{I}|$  can be computed brute-force, we focus on how to compute the values  $|\mathcal{H}_T|$  for all  $T \subseteq V$ . Fix  $T \subseteq V$ . For i > 0, let  $\mathcal{H}_{i,T}$  be the set of functions  $g: V \to \mathsf{adom}(D^\circ)$  such that g can be extended to a homomorphism  $g: q \to D^\circ$  such that for exactly i variables  $x \in V$ , the first component of g(x) is in T, that is, g(x) = (y, b) implies  $y \in T$ . Note that  $\mathcal{H}_{|V|,T} = \mathcal{H}_T$ .

Let  $D_{j,T}^{\circ}$  be the **S**-database obtained from the database  $D^{\circ}$  by cloning every element from the set  $\{(x, a) \in \operatorname{adom}(D^{\circ}) \mid x \in T\}$  exactly j-1 times. Note that  $D_{1,T}^{\circ} = D^{\circ}$  and  $D_{j,T}^{\circ} \in \mathbb{D}$  for all j > 0. Moreover, the following holds.

Claim 4. For j > 0,  $\#q(D_{j,T}^{\circ}) = \sum_{i=0}^{|V|} j^i |\mathcal{H}_{i,T}|$ .

Invoking the equation from Claim 4 for j = 1, 2, ..., |V| + 1, we obtain a system of |V|+1 linear equations where  $|\mathcal{H}_{i,T}|$  are the unknowns,  $j^i$  form the matrix of coefficients, and  $\#q(D_{j,T})$  are the constant terms. Since the matrix is a Vandermonde matrix, this system of equations has a unique solution. Moreover, since the class  $\mathbb{D}$  is closed under cloning, the values  $\#q(D_{j,T}^{\circ})$  can be effectively computed using an oracle for AnswerCount( $\{q\}, \mathbb{D}$ ). Hence there is an algorithm  $solve(q^m, D^{\circ}, T)$  that given  $q^m, D^{\circ}$ , and a set  $T \subseteq V$  computes the value  $|\mathcal{H}_T|$ .

Claim 5. Algorithm  $solve(q^m, D^{\circ}, T)$  is an fpt algorithm with access to an oracle for AnswerCount( $\{q\}, \mathbb{D}$ ), the parameter being the size of the query  $q^m$  (which dominates the size of T).

All we need to show is that *solve* works in time  $f(||q^m||) \cdot poly(||D^\circ||)$  for some computable function f. Since we can use the standard algorithm to solve the system of linear equations in time polynomial in the size of the system, it is enough to show that the system can be constructed in the desired time.

The system has |V| + 1 equation. Since  $0 \le i \le |V|$  and  $1 \le j \le |V| + 1$ , the coefficients  $j^i$  do not depend on the database and can be constructed in the desired time.

For the constant terms  $\#q(D_{j,T}^{\circ})$  we observe that we can compute  $D_{j,T}^{\circ}$  in time bounded by  $f'(||q^m||) \cdot poly(||D^{\circ}||)$  for some computable function f'. Indeed, since  $D^{\circ}$  is a subdatabase of the product database  $D_{q^m} \times D$ , it uses no more than  $||q^m||$  relational symbols. Moreover, every fact in  $D^{\circ}$  has arity not greater than  $||q^m||$  and, thus, cannot give rise to more than  $j^{||q^m||}$  facts. Hence,  $||D_{j,T}^{\circ}|| \leq j^{|q^m|}||D^{\circ}||$  and  $D_{j,T}^{\circ}$  can be computed in the desired time by simply enumerating all facts in database  $D^{\circ}$ . In consequence, there is an fpt algorithm with an oracle that constructs the desired system of equations. This ends the proof of Claim 5.

To conclude, the algorithm that given CQ  $q^m$  and database D computes  $\#q^m(D)$  works as follows. First, we construct the unmarked query q and the database  $D^\circ$ , and compute the size of the set  $\mathcal{I}$ . Then, for all  $T \subseteq V$  we invoke  $solve(q^m, T, D^\circ)$  to compute the values  $|\mathcal{H}_T|$ . Finally, we use the equation from Claim 3 to compute the value  $\#q^m(D)$ .

For the time complexity of the algorithm, we observe that q,  $|\mathcal{I}|$ , and  $D^{\circ}$  can be easily computed by an fpt algorithm. Since the size of the equation in Claim 3 depends only

on the size of the query q, we have no more than a constant number of values  $|\mathcal{H}_T|$  to compute. By Claim 5 each value  $|\mathcal{H}_T|$  can be computed by an fpt algorithm with access to an oracle computing #q(D') for  $D' \in \mathbb{D}$ . Hence, the overall running time is bounded by  $f(||q||) \cdot p(||D||)$  for some computable function f and a polynomial p.

# APPENDIX E. ADDITIONAL DETAILS FOR SECTION 9

For the proof of Lemma 9.2, it remains to establish Points (A) and (B) used in the proof given in the main part of the paper. For the reader's convenience, we repeat the central definitions.

Let I be an instance and  $\mathcal{T}$  a set of TGDs. For each fact in  $\operatorname{ch}_{\mathcal{T}}(I)$ , we want to identify a source fact in I. Start with setting  $\operatorname{src}(R(\bar{c})) = R(\bar{c})$  for all  $R(\bar{c}) \in I$ . Next assume that  $R(\bar{c}) \in \operatorname{ch}_{\mathcal{T}}(I)$  was introduced by a chase step that applies a TGD  $T \in \mathcal{T}$  at a tuple  $(\bar{d}, \bar{d}')$ , and let R' be the relation symbol in the guard atom in  $\operatorname{body}(T)$ . Then we set  $\operatorname{src}(R(\bar{c})) = R'(\bar{d}, \bar{d}')$  if  $\bar{d} \cup \bar{d}' \subseteq \operatorname{adom}(I)$  and  $\operatorname{src}(R(\bar{c})) = \operatorname{src}(R'(\bar{d}, \bar{d}'))$  otherwise. For any guarded set X of I, define  $\operatorname{ch}_{\mathcal{T}}(I)|_X^{\downarrow}$  to contain those facts  $R(\bar{c}) \in \operatorname{ch}_{\mathcal{T}}(I)$  such that the constants in  $\operatorname{src}(R(\bar{c}))$  are exactly those in X.

We shall actually consider such subinterpretations not only of the final result  $ch_{\mathcal{T}}(I)$  of the chase, but also of the instances constructed as part of a chase sequence  $I_0, I_1, \ldots$  for Iwith  $\mathcal{T}$ . In fact, we can define  $I_i|_X^{\downarrow}$  in exact analogy with  $ch_{\mathcal{T}}(I)|_X^{\downarrow}$ , for all  $i \geq 0$ .

**Lemma E.1.** Let  $I_0, I_1, \ldots$  be a chase sequence of I with  $\mathcal{T}$  and  $i \geq 0$ . Then

- (A) for all guarded sets X in I, there is a homomorphism from  $I_i|_X^{\downarrow}$  to  $ch_{\mathcal{T}}(I_i|_X)$  that is the identity on all constants in X;
- (B) if  $c \in \operatorname{adom}(I_i)$  is a null and  $R_1(\bar{c}_1), R_2(\bar{c}_2) \in I_i$  such that c occurs in both  $c_1$  and  $c_2$ , then  $\operatorname{src}(R_1(\bar{c}_1)) = \operatorname{src}(R_2(\bar{c}_2))$ .

*Proof.* The proof of both (A) and (B) is by induction on *i*. We only present the more interesting proof of (A). The induction start holds as  $I_0|_X^{\downarrow} = I_0|_X \subseteq ch_{\mathcal{T}}(I|_X)$ .

For the induction step, assume that  $I_{i+1}$  was obtained from  $I_i$  by applying a TGD  $T = \phi(\bar{x}, \bar{y}) \rightarrow \exists \bar{z} \, \psi(\bar{x}, \bar{z})$  at a tuple  $(\bar{c}, \bar{c}')$ . Let R be the relation symbol used in a guard atom of  $\phi$ , and let Z be the constants in  $\operatorname{src}(R(\bar{c}, \bar{c}'))$ .

Now consider any guarded set X in I. If  $X \neq Z$ , then by definition of  $\cdot|_X^{\downarrow}$  in terms of src, we must have  $I_{i+1}|_X^{\downarrow} = I_i|_X^{\downarrow}$  and it suffices to use the induction hypothesis. Thus assume that X = Z. Then clearly  $I_{i+1}|_X^{\downarrow} \setminus I_i|_X^{\downarrow} = \psi(\bar{c}, \bar{c}'')$  where  $\bar{c}''$  consists of nulls that do not occur in  $I_i$ . By induction hypothesis, there is a homomorphism  $h_i$  from  $I_i|_X^{\downarrow}$  to  $ch_{\mathcal{T}}(I_i|_X)$  that is the identity on all constants in X. Applicability of T at  $(\bar{c}, \bar{c}')$  implies  $\phi(\bar{c}, \bar{c}') \subseteq I_i$  and thus  $\phi(h_i(\bar{c}), h_i(\bar{c}')) \subseteq ch_{\mathcal{T}}(I_i|_X)$ . It follows T has been applied at  $(h(\bar{c}), h(\bar{c}'))$  in (any fair chase sequence that produces)  $ch_{\mathcal{T}}(I_i|_X)$ . As a consequence, there are constants  $\bar{d}$  such that  $\psi(h(\bar{c}), \bar{d}) \subseteq ch_{\mathcal{T}}(I_i|_X)$ . We extend  $h_i$  to  $h_{i+1}$  so that  $h_{i+1}(\bar{c}'') = \bar{d}$ . Clearly,  $h_{i+1}$  is a homomorphism from  $I_{i+1}|_X^{\downarrow}$  to  $ch_{\mathcal{T}}(I_{i+1}|_X)$ .

We next prove the part of Theorem 9.7 that is concerned with contract treewidth. The proof uses minors. We recall that an undirected graph G is a *minor* of an undirected graph H if G can be obtain from H by contracting edges and then taking a subgraph.

**Lemma E.2.** Let  $(\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$  be an OMQ and  $k \geq 1$ . Then  $Q_k^{CTW}$  is a  $CTW_k$ -approximation of Q.

Proof. Let  $Q(\bar{x}) = (\mathcal{O}, \mathbf{S}, q) \in (\mathbb{G}, \mathbb{UCQ})$ . By construction of  $Q_k^{CTW} = (\mathcal{O}, \mathbf{S}, q_k^{CTW})$ , it is clear that Points 1 and 2 of the definition of  $CTW_k$ -approximations are satisfied. It thus remains to establish Point 3.

Thus let  $P(\bar{x}) = (\mathcal{O}', \mathbf{S}, p) \in (\mathbb{G}, \mathbb{UCQ})$  such that  $P \subseteq Q$  with p of contract treewidth at most k. We have to show that  $P \subseteq Q_k^{\text{CTW}}$ . Let D be an **S**-database and let  $\bar{c} \in P(D)$ . Thus there is a homomorphism h from some CQ  $p'(\bar{x})$  in p to  $ch_{\mathcal{O}'}(D)$  such that  $h(\bar{x}) = \bar{c}$ .

The general strategy of the proof is the same as in the proof of Lemma 9.11, but there is an additional complication. Ideally, we would like to use the homomorphism h and the fact that p' has contract treewidth at most k to construct from D a database D'' such that the following three conditions are satisfied:

(a)  $\bar{c} \in P(D'');$ 

(b) the contract treewidth of  $(D'', \bar{c})$  is at most k;

(c) there is a homorphism from D'' to D that is the identity on  $\bar{c}$ .

Let us briefly argue how this helps to prove Lemma E.2. Point (a) and  $P \subseteq Q$  imply that there is a homomorphism g from some CQ  $q'(\bar{x})$  in q to  $ch_{\mathcal{O}}(D'')$  with  $g(\bar{x}) = \bar{c}$ . We obtain a CQ  $\hat{q}(\bar{x})$  from q' by identifying variables, achieving that for all distinct variables  $y_1, y_2$  in  $\hat{q}$ ,  $g(y_1) = g(y_2)$  implies that  $y_1 = y_2 \in \hat{q}$ . Point (b) then implies that  $\hat{q}(\bar{x})$  is a CQ in  $q_k^{\text{CTW}}$ and we may use Point (c) to show that  $\bar{c} \in Q_k^{CTW}(D)$ , as required.

The additional complication is as follows. To ensure Point (b), it is necessary that the homomorphism h from p' to D that we use in the construction of D'' is 'as injective as possible'. Intuitively, this is because an injective homomorphism provides a much closer link between p' and D, and such a close link is needed to transfer the bound on contract treewidth from p' to D''. In particular, non-injectivities on answer variables must be avoided as much as possible. To address this issue, we first construct from  $(D, \bar{c})$  another pointed database  $(D', \bar{c}')$  and a homomorphism h' from D' to D with  $h(\bar{c}') = \bar{c}$ , breaking as many non-injectivities on answer variables as possible. We then construct D'' starting from D' and h' rather than from D and h.

We now describe the construction of  $(D', \bar{c}')$  and h' in detail. Let ' $\sim$ ' denote the smallest equivalence relation on the variables in  $\bar{x}$  such that  $x_1 \sim x_2$  whenever p' has an  $\bar{x}$ -component S such that  $x_1, x_2 \in S$ . We construct  $(D', \bar{c}')$  such that:

- (1) there is a homomorphism h' from p' to  $\mathsf{ch}_{\mathcal{O}'}(D')$  such that  $h'(\bar{x}) = \bar{c}'$  and  $h'(x_1) = h'(x_2)$ , with  $x_1, x_2 \in \bar{x}$ , implies  $x_1 \sim x_2$ ;
- (2) there is a homomorphism from D' to D that maps  $\bar{c}'$  to  $\bar{c}$ .

Informally, the condition on h' in Point 1 says that h' avoids non-injectivities on answer variables as much as possible. Let  $\mathcal{C}_1, \ldots, \mathcal{C}_m$  be the equivalence classes of ' $\sim$ '. Define

$$D' = \{ R(c_1^{i_1}, \dots, c_n^{i_n}) \mid R(c_1, \dots, c_n) \in D \text{ and } 1 \le i_1, \dots, i_n \le m \}.$$

It is easy to see that Point 2 is indeed satisfied as long as we construct  $\bar{c}'$  from  $\bar{c}$  by replacing each component c with some  $c^i$ ,  $i \leq i \leq m$ . To define the homomorphism h' required by Point 1, we need two preliminaries.

First, by definition of '~' we find, for each quantified  $y \in \operatorname{var}(p')$ , at most one *i* such that there is an answer variable  $x \in C_i$  that is reachable from *y* in  $G_{p'}$  without passing an answer variable. Set  $\rho(y) = i$  and  $\rho(y) = 1$  if there is no such *i*. Moreover, for each variable *x* in  $\bar{x}$ , set  $\rho(x) = i$  if  $x \in C_i$ . It is easy to see that when quantified variables  $y_1, y_2$  co-occur in an atom in p', then  $\rho(y_1) = \rho(y_2)$ .

Second, by construction of D' we find for each fact  $\alpha = R(c_1^{i_1}, \ldots, c_n^{i_n}) \in D'$  a homomorphism  $g_\alpha$  from D to D' such that  $g_\alpha(c_j) = c_j^{i_j}$  for  $1 \le j \le n$ . We can extend  $g_\alpha$  to a homomorphism from  $\mathsf{ch}_{\mathcal{O}'}(D)$  to  $\mathsf{ch}_{\mathcal{O}'}(D')$ . We now define h' as follows:

- if  $x \in \operatorname{var}(p_i)$  and  $h(x) \in \operatorname{adom}(D)$ , then  $h'(x) = h(x)^{\rho(x)}$ ;
- if  $x \in \operatorname{var}(p_i)$  and  $h(x) \notin \operatorname{adom}(D)$  is in the tree-like structure that the chase has generated below fact  $R(c_1, \ldots, c_n)$ ,<sup>10</sup> then  $h'(y) = g_\alpha(h(y)), \ \alpha = R(c_1^{\rho(x)}, \ldots, c_n^{\rho(x)}).$

Moreover, set  $\bar{c}' = h'(\bar{c})$ . We argue that h' is indeed a homomorphism from p' to  $ch_{\mathcal{O}'}(D')$ . Let  $R(\bar{y})$  be an atom in p'. First assume that  $h(y) \in adom(D)$  for all variables y in  $\bar{y}$ . Let  $\alpha = R(h'(\bar{y}))$ . Then  $g_{\alpha}$  is a homomorphism from  $ch_{\mathcal{O}'}(D)$  to  $ch_{\mathcal{O}'}(D')$  with  $g_{\alpha}(h(\bar{y})) = h'(\bar{y})$ . Together with  $R(h(y)) \in ch_{\mathcal{O}}(D)$ , this yields  $R(h'(y)) \in ch_{\mathcal{O}}(D')$  as required.

Now assume that  $\bar{y}$  contains at least one variable y with  $h(y) \notin \operatorname{adom}(D)$ . Then y is a quantified variable. By definition of  $\rho$ ,  $\rho(y)$  must be identical for all quantified variables y in  $\bar{y}$ , and it must also be identical to  $\rho(x)$  for all answer variables in  $\bar{y}$ . This means that h'(y) is defined based on the same homomorphism  $g_{\alpha}$  for all variables y in  $\bar{y}$ , and in particular  $g_{\alpha}(h(\bar{y})) = h'(\bar{y})$ . From  $R(h(y)) \in \operatorname{ch}_{\mathcal{O}}(D)$ , we again obtain  $R(h'(y)) \in \operatorname{ch}_{\mathcal{O}}(D')$  as required.

We next construct an S-database D'' that satisfies Points (a) to (c) above, in a slightly modified form:

- (3) there is a homomorphism h'' from p' to  $ch_{\mathcal{O}'}(D'')$  that maps  $\bar{x}$  to  $\bar{c}'$ ;
- (4) the contract treewidth of  $(D'', \bar{c}')$  is at most k;
- (5) there is a homomorphism from D'' to D' that is the identity on  $\overline{c'}$ .

Set

$$\Gamma = \{h'(\bar{y} \cap \bar{x}) \mid R(\bar{y}) \in p'\} \cup \{h'(S \cap \bar{x}) \mid S \ \bar{x}\text{-component of } p'\}$$

and note the tight connection to the definition of contracts, in which edges step from atoms (first set in the definition of  $\Gamma$ ) and from  $\bar{x}$ -components (second set). For every  $S \in \Gamma$ , let  $D_S$  be the database obtained from D' by renaming every constant  $c \notin S$  to  $c^S$ . Now define

$$D'' = \bigcup_{S \in \Gamma} D_S.$$

It is easy to see that Point 5 is satisfied. We now argue that Points 3 and 4 also hold. For Point 3, we have to construct a homomorphism h'' from p' to  $ch_{\mathcal{O}'}(D'')$  with  $h''(\bar{x}) = \bar{c}'$ . Start with setting h''(x) = h'(x) for all  $x \in \bar{x}$ , and thus  $h''(\bar{x}) = \bar{c}'$  as required. It remains to define h'' for the quantified variables in p'. We do this per  $\bar{x}$ -component. Thus let S be an  $\bar{x}$ -component of p'. Then  $h(S \cap \bar{x}) \in \Gamma$ . It is not hard to prove that  $ch_{\mathcal{O}'}(D'') = \bigcup_{S \in \Gamma} ch_{\mathcal{O}'}(D_S)$ . Clearly, there is a homomorphism  $h_S$  from D' to  $D_S$  with  $h_S(c) = c$  for all  $c \in S$ , and  $h_S$  can be extended to a homomorphism from  $ch_{\mathcal{O}'}(D')$  to  $ch_{\mathcal{O}'}(D_S)$ . Define  $h''(y) = h_S \circ h'(y)$  for all  $y \in S$ . It can be verified that h'' is indeed a homomorphism. Details are omitted.

To prove Point 4, we show that  $contract(G_{D''})$  is a minor of  $contract(G_{p'})$ . Here, by  $contract(G_{D''})$  we mean  $contract(G_{q_D})$  where  $q_D$  is D viewed as a CQ with answer variables  $\bar{c}$ . To this end, we first note that

(\*) if  $\{a, b\}$  is an edge in contract $(G_{D''})$ , then there are  $x_a, x_b$  such that  $h'(x_a) = a, h'(x_b) = b$ , and  $\{x_a, x_b\}$  is an edge in contract $(G_{p'})$ .

 $<sup>^{10}</sup>$ This can be made precise in the same way as in the proof of Lemma 9.2. We prefer to remain on the intuitive level here to not distract from the main proof.

Thus let  $\{a, b\}$  be an edge in  $\operatorname{contract}(G_{D''})$ . By construction of D'', this implies that there is an  $S \in \Gamma$  with  $\{a, b\} \subseteq S$ . Consequently, p' contains an atom  $R(\bar{y})$  such that there are  $x_a, x_b \in \bar{y} \cap \bar{x}$  with  $h'(x_a) = a$  and  $h'(x_b) = b$ , or p' has an  $\bar{x}$ -component S such that there are  $x_a, x_b \in S \cap \bar{x}$  with  $h'(x_a) = a$  and  $h'(x_b) = b$ . In both cases,  $\{x_a, x_b\}$  is an edge in  $\operatorname{contract}(G_{p'})$ . At this point, we are done if h' is injective on  $\bar{x}$  because then  $\operatorname{contract}(G_{D''})$  is a subgraph of  $\operatorname{contract}(G_{p'})$ . But this need not be the case. However, Point 1 above implies that if  $h'(x) = h'(x'), x, x' \in \bar{x}$ , then we find a sequence of variables  $x_1, \ldots, x_n$  from  $\bar{x}$  such that  $x_1 = x, x_n = x'$ , and  $x_i$  is connected to  $x_{i+1}$  in  $G_{p'}$  via a path whose non-end nodes are all from outside  $\bar{x}$ . Thus,  $\operatorname{contract}(G_{p'})$  contains edges  $\{x_1, x_2\}, \ldots, \{x_{n-1}, x_n\}$ . If we contract all these edges, we obtain a minor G of  $\operatorname{contract}(G_{p'})$  that h' maps injectively into  $\operatorname{contract}(G_{D''})$  and (\*) still holds. Thus  $\operatorname{contract}(G_{p'})$  as the latter contains G as a minor.

Now back to the main proof. From  $\vec{c}' \in P(D'')$ , we obtain  $\vec{c}' \in Q(D'')$ . Consequently, there is a homomorphism g from some CQ q' in q to  $ch_{\mathcal{O}}(D'')$  such that  $g(\bar{x}) = \vec{c}'$ . Let  $\hat{q}$ denote the collapsing of q' that is obtained by identifying  $y_1$  and  $y_2$  whenever  $g(y_1) = g(y_2)$ with at least one of  $y_1, y_2$  a quantified variable and adding  $x_1 = x_2$  whenever  $g(x_1) = g(x_2)$ and  $x_1, x_2$  are both answer variables. Note that g is an injective homomorphism from  $\hat{q}$ to  $ch_{\mathcal{O}}(D'')$ , that is, if  $g(y_1) = g(y_2)$  then  $y_1$  and  $y_2$  are answer variables and  $y_1 = y_2 \in \hat{q}$ . In what follows, we use this fact to show that the contract treewidth of  $\hat{q}$  is at most k. This finishes the proof as it means that  $\hat{q}$  is a CQ in  $q_k^{\text{CTW}}$ , and thus g witnesses that  $\vec{c}' \in Q_k^{\text{CTW}}(D'')$ . Points 2 and 5 above yield a homomorphism g' from D'' to D such that  $g'(\vec{c}') = \bar{c}$ . We can extend g' to a homomorphism from  $ch_{\mathcal{O}}(D'')$  to  $ch_{\mathcal{O}}(D)$ . It is thus easy to see that  $\bar{c} \in Q_k^{\text{CTW}}(D)$ .

Since g is injective and by definition of  $G_{\hat{q}}$ , it suffices to show that if  $\{x_1, x_2\}$  is an edge in contract $(G_{\hat{q}})$ , then  $\{g(x_1), g(x_2)\}$  is an edge in contract $(G_{D''})$ . Thus let  $\{x_1, x_2\}$  be an edge in contract $(G_{\hat{q}})$ .

First assume that  $\{x_1, x_2\}$  is an edge in the restriction of  $G_{\widehat{q}}$  to nodes  $\overline{x}$ . Then  $\widehat{q}$  contains an atom  $R(\overline{z})$  such that  $x_1, x_2 \in \overline{z}$ . This implies that  $g(x_1), g(x_2)$  occur in the fact  $R(g(\overline{z})) \in \mathsf{ch}_{\mathcal{O}}(D'')$ . Since  $\mathcal{O} \in \mathbb{G}$ , D'' must contain a fact in which both of  $g(x_1), g(x_2)$  occur. Thus,  $\{g(x_1), g(x_2)\}$  is an edge in  $\mathsf{contract}(G_{D''})$ .

Now assume that  $x_1, x_2$  co-occur in some  $\bar{x}$ -component of  $G_{\widehat{q}}$ . Then  $G_{\widehat{q}}$  contains a path  $z_1, \ldots, z_n$  such that  $z_1 = x_1, z_n = x_n$ , and  $z_2, \ldots, z_{n-1}$  are quantified variables. Let  $z_{i_1}, \ldots, z_{i_k}$  denote the subsequence of  $z_1, \ldots, z_n$  obtained by dropping all  $z_i$  such that  $g(z_i)$  is a constant that was introduced by the chase. Since  $\mathcal{O} \in \mathbb{G}$ ,  $\{z_{i_j}, z_{i_{j+1}}\}$  is an edge in  $G_{\mathcal{D}''}$  for  $1 \leq j < k$ . We know that  $g(z_{i_j}) \notin \vec{c}'$  for  $2 \leq j < k$  since if  $g(z_{i_j}) = a \in \vec{c}'$ , then  $z_{i_j}$  was identified with some  $x \in \bar{x}$  such that g(x) = a during the construction of  $\widehat{q}$ , in contrary to the fact that  $z_{i_j}$  is a quantified variable. It follows that  $\{g(x_1), g(x_2)\}$  is an edge in contract $(G_{\mathcal{D}''})$ .

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