On Bounded Positive Existential Rules

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Abstract. We consider the existential rule framework, which generalizes Horn description logics. We study and compare several boundedness notions in this framework. Our main result states that (strongly-) bounded rules are exactly those at the intersection of two well-known abstract classes of existential rules, namely *fes* (finite expansion sets, which ensure the finiteness of the core chase) and *fus* (finite unification sets, which correspond to UCQ-rewritable rules).

1 Introduction

Existential rules [6, 12, 21] are a fragment of first-order logic generalizing most ontological languages studied in ontology-mediated query answering (OMQA), in particular Horn description logics [13, 22, 23]. In the OMQA setting, databases (or fact bases) are added with an ontological layer, which allows to deduce new facts from incomplete datasources, thereby enriching answers to database queries.

As OMQA can be directly implemented on top of relational database systems, many research efforts have been devoted to make the paradigm efficient. At the core of the techniques developed for existential rules, and to some extent for Horn description logics, we find the two classical paradigms for processing rules, namely forward chaining and backward chaining. In the OMQA setting, both approaches are recast as ways of reducing the problem to a classical database query answering problem, by embedding the rules into the facts or into the query. Forward chaining is decomposed into a materialization step (applying the rules to the data, hence materializing inferences into the data) followed by the evaluation of the query against the enriched database. Backward chaining is decomposed into a query rewriting step (rewriting the query using the rules) followed by the evaluation of the rewritten query against the database, thereby leaving the data untouched.

Both approaches rely on a fixpoint operator to cope with rule semantics. Indeed, materialization should continue until the point where only redundant facts are added to the dataset, while rewriting should continue until the point where only redundant queries are added to the rewriting set. It is understood that both processes may not terminate since entailment with existential rules is undecidable (e.g., [14]). Deciding halting of these processes is undecidable as well [17, 5]. Following the terminology introduced in [5], we say that a set of existential rules is a *finite expansion set (fes)* if it ensures that a finite sound and complete materialization can be computed for any fact base, and a *finite unification set (fus)* if it ensures that any conjunctive query can be rewritten into a finite sound and complete set of conjunctive queries (such a set being seen as a union of conjunctive queries). As concrete examples of *fes* rules, one can cite (plain) datalog [1] and sets of rules satisfying various acyclicity conditions [16, 2]. Some prominent classes of *fus* rules are linear rules (which generalize some DL-Lite dialects [13, 12]), sticky rules [10] and more generally rules with the "backward shyness" property [25]. Note that [5] defines a third property ensuring decidability of OMQA, namely bounded-treewidth sets (which contains $\mathcal{EL}$ [23] and the family of guarded rules [9, 7]), however this class is out of the scope of this paper.

To *fes* (resp. *fus*) rules is naturally associated a finite breadth-first materialization (resp. query rewriting) process, whose maximal number of steps generally depends not only on the set of rules but also on the data (resp. on the input query). In contrast, bounded rules are exactly those rules that can be evaluated *without a fixpoint operator*. A set of rules is said to be *bounded* if breadth-first materialization computes all consequences from a knowledge base (composed of a fact base and the rules) in a predefined number of steps k. More precisely, there is k *independent* from any fact base, such that the materialization of any fact base at step $k' > k$ is equivalent to that obtained at step k. As relational database systems may lack a fixpoint operator (see for example MySQL), bounded rules form an interesting intersection point between databases and ontologies, because they can be seamlessly evaluated on any relational system, which is not the case in general.

The goal of this work is to further investigate the properties of bounded existential rules, in particular the precise relationships between *fes*, *fus* and bounded sets of rules.

Our contributions are more precisely the following:

1. We first define a breadth-first query rewriting technique which is precisely the dual of breadth-first materialization. Let $K = (F, \mathcal{R})$ be any knowledge base, where F is a fact base and $\mathcal{R}$ a set of existential rules, and let q be a (Boolean) conjunctive query. From earlier work on existential rules, we know that K entails q iff there is k (depending on $\mathcal{R}$ and F) such that F^k, the saturation of F at step k, entails q (e.g., [11, 4]); equivalently, K entails q iff there is k' (depending on $\mathcal{R}$ and q) such that F entails $Q_{k'}$, the set of rewritings of q obtained at step k' (see [20, 18] for practical algorithms). We define a variant of the breadth-first query rewriting technique from [20] that fulfills the following property: for any $i \geq 0$, F^i entails q iff F entails Q_i (Theorem 1), hence $k = k'$ in the above sentence.
2. We point out that boundedness can also be defined in terms of query rewriting instead of materialization, and using Theorem 1, we obtain the same bound for both definitions: for any k, it holds that F^k is equivalent to F^{k+1} for all F *iff* it holds that Q_k is equivalent to Q_{k+1} for all q (Theorem 2). We also show that the notion of "bounded-depth derivation property" introduced in [12] is equivalent to *fus*, and define variants of this property corresponding to *fes* and boundedness respectively.
3. By definition, every bounded set of rules is both *fes* and *fus*. The question of whether the reciprocal statement holds was open. We show that, indeed, bounded rules are exactly those at the intersection of *fes* and *fus* (Theorem 3).

2 Preliminaries

We consider a first-order setting with constants but no other function symbols. A *term* is either a constant or a variable. In the examples we will denote constants by letters at the beginning of the alphabet (a, b, ...,) and variables by letters at the end of the alphabet (v, w, x, y, z). An *atom* is of the form $\mathrm{p}(t_1, \ldots, t_k)$ where p is a predicate of arity k and the t_i are terms. Given an atom or set of atoms A, $\mathrm{vars}(A)$, $\mathrm{consts}(A)$ and $\mathrm{terms}(A)$ denote its set of variables, constants and terms, respectively. We denote by $\models$ the classical logical consequence and by $\equiv$ the logical equivalence. Given two sets of atoms A and A', a *homomorphism* h from A to A' is a substitution of $\mathrm{vars}(A)$ by $\mathrm{terms}(A')$ such that $h(A) \subseteq A'$. If there is a homomorphism h from A to A', we say that A *maps* to A' (by h), which is also denoted by $A \geq A'$. It is convenient to extend any substitution s to unchanged terms (we set $s(t) = t$ for all considered constants and unchanged variables).

A *fact* is an existentially closed conjunctions of atoms. We denote by F a *fact base*, that is a set of facts. Since a conjunction of facts is equivalent to a single fact, we also see a fact base as an existentially closed conjunction of atoms. A *Boolean conjunctive query* (in short CQ) is also an existentially closed conjunction of atoms. Next, fact bases and conjunctive queries will be seen as sets of atoms. The answer to a CQ q in a fact base F is *true* iff $F \models q$. It is well known that $F \models q$ iff $q \geq F$. A *union of conjunctive queries* (UCQ) $Q = \ q_1 \vee q_2 \ldots \vee q_n\ $ is seen as a set of CQs $Q = \{q_1, \ldots, q_n\}$. The answer to Q in F is *true* iff $F \models Q$, i.e., $F \models q_i$ for some $q_i \in Q$.

An *existential rule* $\ r = \forall \mathbf{x}, \mathbf{y}(B[\mathbf{x}, \mathbf{y}] \rightarrow \exists \mathbf{z}\, H[\mathbf{x}, \mathbf{z}])$ is a closed formula where B is a conjunction of atoms constituting the body of the rule, H is a conjunction of atoms for the head of the rule, $\mathbf{x}$ and $\mathbf{y}$ are sets of universally quantified variables, and $\mathbf{z}$ is the set of existentially quantified variables of the rule. The variables in $\mathbf{x}$, i.e., those shared by B and H, are called the *frontier variables* of the rule. In the following we will refer to a rule as a pair of sets of atoms (B, H), interpreting their common variables as the frontier. In the examples, we will use the simplified notation $B \rightarrow H$, for instance the rule $\forall x(q(x) \rightarrow \exists y\ (p(x, y) \wedge q(y)))$ will be written $q(x) \rightarrow p(x, y), q(y)$. A set of rules is denoted by $\mathcal{R}$. We implicitly assume that all rules employ disjoint sets of variables. A *knowledge base* (KB) $K = (F, \mathcal{R})$ is a pair where F is a fact base and $\mathcal{R}$ is a set of rules. The *conjunctive query entailment problem* consists in deciding for given KB K and CQ q whether $K \models q$ (where K is seen as the first order theory associated with $F \cup \mathcal{R}$). It has long been shown that this problem is undecidable (this follows e.g., from [14]).

A rule $r = (B, H)$ is *applicable* to a fact base F if there is a homomorphism h such that $h(B) \subseteq F$. The application of r to F with respect to a homomorphism h is denoted by $\alpha(F, r, h)$ and defined as $\alpha(F, r, h) = F \cup h^{\mathrm{safe}}(H)$ where h^{safe} is a *safe* extension of h to H, i.e., it substitutes existential variables from H with fresh variables (not used elsewhere). It holds that $F, \mathcal{R} \models q$ iff there is a fact base F' derived from F with rules in $\mathcal{R}$, [1] such that $F' \models q$.

[1] i.e., F' is obtained by a sequence of fact bases $F(= F_0), F_1, \ldots, F_k(= F')$ such that, for all $i > 0$, $F_i = \alpha(F_{i-1}, r_i, h)$ with $r_i \in \mathcal{R}$ and h a homomorphism from the body of r_i to F_{i-1}.

We now define fact materialization by (breadth-first) forward chaining, a useful tool, also known as saturation or (breadth-first) chase. [2] The *one-step saturation* of F with $\mathcal{R}$, denoted by $\alpha(F, \mathcal{R})$, is defined as $\alpha(F, \mathcal{R}) = F \cup_{(r,h)} h^{\text{safe}}(H)$ for all $r = (B, H) \in \mathcal{R}$ and h homomorphism from B to F. The *k-saturation* of F with $\mathcal{R}$, denoted by $\alpha^k(F, \mathcal{R})$, is inductively defined as follows: $\alpha^0(F, \mathcal{R}) = F$ and, for any $k > 0$, $\alpha^k(F, \mathcal{R}) = \alpha(\alpha^{k-1}(F, \mathcal{R}), \mathcal{R})$.

Next, when $\mathcal{R}$ is fixed, we will denote the set $\alpha^k(F, \mathcal{R})$ by F^k. Saturation is sound and complete, i.e., for all F, $\mathcal{R}$ and Q, $F, \mathcal{R} \models Q$ iff $F^k \models Q$ for some positive integer k (see e.g., [11, 4]). A set of rules $\mathcal{R}$ is said to be a *fes* (finite expansion set) if for all fact base F there exists a positive constant k such that $F^k \models F^{k+1}$ (hence $F^k \equiv F^{k+1}$) [6]. Note that k generally depends on F. It follows that when $\mathcal{R}$ is *fes*, the saturation process is finite, hence it can be used to decide if $F, \mathcal{R} \models Q$. The following example illustrate the *fes* property.

Example 1 (fes). Let $K = (F, \mathcal{R})$ with $F = \{p(a, b)\}$ and $\mathcal{R} = \{r : p(x, y) \rightarrow p(y, z), p(z, y)\}$. Then $F^0 = F$, $F^1 = F \cup \{p(b, z_0), p(z_0, b)\}$, $F^2 = F^1 \cup \{p(z_0, z_1),$ $p(z_1, z_0)$, $p(b, z_2), p(z_2, b)$, $p(b, z'_0), p(z'_0, b)\}$ (the rule applications corresponding to homomorphisms already found at the preceding step are written in gray font, next we will omit them). We have $F^2 \equiv F^1$ (note that there is no k such that $F^k = F^{k+1}$, even by considering only new homomorphisms at each step, which shows the importance of checking equivalence and not only equality). Actually it holds that $F^2 \equiv F^1$ *for any* F, hence $\mathcal{R}$ is *fes* (and even bounded, see Sect. 4). Let us consider $\mathcal{R}' = \{r : p(x, y) \rightarrow p(y, z)\}$. Then $F^0 = F$, $F^1 = F \cup \{p(b, z_0)\}$, $F^2 = F^1 \cup \{p(z_0, z_1), p(b, z_2)\}$ and so on. There is no k such that $F^k \equiv F^{k+1}$, hence $\mathcal{R}'$ is not *fes*.

Backward chaining is a dual approach to deciding conjunctive query entailment, which involves rewriting the input query using the rules. The key operation is unification between (a subset of) a query and (a subset of) a rule head, which requires particular care due to the presence of existential variables in the rules. For this reason, we use the notion of a piece-unifier (introduced in [6]). Given a subquery $q' \subseteq q$, we call *separating* variables of q' the variables occurring in both q' and $(q \setminus q')$; the other variables from q' are called non-separating. The definition of piece-unifier below ensures that, q' being the unified part of q, only non-separating variables from q' can be unified with an existential variable of the rule.

Definition 1 (Piece Unifier) *Let q be a query and $r = (B, H)$ a rule. A* piece-unifier *of q with r is a triple $\mu = (q', H', u)$ where $q' \neq \emptyset$, $q' \subseteq q$, $H' \subseteq H$, and u is a substitution of $T = \text{terms}(q' \cup H')$ by T such that (i) $u(q') = u(H')$ and (ii) for all existential variable $x \in \text{vars}(H')$ and $t \in T$, with $t \neq x$, if $u(x) = u(t)$, then t is a non-separating variable from q'.*

Given a CQ q, a rule $r = (B, H)$ and a piece-unifier $\mu = (q', H', u)$ the *direct rewriting* of q with r and μ, denoted by $\beta(q, r, \mu)$, is the CQ $u^{\text{safe}}(B) \cup u(q \setminus q')$, where u^{safe} is a safe extension of u to B substituting variables in $\text{vars}(B) \setminus \text{vars}(H')$ with fresh variables.

[2] Several chase variants have been defined, see the last section.

Example 2 (Piece Unifier). Let $r = r(x) \rightarrow p(x,y)$ and $q_1 = \{p(w,v), s(v)\}$. There is no piece-unifier of q_1 with r since, with $q'_1 = \{p(w,v)\}$, v is a separating variable of q'_1, hence cannot be unified with the existential variable y. Let $q_2 = \{s(z), p(z,v), p(w,v), t(w)\}$. The triple $\mu = (q', H', u)$ with $q' = \{p(z,v), p(w,v)\}$, $H' = \{p(x,y)\}$ and $u = \{x \mapsto z, y \mapsto v, w \mapsto z\}$ is a piece-unifier of q_2 with r, which yields the direct rewriting $\{r(z), s(z), t(z)\}$.

It holds that $F, \mathcal{R} \models q$ iff there is a rewriting q' of q with rules in $\mathcal{R}$, [3] such that $F \models q'$. A set of rewritings Q of q (with $\mathcal{R}$) is said to be *sound* and *complete* if for any F it holds that $F, \mathcal{R} \models q$ iff there is $q' \in Q$ such that $F \models q'$. When Q is finite it can be seen as a UCQ, hence the previous condition can then be recast as follows: $F, \mathcal{R} \models q$ iff $F \models Q$. The set $\mathcal{R}$ is said to be *fus* (finite unification set) if for any q, there is a finite sound and complete set of rewritings of q with $\mathcal{R}$ [6, 20].

Similarly in spirit to saturation, one can consider breadth-first query rewriting: starting from the UCQ $Q = \{q\}$, at each step we compute all the direct rewritings of CQs in the current UCQ. Formally: the one-step rewriting of a UCQ Q with $\mathcal{R}$ is $\beta(Q, \mathcal{R}) = Q \cup_{(q,r,\mu)} \{\beta(q, r, \mu)\}$ where $q \in Q$, $r \in \mathcal{R}$ and μ is a piece-unifier of q with r. Then, the *(breadth-first) k-rewriting* of Q with $\mathcal{R}$, denoted by $\beta_k(Q, \mathcal{R})$, is inductively defined as follows: $\beta_0(Q, \mathcal{R}) = Q$, and for all $k > 0$, $\beta_k(Q, \mathcal{R}) = \beta(\beta_{k-1}(Q, \mathcal{R}), \mathcal{R})$.

It holds that $F, \mathcal{R} \models q$ iff $F \models \beta_k(\{q\}, \mathcal{R})$ for some positive integer k (follows from [4]). This property yields an alternative characterization of *fus*: a set of rules is *fus* iff for all q, there is k such that $\beta_k(\{q\}, \mathcal{R}) \equiv \beta_{k+1}(\{q\}, \mathcal{R})$. [4]

Example 3 (fus).

Let $r = p(x,y), p(y,z) \rightarrow p(z,t)$. Let $q' = \{p(v,a)\}$, where a is a constant: since t is an existential variable, there is no piece-unifier of q' with r.
Let $q'' = \{p(a,v)\}$.
$\beta_1(\{q''\}, \{r\}) = \{q''\} \cup \{\{p(x_0,y_0), p(y_0,a)\}\}$;
$\beta_2(\{q''\}, \{r\}) = \beta_1(\{q''\}, \{r\}) \cup \{\{p(x'_0,y'_0), p(y'_0,a)\}\}$, where the last CQ corresponds to the piece-unifier already found in the preceding step. Hence, $\beta_2(\{q''\}, \{r\}) = \beta_1(\{q''\}, \{r\})$ if we restrict the computation to new piece-unifiers.
Finally, let $q = \{p(v,w)\}$.
$\beta_1(\{q\}, \{r\}) = \{q\} \cup \{q_1 = \{p(x_0,y_0), p(y_0,v)\}\}$.
$\beta_2(\{q\}, \{r\}) = \beta_1(\{q\}, \{r\}) \cup \{\{p(x_1,y_1), p(y_1,y_0), p(x_0,y_0)\}\}$ (we consider only new piece-unifiers). Since existential variables can only be unified with non-separating variables, there is only one new piece-unifier $(\{p(x_0,v)\}, \{p(z,t)\}, \{z \mapsto y_0, t \mapsto v\})$, which yields q_1.
$\beta_3(\{q\}, \{r\}) = \beta_2(\{q\}, \{r\}) \cup \{\{p(x_2,y_2), p(y_2,y_1), p(x_1,y_1)\}\}$, where the new the piece-unifier is $(\{p(x_0,y_0), p(y_1,y_0)\}, \{p(z,t)\}, \{z \mapsto y_1, x_0 \mapsto y_1, t \mapsto y_0\})$. And so on. There is no k such that $\beta_k = \beta_{k+1}$ (up to bijective variable renaming), however any UCQ β_i is equivalent to q. As these examples suggest it, $\{r\}$ is indeed *fus*.

[3] i.e., q' is obtained by a sequence of direct rewritings $q(= q_0), q_1, \ldots, q_k(= q')$ such that, for all $i > 0$, $q_i = \beta(q_{i-1}, r_i, \mu)$ with $r_i \in \mathcal{R}$ and μ a piece-unifier of q_{i-1} with r_i.

[4] The breadth-first rewriting algorithm in [20] builds $\beta(\beta_i(Q, \mathcal{R}), \mathcal{R})$ by considering only queries that are not contained in a query from $\beta_i(Q, \mathcal{R})$; in this case the *fus* condition becomes: there is k such that $\beta_{k+1}(Q, \mathcal{R}) = \beta_k(Q, \mathcal{R})$.

Note that there is k such that $F \models \beta_k(\{q\},\mathcal{R})$ if and only if there is k' such that $\alpha^{k'}(F,\mathcal{R}) \models q$. However, the above breadth-first rewriting is not exactly the dual of breadth-first saturation, in the sense that $\alpha(F,\mathcal{R}) \models q$ does not imply $F \models \beta(\{q\},\mathcal{R})$. In other words, a single step of breadth-first rewriting is not able to "simulate" a step of saturation. Let us illustrate this observation with a simple example.

Example 4 (Saturation vs rewriting step). Let $K = (F,\mathcal{R})$ with $F = \{p_0(a), q_0(a)\}$ and $\mathcal{R} = \{r_p : p_0(x) \rightarrow p_1(x); r_q : q_0(x) \rightarrow q_1(x)\}$. Let $q = \{p_1(u), q_1(u)\}$. A single saturation step $\alpha(F,\mathcal{R}) = \{p_0(a), q_0(a), p_1(a), q_1(a)\}$ allows to entail q. However, a single rewriting step $\beta_1(\{q\},\mathcal{R}) = \{\{p_1(u), q_1(u)\}, \{p_0(u), q_1(u)\}, \{p_1(u), q_0(u)\}\}$ does not allow to prove that $K \models q$, i.e., $F \not\models \beta_1(\{q\},\mathcal{R})$. The trouble is that each direct rewriting is performed with respect to a single rule, hence the desired CQ $\{p_0(u), q_0(u)\}$, which requires to rewrite q with both r_p and r_q, is obtained only at the second rewriting step (from $\{p_0(u), q_1(u)\}$ or from $\{p_1(u), q_0(u)\}$).

3 A New Breadth-First Query Rewriting

In order to obtain the precise dual of saturation, we define another breadth-first rewriting mechanism able to unify a CQ with several rules from $\mathcal{R}$ at once. Instead of a piece-unifier, we consider an "aggregated unifier" (as introduced in [19] for algorithmic purposes), which aggregates several piece-unifiers of a CQ with rules from $\mathcal{R}$, provided that these piece-unifers are compatible (briefly, they involve disjoint subsets of the query and unify common variables in a way that does not lead to unify different constants together). To avoid technical developments, we will consider here an alternative way of defining exactly the same kind of rewriting by modifying the set of rules instead of the unifier (this alternative definition is not practically relevant but it is suitable for our study).

Let $\mathcal{R}' = \{r_1, \ldots, r_l\}$ be a set of rules with each $r_i = (B_i, H_i)$. We recall that distinct rules have disjoint sets of variables. The aggregated rule assigned to $\mathcal{R}'$, denoted by $r_1 \diamond \ldots \diamond r_l$, is defined as $B_1 \wedge \ldots \wedge B_l \rightarrow H_1 \wedge \ldots H_l$. Let $\mathcal{R}^\diamond$ be the (infinite) set of aggregated rules assigned to multisubsets of $\mathcal{R}$ (i.e., an aggregated rule may involve several "copies" of the same rule from $\mathcal{R}$, with a safe renaming of variables in each copy).

Then, for any UCQ Q, $\beta^\diamond(Q,\mathcal{R}) = Q \cup_{(q,r,\mu)} \{\beta(q,r,\mu)\}$, where $q \in Q$, $r = r_1 \diamond \ldots \diamond r_l \in \mathcal{R}^\diamond$ with $l \leq |q|$, and μ is a piece-unifier of q with r. We denote by $\beta^\diamond_k(Q,\mathcal{R})$ the associated breadth-first k-rewriting. [5]

Example 5. Consider again Ex. 4. We have $\beta^\diamond_1(\{q\},\mathcal{R}) = \beta_1(\{q\},\mathcal{R}) \cup \{\{p_0(u), q_0(u)\}\}$, where the additional query is obtained by unifying q with the aggregated rule $r_1 \diamond r_2 = p_0(x_0), q_0(x_1) \rightarrow p_1(x_0), q_1(x_1)$.

We now prove that the new breadth-first rewriting fulfills the desired properties.

Lemma 1 *For all $F,\mathcal{R}$ and q, it holds that $\alpha(F,\mathcal{R}) \models q$ iff $F \models \beta^\diamond(\{q\},\mathcal{R})$.*

[5] We could state $\beta^\diamond(Q,\mathcal{R}) = \beta(Q,\mathcal{R}^\diamond)$, however it must be clear that, for each CQ, only a finite subset of $\mathcal{R}^\diamond$ needs to be considered.

Proof:(Sketch) ($\Rightarrow$) Let $F^1 = \alpha(F, \mathcal{R})$. As $F^1 \models q$ there is h such that $h(q) \subseteq F^1$. Let q_0 be the largest subset of q such that $h(q_0) \subseteq F$ and $\{q_1, \ldots, q_l\}$ be the partition of $q \setminus q_0$ such that each q_i ($0 < i \leq l$) maps to the atoms produced by the application of a rule $r_i = (B_i, H_i) \in \mathcal{R}$ to F with a homomorphism h_i, i.e., $h(q_i) \subseteq h_i^{\mathrm{safe}}(H_i)$ (and $F \cup h_1^{\mathrm{safe}}(H_1) \cup \ldots \cup h_l^{\mathrm{safe}}(H_l) \subseteq F^1$). For each $i > 0$, let $H_i' \subseteq H_i$ denote the useful part of H_i, i.e., $h(q_i) = h_i^{\mathrm{safe}}(H_i')$. If $q_0 = q$, i.e., $F \models q$, then $F \models \beta^\diamond(\{q\}, \mathcal{R})$ since $q \in \beta^\diamond(\{q\}, \mathcal{R})$. Otherwise, let $r^\diamond = r_1 \diamond \ldots \diamond r_l$ and μ be the piece-unifier of q with $r^\diamond$ naturally associated with the homomorphisms h and $h_1 \cup \ldots \cup h_l$ (i.e., $\mu = (q_1 \cup \ldots \cup q_l, H_1' \cup \ldots \cup H_l', u)$ where for all terms e and e' in the domain of u, $u(e) = u(e')$ iff $(h \cup h_1^{\mathrm{safe}} \cup \ldots \cup h_l^{\mathrm{safe}})(e) = (h \cup h_1^{\mathrm{safe}} \cup \ldots \cup h_l^{\mathrm{safe}})(e')$). We easily check that $F \models \beta(q, r^\diamond, \mu)$. Since $\beta(q, r^\diamond, \mu) \in \beta^\diamond(\{q\}, \mathcal{R})$, we obtain that $F \models \beta^\diamond(\{q\}, \mathcal{R})$.

($\Leftarrow$) If $F \models q$ then $\alpha(F, \mathcal{R}) \models q$. Otherwise, we know there is $q_1 \neq q$ in $\beta_1^\diamond(\{q\}, \mathcal{R})$ s.t. $F \models q_1$ where q_1 is obtained by rewriting $q' \subseteq q$ with an aggregated rule $r^\diamond = r_1 \diamond \ldots \diamond r_l$ and a piece-unifier $(q', H_1' \cup \ldots \cup H_l', u)$. Let h' be a homomorphism from q_1 to F. For each $r_i = (B_i, H_i)$ composing $r^\diamond$, $h' \circ u^{\mathrm{safe}}$ is a homomorphism from B_i to F. Hence, $(h' \circ u)^{\mathrm{safe}}(H_i) \subseteq \alpha(F, \mathcal{R})$. We build the following homomorphism h from q to $\alpha(F, \mathcal{R})$: for all $x \in \mathrm{vars}(q)$, if $x \in \mathrm{vars}(q) \setminus \mathrm{vars}(q')$ then $h(x) = h'(x)$, otherwise, let any $e \in H_i'$ such that $u(x) = u(e)$, then $h(x) = (h' \circ u^{\mathrm{safe}})^{\mathrm{safe}}(e)$.

□

Theorem 1. *For all $F, q, \mathcal{R}$ and $k \geq 0$, it holds that $\alpha^k(F, \mathcal{R}) \models q$ iff $F \models \beta_k^\diamond(\{q\}, \mathcal{R})$*

Proof: The proof is by induction on k. For $k = 0$, the property is trivially true. Assume the property holds for any $k < n$. First note that, for any $i \geq 1$, $\alpha^i(F, \mathcal{R}) = \alpha^{i-1}(\alpha(F, \mathcal{R}), \mathcal{R})$ and $\beta_i^\diamond(\{q\}, \mathcal{R}) = \beta_{i-1}^\diamond(\beta^\diamond(\{q\}, \mathcal{R}), \mathcal{R})$, which directly follows from the definitions. We have $\alpha^n(F, \mathcal{R}) \models q$ iff
$\alpha^{n-1}(\alpha(F, \mathcal{R}), \mathcal{R}) \models q$ iff
$\alpha(F, \mathcal{R}) \models \beta_{n-1}^\diamond(\{q\}, \mathcal{R})$ (by induction hypothesis) iff
$F \models \beta^\diamond(\beta_{n-1}^\diamond(\{q\}, \mathcal{R}), \mathcal{R})$ (by Lemma 1) iff
$F \models \beta_n^\diamond(\{q\}, \mathcal{R})$.
Hence, $\alpha^k(F, \mathcal{R}) \models q$ iff $F \models \beta_k^\diamond(\{q\}, \mathcal{R})$ holds for any $k \geq 0$. □

This correspondence between α^k and $\beta_k^\diamond$ allows us to rely on the soundness and completeness of breadth-first forward chaining to establish the soundness and completeness of breadth-first rewriting:

Corollary 1. *It holds that $F, \mathcal{R} \models q$ iff $F \models \beta_k^\diamond(\{q\}, \mathcal{R})$ for some positive integer k.*

Breadth-first rewriting yields an alternative definition of *fus*.

Proposition 1 *A set of rules $\mathcal{R}$ is* fus *iff for all query q there is a positive constant k such that $\beta_k^\diamond(\{q\}, \mathcal{R}) \equiv \beta_{k+1}^\diamond(\{q\}, \mathcal{R})$.*

From now on, for a UCQ Q and a fixed set of rules $\mathcal{R}$, we will denote the set $\beta_k^\diamond(Q, \mathcal{R})$ simply by Q_k.

4 Several Notions of Boundedness

We now define bounded rules and clarify their relationships with other properties found in the literature. Two meaningful notions of boundedness can be provided, with the bound being based on fact saturation or on query rewriting.

Definition 2 *A set of existential rules $\mathcal{R}$ is*

(saturation-bounded) if there exists $k \in \mathbb{N}$ such that for all F, $F^k \equiv F^{k+1}$.

(rewriting-bounded) if there exists $k \in \mathbb{N}$ such that for all Q, $Q_k \equiv Q_{k+1}$.

We first show that these two notions precisely coincide.

Theorem 2. *Any set of existential rules $\mathcal{R}$ is saturation-bounded iff it is rewriting-bounded. Moreover, the bound is the same, i.e., for all F and all Q, for all k, $F^k \equiv F^{k+1}$ iff $Q_k \equiv Q_{k+1}$.*

Proof: ($\Rightarrow$) Assume that $\mathcal{R}$ is saturation-bounded and let k be the bound. Then for all Q and F it holds that $F, \mathcal{R} \models Q$ iff $F^k \models Q$. Let q be any query in Q_{k+1}. Since $q \models Q_{k+1}$, by soundness of rewriting, it holds that $q, \mathcal{R} \models Q$; since $\mathcal{R}$ is saturation-bounded, $\{q\}^k \models Q$ hence, by Th. 1, $q \models Q_k$. Since this holds for any query $q \in Q_{k+1}$, we have $Q_{k+1} \models Q_k$. Furthermore, by definition, $Q_k \models Q_{k+1}$. Thus $Q_k \equiv Q_{k+1}$.

($\Leftarrow$) Assume that $\mathcal{R}$ is rewriting-bounded and let k be the bound. Then for all Q and F it holds that $F, \mathcal{R} \models Q$ iff $F \models Q_k$. By soundness of forward chaining, it holds that $F, \mathcal{R} \models F^{k+1}$; since $\mathcal{R}$ is rewriting-bounded, $F \models (F^{k+1})_k$ hence, by Th. 1, $F^k \models F^{k+1}$. Furthermore, by definition, $F^{k+1} \models F^k$. Thus $F^k \equiv F^{k+1}$. $\square$

In light of this, next we will simply say *bounded* rules. In [12], Calì et al. introduced the notion of *bounded-depth derivation property* for existential rules, for which the number of saturation steps is bounded for all query (in short, Q-BDDP). We define the analogous of the bounded-depth derivation property for facts (F-BDDP), as well as a natural property issued from both from (Q-BDDP) and (F-BDDP), we call strong bounded-depth derivation property (strong BDDP). We show that these three properties coincide with the classes *fus*, *fes* and *bounded*.

Definition 3 (Bounded-Derivation Properties) *Let $\mathcal{R}$ be a set of existential rules. Then, $\mathcal{R}$ enjoys the property*

(F-BDD) if for all F there is $k \in \mathbb{N}$ such that for all Q: $F, \mathcal{R} \models Q$ iff $F^k \models Q$

(Q-BDD) if for all Q there is $k \in \mathbb{N}$ such that for all F: $F, \mathcal{R} \models Q$ iff $F^k \models Q$

(strong BDD) if there is $k \in \mathbb{N}$ such that for all F and Q: $F, \mathcal{R} \models Q$ iff $F^k \models Q$.

We now show that these notions respectively correspond to *fes*, *fus* and boundedness. [6]

Proposition 2 *Any set of existential rules is* fes *iff it has the F-BDD Property.*

[6] The three following propositions were first proven by J.-F. Baget and M.-L. Mugnier and presented in a seminar at Oxford University in December 2012.

Proof: ($\Rightarrow$) Let $\mathcal{R}$ be *fes*: for all F, there is k such that $F^k \equiv F^{k+1}$. By soundness and completeness of forward chaining, for any Q we have $F, \mathcal{R} \models Q$ iff there is n such that $F^n \models Q$. For any F and such n, it holds that $F^k \models F^n$. Hence, $F^k \models Q$.

($\Leftarrow$) Assume $\mathcal{R}$ has the F-BDD Property and set $Q = \{F^{k+1}\}$ (where k is the bound of the F-BDD Property). We thus have $F, \mathcal{R} \models F^{k+1}$ iff $F^k \models F^{k+1}$. Forward chaining is sound, so $F, \mathcal{R} \models F^{k+1}$. Hence $F^k \models F^{k+1}$. By definition, $F^{k+1} \models F^k$. Therefore, $F^k \equiv F^{k+1}$. □

Proposition 3 *Any set of existential rules is* fus *iff it has the Q-BDD Property.*

Proof: ($\Rightarrow$) Let $\mathcal{R}$ be *fus*: for all Q, there is k such that $Q^k \equiv Q^{k+1}$. By soundness and completeness of breadth-first rewriting (Corollary 1), for any F, we have $F, \mathcal{R} \models Q$ iff $F \models Q_k$. Equivalently, by Th. 1, $F^k \models Q$. ($\Leftarrow$) Assume $\mathcal{R}$ has the Q-BDD Property. For any $q \in Q_{k+1}$ (where k is the bound of the Q-BDD Property), let us set $F = q$: we have $q, \mathcal{R} \models Q$ iff $(q)^k \models Q$. Breadth-first rewriting is sound, so $q, \mathcal{R} \models Q$. Hence $q \models Q_k$. Since this holds for any $q \in Q_{k+1}$, we have $Q_{k+1} \models Q_k$. Since Q_k is included in Q_{k+1}, we also have $Q_k \models Q_{k+1}$. Therefore, $Q_k \equiv Q_{k+1}$. □

Proposition 4 *Any set of existential rules is bounded iff it has the strong BDD Property.*

Proof: The proof goes like that of Prop. 2.

($\Rightarrow$) Let $\mathcal{R}$ be saturation-bounded and let k such that for all F, $F^k \equiv F^{k+1}$. By soundness and completeness of forward chaining, for any F and Q, we have $F, \mathcal{R} \models Q$ iff $F^k \models Q$.

($\Leftarrow$) Assume $\mathcal{R}$ has the strong BDD Property and set $Q = \{F^{k+1}\}$ (where k is the bound of the strong BDD Property). We thus have $F, \mathcal{R} \models F^{k+1}$ iff $F^k \models F^{k+1}$. Forward chaining is sound, so $F, \mathcal{R} \models F^{k+1}$. Hence $F^k \models F^{k+1}$. By definition, $F^{k+1} \models F^k$. Therefore, $F^k \equiv F^{k+1}$. □

5 Boundedness = fes ∩ fus

We now prove that bounded rules are exactly those at the intersection of *fes* and *fus* classes.

Theorem 3. *$\mathcal{R}$ is* fes *and* fus *iff $\mathcal{R}$ is bounded.*

One direction of the proof ($\Leftarrow$) is straightforward, and follows by Prop.s 2 and 3, simply picking the k of the bound. We dedicate the remaining of this section to the formal development of the other direction. We first consider the set of all objects of the form $(\bar{B}, \bar{H})$ where $\bar{B}$ is a rewriting of a rule body in $\mathcal{R}$ and $\bar{H}$ is the saturation of $\bar{B}$ with $\mathcal{R}$. When $\mathcal{R}$ is *fes*, such objects correspond to rules (i.e., each $\bar{H}$ can be made finite). When moreover $\mathcal{R}$ is *fus*, the set of all rewritings to be considered is finite, hence the set of all rules of interest is finite.

Definition 4 (Rule Completion) *Let $\mathcal{R} = \{r_1, \ldots, r_n\}$ be a* fes *and* fus *set of rules of the form $r_i = (B_i, H_i)$. We define the set $\mathcal{C}_{\mathcal{R}}$ as follows:*

1. *For any* $r_i = (B_i, H_i)$*, let* k_i *be the smallest integer such that* $\beta^{\diamond}_{k_i}(B_i, \mathcal{R}) \equiv \beta^{\diamond}_{k_i+1}(B_i, \mathcal{R})$ *(such a* k_i *exists since* $\mathcal{R}$ *is* fus*).*
2. *For any* $q_{i_j} \in \beta^{\diamond}_{k_i}(B_i, \mathcal{R})$*, let* k_{i_j} *be the smallest integer such that* $\alpha^{k_{i_j}}(q_{i_j}, \mathcal{R}) \equiv \alpha^{k_{i_j}+1}(q_{i_j}, \mathcal{R})$ *(such a* k_{i_j} *exists since* $\mathcal{R}$ *is* fes*).*
3. *Then:*

$$\mathcal{C}_{\mathcal{R}} = \{(\bar{B}, \bar{H}) \mid r_i = (B_i, H_i) \in \mathcal{R},\ \bar{B} \in \beta^{\diamond}_{k_i}(B_i, \mathcal{R}), \bar{H} = \alpha^{k_{i_j}}(\bar{B}, \mathcal{R})\ \}$$

The *bound* associated with $\mathcal{R}$ is $d_{\mathcal{R}} = max_{r_i \in \mathcal{R}, q_{i_j} \in \beta^{\diamond}_{k_i}(B_i, \mathcal{R})}(k_{i_j})$.

Note that $\mathcal{C}_{\mathcal{R}}$ is finite and unique (up to bijective variable renaming). Most importantly, its size depends solely on $\mathcal{R}$.

Proposition 5 *For any* fes *and* fus *set of rules* $\mathcal{R}$*, it holds that* $\mathcal{C}_{\mathcal{R}} \equiv \mathcal{R}$*.*

Proof: The direction $\mathcal{C}_{\mathcal{R}} \models \mathcal{R}$ holds since, for each rule $r_i = (B_i, H_i) \in \mathcal{R}$, $B_i \in \beta^{\diamond}_{k_i}(B_i, \mathcal{R})$, hence there is a rule $\bar{r} = (\bar{B}, \bar{H}) \in \mathcal{C}_{\mathcal{R}}$ with $B_i = \bar{B}$ and $H_i \subseteq \bar{H}$. Direction $\mathcal{R} \models \mathcal{C}_{\mathcal{R}}$ follows from the soundness and completeness of saturation. Indeed, for each rule $(\bar{B}, \bar{H}) \in \mathcal{C}_{\mathcal{R}}$, let $(\bar{B}', \bar{H}')$ be obtained by replacing each frontier variable with a distinct fresh constant (i.e., that does not occur in $\mathcal{R}$). By definition of $\mathcal{C}_{\mathcal{R}}$, we have $\bar{B}', \mathcal{R} \models \bar{H}'$, and equivalently $\mathcal{R} \models \bar{B} \rightarrow \bar{H}$. □

We now show that each saturation step with $\mathcal{C}_{\mathcal{R}}$ can be computed by a bounded number of saturation steps with $\mathcal{R}$ (again with a bound independent from any fact base, Prop. 6). Next, we will show that a single saturation step with $\mathcal{C}_{\mathcal{R}}$ is actually sufficient to saturate any fact base (Prop. 7), therefore it is equivalent to a bounded number of saturation steps with $\mathcal{R}$.

Proposition 6 *Let* $\mathcal{R}$ *be* fes *and* fus *and* $\mathcal{C}_{\mathcal{R}}$ *be the associated completion set. Then: for any fact base* F*,* $\alpha^{d_{\mathcal{R}}}(F, \mathcal{R}) \models \alpha(F, \mathcal{C}_{\mathcal{R}})$ *(where* $d_{\mathcal{R}}$ *is the bound introduced in Def. 4).*

Proof: (Sketch) Let $F' = \alpha^{d_{\mathcal{R}}}(F, \mathcal{R})$. We show that for each rule $\bar{r} = (\bar{B}, \bar{H}) \in \mathcal{C}_{\mathcal{R}}$ and each homomorphism h from $\bar{B}$ to F, $F' \models \alpha(F, \bar{r}, h)$ holds, which suffices to prove that $F' \models \alpha(F, \mathcal{C}_{\mathcal{R}})$ since all rules are applied "in parallel" in a single saturation step. Consider the sequence S of rule applications leading from $\bar{B}$ to $\bar{H}$. The choice of $d_{\mathcal{R}}$ implies that $\alpha^{d_{\mathcal{R}}}(\bar{B}, \mathcal{R}) \equiv \bar{H}$. Let h from $\bar{B}$ to F. The sequence S can be applied "similarly" to F (i.e., each homomorphism h_i associated with a rule application is replaced by $h \circ h_i$), yielding $S(F)$ with $S(F) \models h(\bar{H})$. Since $\bar{H}$ is obtained in at most $d_{\mathcal{R}}$ breadth-first steps, this is also true for $S(F)$, hence $F' \models S(F)$. Since $F \subseteq F'$, we obtain $F' \models F \cup h^{\text{safe}}(\bar{H}) = \alpha(F, \bar{r}, h)$.

□

Proposition 7 *Let* $\mathcal{R}$ *be a set of rules both* fes *and* fus*. For any fact base* F*, it holds that* $\alpha(F, \mathcal{C}_{\mathcal{R}}) \equiv \alpha^k(F, \mathcal{C}_{\mathcal{R}})$ *for all* $k \geq 1$*.*

Proof: (Sketch) We focus on proving that $\alpha(F, \mathcal{C}_{\mathcal{R}}) \models \alpha(\alpha(F, \mathcal{C}_{\mathcal{R}}), \mathcal{R})$ which suffices to derive the thesis. Indeed, we know that for any F' and $\mathcal{R}'$ if $F' \models \alpha(F', \mathcal{R}')$ then

$F' \models \alpha^k(F', \mathcal{R}')$, for all $k \in \mathbb{N}$. Hence $\alpha(F, \mathcal{C}_\mathcal{R}) \equiv \alpha^k(\alpha(F, \mathcal{C}_\mathcal{R}), \mathcal{R})$, in particular for $k = d_\mathcal{R}$. Moreover, as $\mathcal{R}$ is both *fes* and *fus* by Prop. 6 we have that $\alpha(F, \mathcal{C}_\mathcal{R}) \models \alpha(\alpha(F, \mathcal{C}_\mathcal{R}), \mathcal{C}_\mathcal{R})$.

Let $r = (B, H)$ be any rule of $\mathcal{R}$. If r is applicable to $\alpha(F, \mathcal{C}_\mathcal{R})$ with a homomorphism h, then $h(B) \subseteq \alpha(F, \mathcal{C}_\mathcal{R})$. By Prop. 6 we thus have $\alpha^{d_\mathcal{R}}(F, \mathcal{R}) \models h(B)$. By Th. 1, we get that $F \models \beta^\diamond_{d_\mathcal{R}}(\{h(B)\}, \mathcal{R})$, so there exists $h(B)_{rew} \in \beta^\diamond_{d_\mathcal{R}}(\{h(B)\}, \mathcal{R})$ such that $F \models h(B)_{rew}$. Any rewriting sequence from $h(B)$ to $h(B)_{rew}$ can be performed "similarly" from B yielding $B_{rew} \in \beta^\diamond_{d_\mathcal{R}}(\{B\}, \mathcal{R})$ with $B_{rew} \geq h(B)_{rew}$. Besides, by definition of $\mathcal{C}_\mathcal{R}$, we know there exists $\bar{r} = (\bar{B}, \bar{H}) \in \mathcal{C}_\mathcal{R}$ with $\bar{B} = B_{rew}$ and $\bar{H} \equiv \alpha^{d_\mathcal{R}}(B_{rew}, \mathcal{R})$. We show that any derivation sequence from $\bar{B}$ to $\bar{H}$ can be applied to $h(B)_{rew}$ to entail $h(B)$. Since $r = (B, H) \in \mathcal{R}$ and this sequence is applied until saturation, $h(H)$ is also entailed. We conclude that $\alpha(F, \mathcal{C}_\mathcal{R}) \models h(H)$.

□

Proof: [**Proof of Th. 3**] We now prove that if $\mathcal{R}$ is *fes* and *fus* then it is bounded.

For any fact base F and any CQ q, $F, \mathcal{R} \models q$ iff $F, \mathcal{C}_\mathcal{R} \models q$ (Prop. 5). From Prop. 7, $F, \mathcal{C}_\mathcal{R} \models q$ iff $\alpha(F, \mathcal{C}_\mathcal{R}) \models q$. Hence, $F, \mathcal{R} \models q$ iff $\alpha(F, \mathcal{C}_\mathcal{R}) \models q$. It remains to show that there is k independent from F and q such that $\alpha^k(F, \mathcal{R}) \equiv \alpha(F, \mathcal{C}_\mathcal{R})$. From Prop. 6, we have a constant k ($k = d_\mathcal{R}$) independent from F and q such that $\alpha^k(F, \mathcal{R}) \models \alpha(F, \mathcal{C}_\mathcal{R})$; moreover, since $F, \mathcal{R} \models \alpha^k(F, \mathcal{R})$ for any k, we have $\alpha(F, \mathcal{C}_\mathcal{R}) \models \alpha^k(F, \mathcal{R})$. We conclude that $\mathcal{R}$ is bounded. □

6 Concluding Remarks

In this paper, we provide several results that clarify the relationships between fundamental properties of existential rule sets, namely *fes*, *fus* and boundedness. The main result is that bounded rule sets are exactly those that are both *fes* and *fus*.

Recognizing if a set of rules is bounded is a difficult problem, which is already undecidable for plain datalog [1], hence for many *fes* classes of existential rules. A significant exception are monadic datalog programs, for which boundedness is recognizable [15]. An open question is whether boundedness is recognizable for specific classes of existential rules, in particular those known to be *fus*. Whether restricting predicate arity to two could have an impact on the problem decidability is also an interesting issue.

Besides, the halting condition for the saturation process considered here relies on logical equivalence (i.e., $F^k \equiv F^{k+1}$). This condition corresponds exactly to the halting of the chase variant known as the *core* chase [17]. Other chase variants have been proposed in the literature, in particular the restricted chase [8], the skolem chase [24] and the oblivious chase [9], which are known to halt in (increasingly) fewer cases (see, e.g., [3] for examples illustrating the differences between these mechanisms). With each of these variants could be associated a different boundedness notion. Note however that all the chase variants collapse on rules without existential variables (i.e., plain datalog), hence the undecidability of boundedness recognition in plain datalog applies to all these potential variants of boundedness.

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