Querying Class-Relationship Logic in a Metalogic Framework

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Abstract. We introduce a class relationship logic for stating various forms of logical relationships between classes. This logic is intended for ontologies and knowledge bases and combinations thereof. Reasoning and querying is conducted in the DATALOG logical language, which serves as an embracing decidable and tractable metalogic.

Keywords: Querying knowledge bases and ontologies. DATALOG as metalogic. Analytic vs. synthetic knowledge.

1 Introduction

We address a two-level logic for ontologies and knowledge bases dealing with relationships between classes. The proposal is distinguished by encoding of the applied class relationship logic utilizing DATALOG as a formal metalogic.

The proposed class-relationship logic, CRL, offers predicate logical sentences with quantifiers stating relationships between classes. We identify four elementary relationship forms corresponding to the four pairs of quantifier prefixes formed by $\forall$ and $\exists$.

The predominant form is the following relationship between classes c and d

$$\forall x(c(x) \to \exists y(r(x, y) \land d(y)))$$

comprising class inclusion and partonomic ontologies as special cases. These sentences are shaped into a *prima facie* atomic, variable free form, which hides the underlying quantifiers. The entire setup is termed CRL-META.

The embracing DATALOG metalogic enables controlled reasoning of CRL (including, notably, inheritance) and querying of the stated relationships. Thus in CRL-META one may ask queries about for instance which logical relationships there exist between given classes. The DATALOG level may readily be implemented on top of a relational database platform, thereby taking advantage of existing relational query languages with their capabilities for efficient access to large knowledge bases with the CRL level being stored as data.

CRL-META is intended in particular for applications where ontologies are to be combined with – possibly large scale – knowledge bases describing relationships between classes. Bio/pharma-science & -engineering are application areas

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calling for tools for computing, say, various causal and effect relationships in combination with partonomies and ontological inheritance reasoning. In our [1] CRL is further coined into a diagram logic which utilizes the dynamic potential of computer screens. A prototype of this CRL diagram system is available.

Although CRL has affinity to description logics (DL), CRL-META is not an attempt to design a crossover of a DL sub-language and DATALOG, cf. e.g. [2], since there remain certain fundamental differences to DL, notably the adoption of the closed world assumption, as to be discussed. Nor is CRL an extension of DATALOG as such, unlike the DATALOG extension with existential quantification in heads of clauses introduced in [3].

The paper is organized as follows: Following an introduction to the applied class-relationship logic CRL in Section 2, Section 3 and 4 present metalogic inference rules providing reasoning and querying functionalities. Section 5 discusses some common relationships. Section 6 compares CRL and CRL-META with description logic. Section 7 discusses handling of class definitions and various epistemic modes pertaining to knowledge bases and ontologies. The final Section 8 concludes and summarizes.

2 Class-Relationship Logic CRL

First order logic states relations between individuals, and accordingly the quantified variables range over individuals. In formal ontologies and in many knowledge bases, unlike in databases, one is primarily interested in relations between classes rather than individuals. Introducing variables ranging over classes in logic requires either resort to logical type theory or encoding of classes as the sort of individuals in a metalogic set up, cf. [4,5]. We pursue here the latter approach choosing at the object logic level class relationship logic, CRL. This section describes CRL, while the metalogic providing embedding and encoding is deferred to Section 3.

A CRL knowledge base and/or ontology takes form of a finite number of sentences in first order logic. The salient sentence form is the ∀∃-relationship sentence of the elementary form

$$\forall x(c(x) \rightarrow \exists y(r(x,y) \wedge d(y)))$$

stating a relationship between relata classes c and d with relator r. This form may serve to assign the property to members of the class c of being r-related to members in d, cf. [6,7]. This form and related ones are also applied in the biomedical ontologies in [9,10,11,12,13]. In [14] this form is examined for parthood (i.e. part-whole) relationships in particular.

A distinguished case of ∀∃-relationships is the class inclusion[1], c *isa* d,

$$\forall x(c(x) \rightarrow d(x))$$

[1] Since we intend an intensional conception of classes throughout, the present extensional specification of class inclusion is understood to be only necessary but not sufficient, cf. our [8].

It may be conceived to come about logically by setting r to the identity relation. Thus the class inclusion relationship in this view is a special, though prominent, case of the $\forall\exists$-relationship. As a notational convenience therefore we may use $\forall x(c(x) \rightarrow \exists y(r(x, y) \wedge d(y)))$ with r being "=", when the pertinent relationship is the *isa* relation.

The $\forall\exists$ form is foundational and crucial in ontologies because it serves to assign properties to the classes as illustrated in the below sample knowledge base. It appears that inheritance of class properties (cf. the property of being related via r to class d) is catered for implicitly by the first order logic *per se*.

In addition to the $\forall\exists$-relationship in CRL we consider here three more relationship forms

$$\begin{array}{ll} \exists\exists) & \exists x(c(x) \wedge \exists y(d(y) \wedge r(x, y))) \\ \exists\forall) & \exists x(c(x) \wedge \forall y(d(y) \rightarrow r(x, y))) \\ \forall\forall) & \forall x(c(x) \rightarrow \forall y(d(y) \rightarrow r(x, y))) \end{array}$$

We assume throughout that the classes are non-empty, $\exists x c(x)$ for any c, for reasons clarified below, but we are not concerned with the actual, extensional content of the classes. Individuals in classes may be recognized and dealt with by lifting to singleton classes.

The above relationships between classes c and d can be abstracted as triples $Q'Q''(c, r, d)$ where the 3-ary combinator $Q'Q''$ is either of $\forall\exists$, $\exists\exists$, $\exists\forall$, and $\forall\forall$. As special case of $\forall\exists(c, r, d)$ there is the class inclusion written $isa(c, d)$. Thus formally, with the combinator made a predicate, the class relationships may be re-conceived as atomic ground formulae in first order predicate logic where variables may range over (encoded) classes. This abstraction principle forms the basis for the CRL metalogic introduced in Section 3.

2.1 Example Knowledge Base

Consider a sample KB fragment stated first as triples in stylized natural language:

betacell isa cell
pancreas haspart betacell
betacell produces insulin
insulin isa hormone

The corresponding underlying predicate logical form is:

$$\begin{array}{l} \forall x(betacell(x) \rightarrow cell(x))) \\ \forall x(pancreas(x) \rightarrow \exists y(betacell(y) \wedge haspart(x, y))) \\ \forall x(betacell(x) \rightarrow \exists y(insulin(y)) \wedge produces(x, y))) \\ \forall x(insulin(x) \rightarrow hormone(x)) \end{array}$$

where the predicates *insulin* and *hormone* correspond to mass nouns, unlike the other predicates, and as such ontologically are conceived of as referring to portions of the pertinent substance.

These CRL sentences, when using the below CRL metalogic setup, are then imaginary in that they are actually represented as Datalog atomic sentences

$isa(betacell, cell)$
$\forall\exists(pancreas, haspart, betacell)$
$\forall\exists(betacell, produces, insulin)$
$isa(insulin, hormone)$

The elementary deductive closure of a CRL knowledge base KB is defined as the set of elementary sentences of the class-class relationship forms, notably, $\forall x(c(x) \rightarrow \exists y(r(x, y) \wedge d(y)))$ (with *isa* giving a special case) which are entailed in the usual first order logical sense from the sentences in the KB.

For instance, in the example we have

$$\mathrm{KB} \models \forall x(betacell(x) \rightarrow \exists y(produces(x, y) \wedge hormone(y)))$$

corresponding to a would-be inferred atomic fact $\forall\exists(betacell, produces, hormone)$ at the metalogic level. Section 4 introduces metalogic inference rules reflecting the desired deductions at the CRL logical level.

This closure of elementary sentences is finite let alone due to the finite number of classes and binary relations in a KB.

2.2 Knowledge Base Dually as Graph and Natural Logic

The abstraction of class relationships as triples adorned with quantifier prefixes invites an alternative conception of a CRL knowledge base as a directed, labelled graph, where nodes are uniquely labelled with classes, and arcs are labelled (not necessarily uniquely) with quantifier prefix and binary relations representing class-class relationships. There may be multiple arcs between any pair of nodes.

The c class (start) node of such a a triple (c, r, d) is called the subject node, and the d class (end) node is called the object node of the relationship. The ingoing arcs of a node form the inlets and the outgoing ones form the outlets. This knowledge base graph represents a formalization of the notion of semantic network endowed with a precise logical meaning through the above logical explication of triples.

Thus a CRL knowledge base is dually conceived of as

(1) a finite, directed, labelled graph with arcs representing class-class relationships, and
(2) a finite collection of predicate logical sentences of the above stated atomic form.

The graph view is much favored by ontologists, whereas the complimentary predicate logical view determines the permissible logical inferences to be made from the knowledge base.

The considered logical relationship forms as it appears from the above example closely reflect to simple natural language forms. Moreover, the below inference rules support reasoning close to linguistic forms, thereby enabling a natural logic in the sense of [15].

2.3 Ontology Part Proper

The part of a KB consisting of the *isa* triples forms the ontology proper of a CRL knowledge base. In an alternative parlance, if the entire knowledge based is conceived of as an ontology, the *isa* relationships constitutes the skeleton ontology.

Following a common convention arcs showed un-labelled and pointing upwards are *isa* relationships. The concomitant logical explication forces certain restrictions on the shape of this subgraph: The *isa* arrows are to form an acyclic graph except for the (implicit) presence of loops of length one due to $\models \forall x(c(x) \rightarrow c(x))$ for any c. The definition of *isa* relationships ensures further transitivity, making *isa* a preorder becoming a partial order relation with the mentioned acyclicity restriction.

3 CRL Metalogic Level in Datalog

As stated above the CRL level is formalized in a embracing CRL metalogic level, along the lines in [5,8], cf. also the combinatory logic programming principles in [4]. The employed metalogic at the outset is the Datalog subset of first order predicate logic. Datalog consists of definite clauses of the form

$$p_0(t_{01}, ..., t_{0n_0}) \leftarrow p_1(t_{11}, ..., t_{1n_1}) \wedge ... \wedge p_m(t_{m1}, ..., t_{mn_m})$$

where the predicate argument terms t_{ij} are either constants or variables, where variables are implicitly universally quantified.

The $\forall\exists$ relationships cannot be represented in Datalog clauses simply by the well-known rewriting to clause form, since removal of the existential quantifier calls for Skolem functions introducing compound terms.

However, in the use of Datalog as metalogic CRL relationships in the KB are recorded straightforwardly as ground atomic facts (as special cases of the above definite clauses), viz. $Q'Q"(c, r, d)$ supplemented with the *isa* relationships.

In addition to these given (manifest) sentences there are deducibles in the form of triples belonging to the deductive closure being derivable by means of available axioms as to be presented below. These deducibles may be made actually present in the KB (they being of finite extent) or the may remain as virtual triples[2]. Some triples may be furnished with various modes, e.g. epistemic modes as to be explained.

Logical reasoning is then performed at the meta-level by adding appropriate axioms in the form of Datalog clauses.

4 Axioms and Deduction at the CRL Metalogic Level

Appropriate axioms, *CRL-axioms*, have to be introduced so as to reflect the logical entailment of relationship sentences, e.g. with the requirement:

$$\text{KB} \models \forall x(c(x) \rightarrow \exists y(r(x, y) \wedge d(y))) \quad \textit{iff} \quad \text{KB} \cup \textit{CRLaxioms} \vdash \forall\exists(c, r, d)$$

[2] cf. Hasse diagrams in lattice theory, where arcs derivable by transitivity are omitted.

As mentioned we assume that all classes are non-empty (existential import): $\exists x c(x)$ for all classes c. This assumption serve to streamline the inference rules, and it admits further of stating overlap as well as disjointness of a pair of classes. Besides, non-empty classes tend to be suspect from an ontological point of view. Thus, there is no notion of empty class in CRL.

4.1 Partial Ordering of Inclusion

For the inclusion relation further we stipulate

$isa(X, X)$

$isa(X, Z) \leftarrow isa(X, Y) \wedge isa(Y, Z)$

Both way inclusions give rise to synonym classes (if not precluded)

$ident(X, Y) \leftarrow isa(X, Y) \wedge isa(Y, X)$

The *isa* relation is then effectively established as a partial order (that is, reflexive, anti-symmetric, and transitive) at the meta level.

4.2 Inheritance Axioms

Appropriate axioms have to be introduced so as to reflect logical entailment of relationship sentences. The crucial mechanism here is what is generally understood as inheritance. Following our [1], for class relationships $\forall\exists(c, r, d)$ there is an inheritance inference rule

$$\frac{\forall\exists(C, R, D) \qquad isa(C', C) \qquad isa(D, D')}{\forall\exists(C', R, D')}$$

or correspondingly the pair

$$\frac{\forall\exists(C, R, D) \qquad isa(C', C)}{\forall\exists(C', R, D)}$$

$$\frac{\forall\exists(C, R, D) \qquad isa(D, D')}{\forall\exists(C, R, D')}$$

which at the metalogic level may be paraphrased in Datalog as the definite clauses

$\forall\exists(C', R, D) \leftarrow \forall\exists(C, R, D) \wedge isa(C', C)$

$\forall\exists(C, R, D') \leftarrow \forall\exists(C, R, D) \wedge isa(D, D')$

The inference rule and its clausal axiom form, as it appears, expresses inheritance of relationships as properties to sub-classes (first clause), as well as inheritance of more general properties to underlying relationships (second clause). This is reminiscent of the notion of monotonicity in natural logic [15].

For the other class relationship forms following [1] similarly we posit

Relationship inheritance

$$\exists\forall(C,R,D') \leftarrow \exists\forall(C,R,D) \wedge isa(D',D)$$
$$\forall\forall(C',R,D) \leftarrow \forall\forall(C,R,D) \wedge isa(C',C)$$
$$\forall\forall(C,R,D') \leftarrow \forall\forall(C,R,D) \wedge isa(D',D)$$

Relationship generalization:

$$\exists\exists(C',R,D) \leftarrow \exists\exists(C,R,D) \wedge isa(C,C')$$
$$\exists\exists(C,R,D') \leftarrow \forall\exists(C,R,D) \wedge isa(D,D')$$
$$\exists\forall(C',R,D) \leftarrow \exists\forall(C,R,D) \wedge isa(C,C')$$

Weakening of quantifier (recall non-empty classes):

$$\forall\exists(C,R,D) \leftarrow \forall\forall(C,R,D)$$
$$\exists\forall(C,R,D) \leftarrow \forall\forall(C,R,D)$$
$$\exists\exists(C,R,D) \leftarrow \forall\exists(C,R,D)$$
$$\exists\exists(C,R,D) \leftarrow \exists\forall(C,R,D)$$

4.3 Axioms for Inverses

The inverses r^{-1} of the binary relations r may also be appealed to in CRL. The inverse r_{inv} of some relation r is established in CRL-META, say, with the ground atomic auxiliary KB clause

$$inv(r_{inv}, r)$$

with the axiom

$$inv(X,Y) \leftarrow inv(Y,X)$$

Then there is

$$\forall\forall(D,R',C) \leftarrow \forall\forall(C,R,D) \wedge inv(R,R')$$
$$\exists\exists(D,R',C) \leftarrow \exists\exists(C,R,D) \wedge inv(R,R')$$

It is easy to verify that $\forall\exists$ and $\exists\forall$ are connected with

$$\forall\exists(D,R',C) \leftarrow \exists\forall(C,R,D) \wedge inv(R,R')$$

but not *vice versa*, conforming with

$$\exists x(c(x) \wedge \forall y(d(y) \rightarrow r(x,y))) \quad \models \quad \forall y(d(y) \rightarrow \exists x(c(y) \wedge r(x,y)))$$

5 Miscellaneous Relationship Patterns

Having described the logical aspects of of CRL-META, we now turn to the pragmatics of the language.

5.1 Classification Hierarchies

Ontologies, being fundamentally clasifications, are often tree-shaped or close to hierarchical. Consider a hierarchical classification (bi-partitioning) of a class a into classes b and c. In CRL this is specified by the two sentences

$$isa(b,a) \text{ and } isa(c,a)$$

The classes b and c are then disjoint in so far that there is no overlapping class below b and c. If overlap between classes b and c is intended this is achieved in CRL by introducing a class, say, bc accompanied by $isa(bc, b)$ and $isa(bc, c)$, recalling that classes are understood to be non-empty. The question of overlap of a pair of classes is settled in CRL-META with the clause

$$overlap(C, D) \leftarrow isa(X, C) \wedge isa(X, D)$$

checking for existence of a common subclass X.

Complementarily, disjointness is answered by

$$disjoint(C, D) \leftarrow \not\forall\ overlap(C, D)$$

appealing to DATALOG$^{\not\forall}$, that is DATALOG extended with negation as failure.

The appeal to Closed World Assumption (CWA) conforms with presence only of positive knowledge (as in relational databases) in a CRL KB.

In description logic (DL), see e.g. [2], the sample classification is expressed by $b \sqsubseteq a$ and $c \sqsubseteq a$ and $b \sqcap c \sqsubseteq \bot$, where the latter sentence specifies disjointness (non-overlap of classes). One may observe that the move from bi-partitioning to n-partitioning of classes in ontological classifications would severely complicate the expressing of disjointness. The difference between CRL and DL here is bound up with the principle of Closed World Assumption vs. Open World Assumption.

5.2 Inverse and Reciprocal Relations

For any relation r the inverse individual relation r_{inv} is bound to exist mathematically. By contrast, given the class relationship $\forall\exists(c, r, d)$, the class relationship $\forall\exists(d, r_{inv}, c)$ may or may not be in effect in a knowledge base. In the positive case the two relationships are called reciprocals in [11], and we say that they form a tight relationship in case of co-presence.

Commonly occurring tight relationships are the parthood class relationships discussed in [14,11]. Given a binary mereological relation, *part*, expressing parthood at the instance level, cf. e.g. [17], the relationship

$$\forall\exists(C, part, D)$$

expresses that everything in C has a part instance in D. Dually

$$\forall\exists(D, part_{inv}, C)$$

expresses that everything in D is part of something in C. These reciprocals are independent; co-presence is possible but not mandatory.

5.3 Composite Relations

Queries to a CRL knowledge base may be stated in CRL-META simply as goal clauses. In knowledge bases it may be of interest to identify relationships between some given classes, say c and d. This may be done in CRL-META simply by a goal clause $\leftarrow \forall\exists(c, R, d)$. In the course of computing answers there may be appealed to the various clausal inference rules, e.g. the inheritance rules.

Relationships with composition of relations may be deductively queried with additional $(n + 2)$-ary predicates in CRL-META as e.g. in

$$\forall\exists(C, R_1, R_2, ..., R_n, D) \leftarrow \forall\exists(C, R_1, C_1) \wedge ... \wedge \forall\exists(C_{n-1}, R_n, D)$$

that is, with an additional $(n + 2)$-ary predicate. The mathematical properties of composed class relationships are examined in [16].

6 Comparison with Description Logic

The class inclusion, $isa(c, d)$, has as counterpart the description logic sentence $c \sqsubseteq d$. More interestingly one may observe that ∀∃-relationships are closely related to formulations using the two-argument ∃-operator (peirce-product) in description logic in that $\forall\exists(c_1, r, c_2)$ with the predicate logical specification $\forall x(c_1(x) \rightarrow \exists y(r(x, y) \wedge c_2(y)))$ in description logic (see e.g. [2]), becomes

$$c_1 \sqsubseteq \exists r.c_2$$

The independent reciprocal $c_2 \sqsubseteq \exists r1.c_1$, where $r1$ is the inverse of r, i.e. r^{-1}, is absent or present at the discretion of the domain analyst. The ∃∃-relationships do not seem to have any simple counterparts in description logic.

As a principal difference to description logic the class relationship logic appeals to the Closed World Assumption (CWA), according to which a relationship fails to hold if it is not either given or deducible in the considered domain specification. This implies that two classes are conceived to be disjoint unless there is given a third proper class which is a common subclass of the two classes in question. This principle is applied in relational databases and seems also to conform with ontology practice. It is, however, in contrast to description logic, where disjointness is to be specified explicitly, say, with $c \sqcap d \equiv \bot$.

More generally our abandoning of classic logic in favour of CRL-META implies that relationship logic specifications are bound to be logically consistent as logic programs, unlike description logic specifications. This may be viewed as a deficiency; however, consistency constraints may be formulated at the introduced metalogic level in a well-known manner, say by imposing constraint clauses defining a distinguished predicate, $error(X)$, whose extension, if nonempty when invoked, is construed as inconsistency.

The ∀-operator in description logic in

$$c \sqsubseteq \forall r.d$$

expresses $\forall x(c(x) \rightarrow \forall y(r(x, y) \rightarrow d(y)))$ not to be confused with the ∀∀-relationship in CRL as defined previously.

7 Coping with Ontological Definitions

Consider the following situation with 3 class relationships, say $\forall\exists(a, r, b)$, $\forall\exists(c, r, d)$, and $isa(d, b)$, viz.

$$\begin{array}{ccc} a & -r\rightarrow & b \\ & & \uparrow \\ c & -r\rightarrow & d \end{array}$$

One might here be tempted to deduce a second inclusion relationship added below and supposedly derived as a kind of inheritance relationship

$$\begin{array}{ccc} a & -r\rightarrow & b \\ (\uparrow) & & \uparrow \\ c & -r\rightarrow & d \end{array}$$

Appealing to common sense, for instance dog owners may be thought of as pet owners given that dogs are pets. However, this example is seductive but misleading. This fallacy may more specifically be ascribed to misleading use of the monotonicity of the Peirce product, which may be stated (cf. e.g [18], see also [6]) as:

$$(r : d)\ isa\ (r : b) \qquad if \qquad d\ isa\ b$$

In Description Logic there is the corresponding

$$\exists r.d \sqsubseteq \exists r.b \quad if \quad d \sqsubseteq b$$

This problem is reminiscent of the historical 19th century discussion of the so-called De Morgan Argument, an important issue in pre-Fregean logic of relations, see the comprehensive and instructive account in [19]. The De Morgan Argument is often rendered as *"Si est caput hominis, et animalis"*, that is "Whatever is head of a man is a head on an animal".

What is at stake here is the distinction between "only-if" definitions and full "if-and-only-if" definitions.

Consider

$$\begin{array}{ccc} cell & & insulin \\ \nwarrow & & \nearrow\ produces \\ & beta\text{-}cell & \end{array}$$

which expresses that the KB contains

$$isa(betacell, cell)$$
$$\forall\exists(betacell, produces, insulin)$$

If we wish to achieve the complete definition of beta-cell this could be amended with

$$isa(X, betacell) \leftarrow isa(X, cell) \wedge \forall\exists(X, produces, insulin)$$

One may introduce the convention that such "if" part of a class definition is implied by default for class nodes having more than one outlet triplet.

In cases where one does not wish to achieve this definitional effect one may use instead

$$\begin{array}{ccc} cell & & insulin \\ \nwarrow & & \nearrow\ produces \\ & insulin\text{-}producing\text{-}cell & \\ & \uparrow & \\ & beta\text{-}cell & \end{array}$$

relying on a convention that class nodes with a single outlet are not treated as if-and-only-if definitions. So this latter formulation is open for other cell types as potential candidates for insulin production.

7.1 Mode Options

In order to cater for the situation that one or more outlet triplets $\forall\exists(c, r, d)$ for a class c in the KB are not to participate in the completed definition of c, we suggest that such relationships are tagged as "observable". This annotation is to tell that the relationship does not contribute to the "only-if" definition of c. Apart from this it is to function as any other KB relationship.

The distinction between definition-contributing relationships and the suggested (presumably empirically based) observables is reminiscent of the analytic/synthetic distinction and the *a priori/a posteriori* distinction among propositions.

Straightforwardly an additional inferential mode tag may distinguish between given and deduced relationships in the knowledge base. This further invites gracefully degraded compound relationships (e.g. causal ones) according to the length of the (shortest) deduction.

8 Summary

We have described a logic for ontology structured knowledge representation. Prominently the logic comes with a two-level (i.e. meta) architecture facilitating controlled reasoning and deductive querying about classes and their relationships. Informally CRL-META bears similarity to DL languages, however, it appeals to the Closed World Assumption, contrast the Open World Assumption of DL. As argued, CWA for class relationships might be relevant for comprehensive ontologies, be they hierarchical or trans-hierarchical. The limited expressivity of CRL-META *vis-à-vis* DL (in particular with respect to classical negation) may be compensated by the potential for implementation of the decidable and tractable DATALOG (cf. [2]) meta-level on a relational database platform.

The atomic form of relationships considered here may subject to enrichment with compound classes and relations, e.g. classes formed as conjunctions of classes. In the perspective of natural logic this would open for enrichment of the applied simple linguistic forms with relative clauses, and adnominal and adverbial prepositional phrases.

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