Extending OWL Ontologies by Cartesian Types to Represent N-ary Relations in Natural Language

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Abstract
Arbitrary \( n \)-ary relations (\( n \geq 1 \)) can in principle be realized through binary relations obtained by a reification process that introduces new individuals to which the additional arguments are linked via accessor properties. Modern ontologies which employ standards such as RDF and OWL have mostly obeyed this restriction, but have struggled with it nevertheless. Additional arguments for representing, e.g., valid time, grading, uncertainty, negation, trust, sentiment, or additional verb roles (for ditransitive verbs and adjuncts) are often better modeled in relation and information extraction systems as direct arguments of the relation instance, instead of being hidden in deep structures. In order to address non-binary relations directly, ontologies must be extended by Cartesian types, ultimately leading to an extension of the standard entailment rules for RDFS and OWL. In order to support ontology construction, ontology editors such as Protégé have to be adapted as well.

1 Description Logics, OWL, and RDF

Relations in description logics (DLs) are either unary (so-called concepts or classes) or binary (roles or properties) predicates (Baader et al., 2003). As the designers of OWL (Smith et al., 2004; Hitzler et al., 2012) decided to be compatible with already existing standards, such as RDF (Cyganiak et al., 2014) and RDFS (Brickley and Guha, 2014), as well as with the universal RDF data object, the triple,

\[
\text{subject predicate object}
\]
a unary relation such as \( C(a) \) (class membership) becomes a binary relation via the RDF type predicate:

\[
a \ \text{rdf:type} \ C
\]

For very good reasons (mostly for decidability), DLs usually restrict themselves to decidable function-free two-variable subsets of first-order predicate logic. Nevertheless, people have argued for relations of more than two arguments, some of them still retaining decidability and coming up with a better memory footprint and a better complexity for the various inference tasks than their triple-based relatives (Krieger, 2012). This idea conservatively extends the standard triple-based model towards a more general tuple-based approach (\( n + 1 \) being the arity of the predicate):

\[
\text{subject predicate object}_1 \ldots \text{object}_n
\]

Using a standard relation-oriented notation, we often interchangeably write

\[p(s, o_1, \ldots, o_n)\]

Here is an example, dealing with diachronic relations (Sider, 2001), relation instances whose object values might change over time, but whose subject values coincide with each other. For example (quintuple representation),

\[
peter \ \text{marriedTo} \ liz \ 1997 \ 1999 \ \ \ \ \text{peter} \ \text{marriedTo} \ lisa \ 2000 \ 2010
\]
or (relation notation)

\[
\text{marriedTo}(peter, liz, 1997, 1999) \ \ \ \ \text{marriedTo}(peter, lisa, 2000, 2010)
\]

which we interpret as the (time-dependent) statement that Peter was married to Liz from 1997 until 1999 and to Lisa from 2000–2010.
In a triple-based setting, semantically representing the same information requires a lot more effort. There already exist several approaches to achieve this (Krieger, 2014), all coming up with at least one brand-new individual (introduced by a hidden existential quantification), acting as an anchor to which the object information (the range information of the relation) is bound through additional properties (a kind of reification). For instance, the so-called N-ary relation encoding (Hayes and Welty, 2006), a W3C best-practice recommendation, sticks to binary relations/triples and uses a container object to encode the range information (ppt1 and ppt2 being the new individuals):

\[
\begin{align*}
\text{peter marriedTo ppt1} & \quad \text{peter marriedTo ppt2} \\
ppt1 \text{ rdf:type nary:PersonPlusTime} & \quad ppt2 \text{ rdf:type nary:PersonPlusTime} \\
ppt1 \text{ nary:value liz} & \quad ppt2 \text{ nary:value lisa} \\
ppt1 \text{ nary:starts "1997"^^xsd:gYear} & \quad ppt2 \text{ nary:starts "2000"^^xsd:gYear} \\
ppt1 \text{ nary:ends "1999"^^xsd:gYear} & \quad ppt2 \text{ nary:ends "2010"^^xsd:gYear}
\end{align*}
\]

As we see from this small example, a quintuple is represented by five triples. The relation name is retained, however, the range of the relation changes from, say, Person to the type of the container object which we call here PersonPlusTime.

Rewriting ontologies to the latter representation is clearly time consuming, as it requires further classes, redefines property signatures, and rewrites relation instances, as shown by the marriedTo example. In addition, reasoning and querying with such representations is extremely complex, expensive, and error-prone. Unfortunately, the former tuple-based representation which argues for additional (temporal) arguments is not supported by ontology editors today, as it would require to deal with general relations.

## 2 What this Paper is (Not) About & Related Approaches

We would like to make clear that this paper is not about developing a theory for yet another new DL which permits n-ary relations. The approach presented here suggests that the concepts of domain and range of a relation are still useful when extending a binary relation with more arguments, instead of talking about the arity of a relation in general. We furthermore suggest in Section 6 to introduce so-called extra arguments which neither belong to the domain nor the range of a relation, and can be seen, as well, should be used as a kind of relation instance annotation. In the course of the paper, we also indicate that most of the entailment rules for RDFS (Hayes, 2004) and OWL Horst/OWL 2 RL (ter Horst, 2005; Motik et al., 2012) can be extended by Cartesian types and n-ary relations, and present an incomplete set of rules in Figure 1. Our approach takes a liberal stance in that it neither ask for the “nature” or “use” of the arguments (e.g., whether they are time points), nor for a (sound, complete, terminating, . . .) set of tableau or entailment rules. In fact, if we would take this into account, we would end up in a potentially infinite number of different sets of rules, some of them requiring additional (lightweight) tests and actions, going beyond simple symbol matching; see (Krieger, 2012) for such a set of rules that model valid time, turning binary relations into quaternary ones. For various reasons, we propose a general restriction on the use of Cartesian types in Section 5, viz., to avoid typing individuals with Cartesian types and to maintain still singleton typing. The practical accomplishment of this paper lies in an extension of the Protégé editor for Cartesian types and n-ary relations that should be complemented by application-independent, but also domain-specific rules for a given application domain (e.g., to address valid time).

Since the early days of KL-ONE, DLs supporting relations with more than two arguments have been discussed, e.g., NARY\textsuperscript{KANDOR} (Schmolze, 1989), C\textsubscript{L,F,R} (De Giacomo and Lenzerini, 1994), D\textsubscript{L,R} (Calvanese et al., 1997), or G\textsubscript{F,1′} (Lutz et al., 1999). Especially Schmolze (1989) argued that “the advantages for allowing direct representation of n-ary relations far outweigh the reasons for the restriction” (i.e., restricting \(n \leq 2\)). To the best of our knowledge and with the exception of NARY\textsuperscript{KANDOR}, these DL languages have still remained theoretical work. In (Krieger, 2013), we presented an implemented theory-agnostic forward chainer, called HFC, which is comparable to popular semantic repositories such as Jena or OWLIM and which supports arbitrary n-tuples. The engine is able to run non-built-in entailment rule sets à la OWL Horst/OWL 2 RL and comes with a conservative extension of these OWL
dialects for valid time (Krieger, 2012). Further rule regimes are possible as long as they are expressible in HFC’s rule language which permits standard symbol matching, additional LHS tests, and RHS actions.

3 Extending Ontologies through Cartesian Types

Modern ontologies make use of standards, defined and coordinated by the W3C, such as XSD, RDF, RDFS, or OWL. OWL, as an instance of the description logic family, describes a domain in terms of classes (concepts), binary properties (roles), and instances (individuals). Complex expressions, so-called axioms, are defined via concept-forming operators (viz., subsumption and equivalence). The entirety of all such axioms which can be separated into those dealing with terminological knowledge (TBox), relational knowledge (RBox), and assertional knowledge (ABox), is usually called an ontology today.

Ontology editors which are geared towards RDF and OWL are thus not able to define n-ary relations directly in the RBox, nor are they capable of stating arbitrary tuples (instances of n-ary relations) in the ABox (together with Cartesian types in the TBox; see below). This would require an extension of the triple data model, or equivalently, allowing for n-ary relations (n > 2).

Formally, the extension of a binary relation p, can be seen as a (potentially infinite) set of pairs (s, o), coming from the Cartesian product of its domain D and range R: p ⊆ D × R. We then often say that a relation p is defined on D, say, the marriedTo relation is defined on Person.

Now, in order to allow for more than two arguments, we decompose R, leading to p ⊆ D × R1 × · · · × Rn. Note that we still make a distinction between domain D and range R = R1 × · · · × Rn, and still say that p is defined on D. Coming back to the previous section and the quaternary marriedTo relation, we can say that

marriedTo ⊆ Person × Person × Year × Year

For reasons that will become clear in a moment, not only the range but also the domain of a relation can, in principle, be deconstructed: p ⊆ (D1 × · · · × Dm) × (R1 × · · · × Rn). When it is clear from the context, we often omit the parentheses and simply write p ⊆ D1 × · · · × Dm × R1 × · · · × Rn. We then say that the domain of p is D1 × · · · × Dm and the range is R1 × · · · × Rn, thus p becomes an (m + n)-ary relation. Again, we say that p is defined on Dm × · · · × Dm.

Graphically, such an extension is easy write down. Let us start, again, with binary relations and let us picture the resulting graph for the following set \{p(a, b), q(b, c), q(b, d), r(b, e)\} of binary relation instances by using directed labeled edges:

Ontology editors such as Protégé (Horridge, 2004) essentially use such a representation: properties are defined on certain classes and ontology or ABox) population reduces to filling missing range arguments for specific instances.

But how do we depict the following set of relation instances

\{r((a, b, c), (d)), p((a, b, c), (a, x)), q((a, x), (y, z))\}

of arity 4 and 5, resp? Quite easy, simply by replacing individuals (= singles) in domain and range position through general tuples:

(d) ↦ (a, b, c) \xrightarrow{p} (a, x) \xrightarrow{q} (y, z)

The “problem” with this kind of graph representation is that we are still using a kind of container (denoted by the parentheses) which groups both domain elements Di (1 ≤ i ≤ m) and range elements Rj (1 ≤ j ≤ n). But this is something we want to avoid as explicated before (recall the N-ary relation encoding example from Section 1).

The answer to all this is already laying before us and has already been introduced, viz., Cartesian types (remember the \(\times_i D_i\) and \(\times_j R_j\) notation). This, however, will require to extend the descriptive expressiveness of the TBox, RBox, and ABox of an ontology.
4 Cartesian Types in TBox, RBox, and ABox

Protégeé (and other ontology editors such as TopBraid) displays the class subsumption hierarchy using indentation, e.g.,

\[ \text{\# Entity} \]
\[ \text{\# Object} \]
\[ \text{\# Agent} \]
\[ \quad \text{\# Group} \]
\[ \quad \text{\# Person} \]
\[ \quad \quad \text{\# Man} \]
\[ \quad \quad \text{\# Woman} \]

These concepts can be seen as singles (or singletons), representing a Cartesian product of only one element. Thus the class Person can be seen as the tuple \((\text{Person})\), consisting of one tuple element. Similarly, when considering the marriedTo relation, we might view the range type as the Cartesian type \((\text{Person,Year,Year})\). Clearly, neither does \((\text{Person})\) subsume \((\text{Person,Year,Year})\), nor does the opposite case hold—they are incompatible, for which we write

\[(\text{Person}) \nRightarrow (\text{Person,Year,Year})\]

However, the following subsumption relations do hold, given the above type hierarchy:

\[(\text{Man,Year,Year}) \subseteq (\text{Person,Year,Year})\]
\[(\text{Woman,Year,Year}) \subseteq (\text{Person,Year,Year})\]
\[(\text{Person,Year,Year}) \subseteq (\text{Agent,Year,Year})\]
\[(\text{Group,Year,Year}) \subseteq (\text{Agent,Year,Year})\]

Now let \(\mathcal{C}\) denote the set of concepts, \(\mathcal{R}\) denote the set of all relations, and \(\mathcal{I}\) denote the set of all instances. Quite naturally, the subsumption relation for concepts \(\subseteq \subseteq \mathcal{C} \times \mathcal{C}\) can be easily extended to Cartesian types:

\[\times_{i=1}^{m} C_i \subseteq \times_{j=1}^{n} D_j \iff m = n \text{ and } C_i \subseteq D_i, \text{ for all } i \in \{1, \ldots, m\}\]

Given such an extension, many of the standard entailment rules from (Hayes, 2004) and (ter Horst, 2005) can be easily adjusted, but also two new rules, called \((\text{ctsub})\) and \((\text{ctequiv})\), need to be introduced which propagate Cartesian type subsumption and equivalence down to their component classes (see Figure 1 for a representative, non-complete set of extended rules).

5 A Restriction on the Use of Cartesian Types

The extension introduced so far would even allow us to type individuals \(a \in \mathcal{I}\) with any Cartesian type \(\times_{i=1}^{m} C_i (m \geq 1)\) for which we might then write \(\times_{i=1}^{m} C_i(a)\). This would make it possible to naturally extend, e.g., the universal instantiation schema \((\text{rdfs9})\) from Hayes (2004) with Cartesian types, viz.,

\[(\text{rdfs9}) \times_{i=1}^{m} C_i(a) \land \times_{j=1}^{n} C_j \subseteq \times_{i=1}^{m} D_i \rightarrow \times_{i=1}^{m} D_i(a)\]

Such an extension is attractive, but has severe drawbacks. It makes domain and range inference more complex and would require a stronger descriptive apparatus, as it will become necessary to group and access parts of the domain and/or range arguments in order to indicate the true number of arguments of a relation, but also to indicate the proper argument types. This would become important when checking relation instances against their relation signature.

Consider, for instance, a quaternary relation \(p \subseteq \mathbb{D} \times \mathbb{R}_1 \times \mathbb{R}_2 \times \mathbb{R}_3\) that seems to come with three range arguments. However, by typing individuals with Cartesian types, the above relation can be binary, ternary (two possibilities), or quaternary, depending on how we interpret the range arguments:

- \(p \subseteq \mathbb{D} \times (\mathbb{R}_1 \times \mathbb{R}_2 \times \mathbb{R}_3)\)
- \(p \subseteq \mathbb{D} \times (\mathbb{R}_1 \times \mathbb{R}_2) \times \mathbb{R}_3\)
- \(p \subseteq \mathbb{D} \times (\mathbb{R}_1 \times \mathbb{R}_2) \times \mathbb{R}_3\)

And there are even further complex embeddings possible (remember type theory), such as

- \(p \subseteq \mathbb{D} \times (\mathbb{R}_1 \times (\mathbb{R}_2 \times \mathbb{R}_3))\)
- \(p \subseteq \mathbb{D} \times (\mathbb{R}_1 \times (\mathbb{R}_2 \times \mathbb{R}_3))\)
Extra Arguments

This section deals with what we call extra arguments, arguments that neither belong to the domain nor the range of an \((m+n)\)-ary relation, but can be seen as a kind of additional annotation, belonging to specific relation instances.\(^1\)

Let us start with a binary relation \((m, n = 1)\) and consider, again, the non-temporal version of \textit{marriedTo} which is a true symmetric relation, expressed by the following instantiated entailment rule:

\[
\text{marriedTo}(i, j) \rightarrow \text{marriedTo}(j, i)
\]

Now, if we add time \((b = \text{begin}; e = \text{end})\), it becomes a quaternary relation as indicated before (for better readability, we separate the domain and range arguments from one another by using parentheses):

\[
\forall \text{marriedTo}(i, (j, b, e)) \rightarrow \text{marriedTo}(j, (i, b, e))
\]

In this sense, the temporal interval \([b, e]\) specifies the valid time in which the fluent (the atemporal statement) \textit{marriedTo} \((i, j)\) is true. By applying the extended rule (\text{rdfp3}) from Figure 1 for symmetry, we see that something clearly goes wrong:

\[
\forall \text{marriedTo}(i, (j, b, e)) \rightarrow \text{marriedTo}(j, (b, e), i)
\]

\(^1\)This is like having annotation properties for relation instances, but OWL unfortunately offers this service only for classes, properties, and individuals.
as symmetric relations assume the same number of arguments in domain and range position! Our example above thus needs to be modified. One solution would be to reduplicate the starting and ending points, so we would end up in a sexternary relation:

\[
marriedTo((i, b, e), (j, b, e)) \rightarrow marriedTo((j, b, e), (i, b, e))
\]

This is not an appealing solution as the structures become larger, and rules and queries are harder to formulate, read, debug, and process. We thus like to extend relations \( p \subseteq D_1 \times \cdots \times D_m \times R_1 \times \cdots \times R_n \) by further arguments \( A_1 \times \cdots \times A_o \), so that \( p \) becomes

\[
p \subseteq D_1 \times \cdots \times D_m \times R_1 \times \cdots \times R_n \times A_1 \times \cdots \times A_o
\]

or simply write \( p \subseteq D \times R \times A \). For the \( marriedTo \) example, we might choose \( \text{Person} \) from the ontology above and the XSD type \( \text{gYear} \): \( D = \text{Person}, R = \text{Person}, A = \text{gYear} \times \text{gYear} \).

Thus by having these extra arguments, we can keep the entailment rules from Figure 1, extended, of course, by the additional annotations.\(^2\) Besides having extra arguments for valid time, other areas are conceivable here, viz., transaction time, space, sentiment, uncertainty, negation, vagueness, or graded information.

### 7 Extensions to Protégé

In order to make Cartesian types available in Protégé, we will extend the \( \text{OWL Classes}, \text{Properties}, \) and \( \text{Individuals} \) tabs.

**TBox: OWL Classes Tab**
- \textit{subclass explorer} pane (left column) extension of the subclass hierarchy towards Cartesian types.
- \textit{class editor} pane (right column) depicting the right properties defined on a Cartesian type (domain); depicting the right Cartesian range types for the defined properties.

**RBox: Properties Tab**
- \textit{property browser} pane (left column) extension of the property hierarchy towards Cartesian types.
- \textit{property editor} pane (right column) extension of the domain and range boxes towards Cartesian types.
- \textit{new: extra arguments} (part of the \textit{property editor} pane) further definition box for the extra arguments.

**ABox: Individuals Tab**
- \textit{class browser} pane (left column) extension of the subclass hierarchy towards Cartesian types.
- \textit{instance browser} pane (middle column) possibility to generate sequence instances defined on Cartesian types (= sequences of instances of singleton types).
- \textit{property editor} pane (right column) depicting the right properties defined on a sequence instance; allowing to choose or construct the range arguments; allowing to choose or construct the extra arguments.

Not only the graphical user interface needs to be extended, but also the internal representation (representation of tuples instead of triples), together with a modification of the input and output routines. We plan to have finished a first version of the extensions to Protégé in Spring 2015 and to present it at the workshop.

\(^2\)Depending on the application domain, these annotations might find their way as (potentially aggregated) extra arguments in the relation instances of the consequence of a rule, e.g., in (rdfp4). We will look into this in more detail at the workshop.
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References

Baader, F., D. Calvanese, D. McGuinness, D. Nardi, and P. Patel-Schneider (2003). The Description Logic Handbook. Cambridge: Cambridge University Press.

Brickley, D. and R. Guha (2014). RDF Schema 1.1. Technical report, W3C.

Calvanese, D., G. De Giacomo, and M. Lenzerini (1997). Conjunctive query containment in description logics with n-ary relations. In Proceedings of the International Workshop on Description Logics, pp. 5–9.

Cyganiak, R., D. Wood, and M. Lanthaler (2014). RDF 1.1 concepts and abstract syntax. Technical report, W3C.

De Giacomo, G. and M. Lenzerini (1994). Description logics with inverse roles, functional restrictions, n-ary relations. In Proceedings of the 4th European Workshop on Logics in Artificial Intelligence, pp. 332–346.

Hayes, P. (2004). RDF semantics. Technical report, W3C.

Hayes, P. and C. Welty (2006). Defining N-ary relations on the Semantic Web. Technical report, W3C.

Hitzler, P., M. Krötzsch, B. Parsia, P. F. Patel-Schneider, and S. Rudolph (2012). OWL 2 web ontology language primer (second edition). Technical report, W3C.

Horridge, M. (2004). A practical guide to building OWL ontologies with the Protégé-OWL plugin. Technical report, University of Manchester.

Krieger, H.-U. (2012). A temporal extension of the Hayes/ter Horst entailment rules and an alternative to W3C’s n-ary relations. In Proceedings of the 7th International Conference on Formal Ontology in Information Systems (FOIS), pp. 323–336.

Krieger, H.-U. (2013). An efficient implementation of equivalence relations in OWL via rule and query rewriting. In Proceedings of the 7th IEEE International Conference on Semantic Computing (ICSC), pp. 260–263.

Krieger, H.-U. (2014). A detailed comparison of seven approaches for the annotation of time-dependent factual knowledge in RDF and OWL. In Proceedings of the 10th Joint ACL-ISO Workshop on Interoperable Semantic Annotation.

Lutz, C., U. Sattler, and S. Tobies (1999). A suggestion for an n-ary description logic. In Proceedings of the International Workshop on Description Logics, pp. 81–85.

Motik, B., B. Cuenca Grau, I. Horrocks, Z. Wu, A. Fokoue, and C. Lutz (2012). OWL 2 web ontology language profiles. Technical report, W3C.

Schmolze, J. G. (1989). Terminological knowledge representation systems supporting n-ary terms. In Proceedings of the 1st International Conference on Principles of Knowledge Representation and Reasoning, pp. 432–443.

Sider, T. (2001). Four Dimensionalism. An Ontology of Persistence and Time. Oxford University Press.

Smith, M. K., C. Welty, and D. L. McGuinness (2004). OWL Web Ontology Language Guide. Technical report, W3C.

ter Horst, H. J. (2005). Completeness, decidability and complexity of entailment for RDF Schema and a semantic extension involving the OWL vocabulary. Journal of Web Semantics 3, 79–115.