How Modular Are Modular Ontologies? Logic-Based Metrics for Ontologies with Imports

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Abstract. Many large ontologies are developed modularly, often using import statements, which are supported by the OWL standard. However, import statements do not provide logical guarantees such as local completeness, which is an established quality criterion for ontology modules: an ontology is locally complete if it uses terms from imported ontologies without changing the knowledge reused from them. To measure the extent to which ontologies separated by import statements are logically modular, we present four new quantitative logic-based metrics: two are strongly related to local completeness and based on module extraction, using some established module notion as a reference; the other two exploit the dependency relation of the atomic decomposition. We formally study the relationship between the measures and evaluate them on a set of ontologies.

1 Introduction

Modularity of ontologies has received much attention in the past decade, given the existence of large and comprehensive ontologies such as SNOMED CT [41] and NCI [16], and considering the observation that modular ontologies can be maintained, comprehended, and reasoned over more easily. There are several ways to develop an ontology modularly. The simplest one is certainly the distribution of the axioms over several files and the use of OWL's import statements. More principled approaches include the use of (a-priori) extensions of DLs supporting modular development [2,4,40] or (a-posteriori) decomposition methods [7,11]. The simple approach based on import statements seems to be used frequently: out of the 438 ontologies in the NCBO BioPortal ontology repository [29], at least 69 are built modular using imports; each of them imports (directly and indirectly) up to 31 other ontologies from within and outside the repository. For example, the Cell Ontology (CL) imports 8 ontologies, including the Gene Ontology (GO).

The use of import statements allows developers not only to reuse an existing ontology in (several) other ontologies, but also to follow the design principle *separation of concerns* [12] or, in ontological terms, to separate (sub-)domains of interest. However, this separation does not provide any logical guarantees, e.g., GO does not need to be a *module* of CL in the strict logical sense that all knowledge about genes that follows from CL already follows from GO. In other words, CL might reuse the vocabulary "borrowed from" GO in a way that changes the knowledge in GO. More generally, if an ontology \mathcal{O} imports a module \mathcal{M} , then it is reasonable to require that \mathcal{O} reuses the vocabulary from \mathcal{M} in a "safe" way, in the sense that (a) \mathcal{O} does not entail any knowledge about that vocabulary or (b) \mathcal{O} does not entail anything *new* about that vocabulary, (i.e., knowledge not already entailed by \mathcal{M}). Guarantee (a) is known as *safety* [5,19] and (b) as *local completeness* [7,25]. Both are strongly related to encapsulation as known from software engineering [36]; moreover, (b) can be formalised using *conservative extensions* [15].

Alas, conservativity is undecidable already for fragments of the DL SROIQ [26] underlying OWL. Approximations are known; e.g., locality [6] is a sufficient condition for conservativity, and its syntactic variant can be computed in polynomial time. Locality is the foundation for the successful family of locality-based modules [6]; it can and has been used to evaluate local completeness qualitatively for ontologies with imports [5,19], concluding that essentially all ontologies satisfy (b) from above [5].

In this paper we introduce four quantitative measures, aka *metrics*, for the quality of imports in ontologies or repositories. Our metrics are based on the general idea of determining how close imported modules are to being modules in a strict sense, i.e., determined by some "reference" notion of a module which itself guarantees local completeness (including, but not restricted to, locality-based modules). Hence they determine the extent to which an ontology with imports uses the vocabulary from the imported ontologies in a "safe" way. The first two metrics capture local completeness by determining the similarity of two graphs: one graph represents the import structure of an ontology or repository, i.e., the nodes are the imported subontologies, and the edges are induced by the imports; the other graph is a reference graph that represents a logical significance relation between importing and imported ontologies which is defined based on an arbitrary logically encapsulating notion of a module. The other two metrics use a reference graph defined via the atomic decomposition of an ontology [11]. which constitutes a partition into subontologies that are atomic w.r.t. some underlying module notion, together with a dependency relation between those atoms. This way they determine the similarity of the import graph to an "ideal" graph that captures the logical dependencies within the ontology, which is different from measuring local completeness.

We define the new metrics and evaluate them on a recent BioPortal snapshot [29]. We expect them to help ontology engineers assess whether and to which degree the importinduced modular structure of their ontology actually reflects the logical dependencies between the constituent ontologies, as represented by the underlying reference graphs. This paper is based on the first author's bachelor thesis [30].

2 Related Work

There is a large amount of work introducing quality criteria for modules and evaluating modules against these criteria; informative overviews are given in [9,20]. Here, the term "module" is to be conceived in a broad sense, referring to ontologies that can be used in combination with other ontologies. These quality criteria can be divided into qualitative and quantitative ones (metrics): qualitative criteria can be either satisfied or violated, and metrics are satisfied to some degree. Some metrics have analogues in software engineering. Criteria are also grouped by the characterised or measured aspects:

- Logical criteria such as local correctness and local completeness [7,25]
- Structural criteria such as size and redundancy [39]

- Criteria transferred from software engineering to ontologies, based on or considering the semantics, such as cohesion and coupling [25,33,34,45]
- User- or developer-centric criteria such as comprehensibility [25], readability [43], or domain coverage [8]

Many of the metrics have been implemented in ontology assessment tools and evaluated empirically [13,20,43].

3 Preliminaries

3.1 Graph Theory

We use *digraphs*, i.e., directed graphs G = (V, E), where V is the (non-empty) set of *nodes* and $E \subseteq V \times V$ the set of *edges*. In the following, let G = (V, E) and G' = (V', E') be digraphs. If $V \subseteq V'$ and $E \subseteq E'$, then G is called a *subgraph* of G'. We denote the digraph $(V, E \setminus E')$ by $G \setminus G'$. To measure the similarity between two digraphs G and G' that share the same nodes, we use the following (asymmetric) variant of the Tversky index [44] of their edge sets, which relates to the notion of specificity from test theory.

Definition 1. Given digraphs G = (V, E) and G' = (V', E') with V = V', the *relative* similarity of G with G' is $RSim(G, G') := |E \cap E'| / |E'|$ if this term is defined, i.e., if $E' \neq \emptyset$. In case $E' = \emptyset$, we set RSim(G, G') := 0 if $E \neq \emptyset$ and RSim(G, G') := 1 if $E = \emptyset$.

As a consequence, if E = E', then $\mathsf{RSim}(G, G') = 1$; if $E \cap E' = \emptyset$, then $\mathsf{RSim}(G, G') = 0$.

3.2 OWL and Import Structures

We assume that the reader is familiar with OWL and the syntax and semantics of the underlying description logic SROIQ, for details see [17,18,24]. An *ontology* O is a finite set of general concept and role inclusions as well as concept and role assertions. Let N_C be a set of concept names, N_R a set of role names and N_I a set of individual names. A *signature* is a set $\Sigma \subseteq N_C \cup N_R \cup N_I$ of *terms*. Given a concept, role, axiom, or ontology X, the set of terms occurring in X is called the *signature of* X, denoted \tilde{X} .

OWL ontologies may contain import statements, which can be used transitively and even cyclically. The *import closure* of an ontology \mathcal{O} is the union of \mathcal{O} and all ontologies imported directly and indirectly by \mathcal{O} . The import structure of \mathcal{O} can be represented by a digraph whose nodes are the imported/importing ontologies and the edges denote the import relation. More generally, an *ograph* is a digraph *G* whose nodes are ontologies.

Example 2. The ograph in Figure 1a consists of ontologies $\mathcal{O}_1, \ldots, \mathcal{O}_5$ and represents the situation where \mathcal{O}_1 imports \mathcal{O}_2 and \mathcal{O}_4 , \mathcal{O}_2 imports \mathcal{O}_3 , and \mathcal{O}_4 imports \mathcal{O}_5 .

In general, an ograph is a means to denote some kind of (logical) significance relation between ontologies. We assume that such relations are reflexive and transitive and thus will often work with the reflexive transitive closure of an ograph G = (V, E), denoted $G^* = (V, E^*)$ and depicted in Figure 1b for the ontologies from Example 2. Importinduced ographs as in Example 2 are a special case, representing the logical significance

$$\begin{array}{cccc} \mathcal{O}_4 \leftarrow \mathcal{O}_5 & & \subset \mathcal{O}_4 \leftarrow \mathcal{O}_5 \bigtriangledown \\ \downarrow & & \downarrow & \swarrow \\ (a) & \mathcal{O}_1 \leftarrow \mathcal{O}_2 \leftarrow \mathcal{O}_3 & & (b) & \subset \mathcal{O}_1 \leftarrow \mathcal{O}_2 \leftarrow \mathcal{O}_3 \circlearrowright \\ & & & & \searrow & \swarrow & \swarrow \end{array}$$

Fig. 1: (a) an exemplary ograph G and (b) its reflexive transitive closure G^*

relation that is *to be expected* from the import (e.g., \mathcal{O}_2 should be significant for \mathcal{O}_1 but not vice versa). Furthermore, an ograph in general does not need to have a unique root or be connected. In this sense, the notion of an ograph even captures repositories of ontologies. For an ograph G = (V, E), let $\mathcal{O}_G := \bigcup V$. If G represents the import structure of an ontology \mathcal{O} , then \mathcal{O}_G is the import closure of \mathcal{O} . Note that ontologies contained in an ograph may share symbols regardless of whether or not they are adjacent.

3.3 Modules and Atomic Decomposition

For an interpretation \mathcal{I} and an ontology \mathcal{O} , we write $\mathcal{I} \models \mathcal{O}$ if \mathcal{I} is a model of \mathcal{O} , and denote the interpretation obtained by restricting \mathcal{I} to the signature Σ with $\mathcal{I}|_{\Sigma}$. The central notion that is used to define a module is that of a conservative extension [15] or, more generally, of Σ -inseparability [22], which is defined as follows.

Let \mathcal{O}_1 and \mathcal{O}_2 be ontologies and Σ a signature. \mathcal{O}_1 and \mathcal{O}_2 are *model inseparable w.r.t.* Σ , written $\mathcal{O}_1 \equiv_{\Sigma}^{mCE} \mathcal{O}_2$, if $\{\mathcal{I}|_{\Sigma} \mid \mathcal{I} \models \mathcal{O}_1\} = \{\mathcal{I}|_{\Sigma} \mid \mathcal{I} \models \mathcal{O}_2\}$. \mathcal{O}_1 and \mathcal{O}_2 are *deductively inseparable w.r.t.* Σ , written $\mathcal{O}_1 \equiv_{\Sigma}^{dCE} \mathcal{O}_2$, if, for all \mathcal{SROIQ} -entailments η over Σ , we have $\mathcal{O}_1 \models \eta$ if and only if $\mathcal{O}_2 \models \eta$. The equivalence relations \equiv^R are defined upon the notion $R \in \{mCE, dCE\}$ which is called an *inseparability relation*.

Other notions of inseparability relations can be defined, see, e.g., [22,38]; in this paper we will consider only $R \in \{\text{mCE}, \text{dCE}\}$. An inseparability relation R induces modules defined as follows [23]. Let \mathcal{M} and \mathcal{O} be ontologies with $\mathcal{M} \subseteq \mathcal{O}$ and Σ a signature. We call \mathcal{M} and R_{Σ} -module of \mathcal{O} if $\mathcal{M} \equiv_{\Sigma}^{R} \mathcal{O}$, and a minimal R_{Σ} -module of \mathcal{O} if \mathcal{M} , but no proper subset of \mathcal{M} , is an R_{Σ} -module of \mathcal{O} . Stronger module notions such as self-contained and depleting R_{Σ} -module exist [23], but are not needed in the following.

Since both notions of inseparability are undecidable already for DLs of moderate expressivity [26,27], extracting R_{Σ} -modules is a computationally very hard problem. Still, there are several successful module extraction methods: some are restricted to fragments of SROIQ, such as the MEX/AMEX approach [14,21]; others are approximation methods, which guarantee that the output is an R_{Σ} -module (often with additional useful properties), but that module is not necessarily minimal. These approaches include locality-based modules (LBMs) [6], reachability-based modules (RBMs) [28,32], and modules based on datalog reasoning [1], and minimal subsumption modules [3]. LBMs come in two flavours (semantic and syntactic), and three variants per flavour (\bot , \neg , nested). We will refer to LBMs in some examples, but the precise definitions are not relevant for understanding those.

Since the techniques developed in the following do not depend on a concrete module extraction approach, we use the general notation x-mod (\cdot, \cdot) , i.e., $\mathcal{M} = x$ -mod (Σ, \mathcal{O}) denotes the module extracted for the signature Σ from the ontology \mathcal{O} using approach x.

Usually Σ is called the *seed signature* for \mathcal{M} . More precisely, the *module extraction* function x-mod(\cdot, \cdot) maps every pair (Σ, \mathcal{O}) to a subset of \mathcal{O} .

In contrast to the extraction of a single module, there are techniques for decomposing an ontology into a collection of subontologies which, in some sense, represent all modules. *Atomic decomposition (AD)* [11] is one such technique. It partitions the input ontology \mathcal{O} into a set of atoms and computes a dependency relation between them, also yielding a base for the set of all modules of \mathcal{O} [10, Lemma 4.15]. AD can be used with any module notion *x* whose function *x*-mod(·, ·) satisfies certain properties, which are called (M0)–(M6) in [10]. LBMs and MEX modules satisfy all of them [10].

Let \mathcal{O} be an ontology and $\mathfrak{F}^{x}(\mathcal{O}) = \{x \operatorname{-mod}(\Sigma, \mathcal{O}) \mid \Sigma \subseteq \mathcal{O}\}$. If x is clear from the context or we do not have a specific x in mind, we simply write $\mathfrak{F}(\mathcal{O})$. Given two axioms $\alpha, \beta \in \mathcal{O}$, we write $\alpha \sim_{\mathcal{O}} \beta$ if, for all $\mathcal{M} \in \mathfrak{F}(\mathcal{O})$, we have $\alpha \in \mathcal{M}$ iff $\beta \in \mathcal{M}$. Obviously $\sim_{\mathcal{O}}$ is an equivalence relation. The *atoms* of \mathcal{O} are the equivalence classes of $\sim_{\mathcal{O}}$, i.e., maximal subsets of axioms that are not separated by any module. We denote atoms by α, b, \ldots and the set of atoms of \mathcal{O} by $\mathfrak{A}(\mathcal{O})$. It is immediate that $\mathfrak{A}(\mathcal{O})$ is a partition of \mathcal{O} into linearly many atoms, and every module $\mathcal{M} \in \mathfrak{F}(\mathcal{O})$ is a disjoint union of atoms. In contrast, not every atom needs to occur in some module, but this is only the case if \mathcal{O} contains certain tautologies [10]. We assume the absence of such tautologies.

Let \mathfrak{a} , \mathfrak{b} be atoms of \mathcal{O} . We say that \mathfrak{a} *depends on* \mathfrak{b} and write $\mathfrak{a} \geq \mathfrak{b}$ if $\mathfrak{a} \subseteq \mathcal{M}$ implies $\mathfrak{b} \subseteq \mathcal{M}$, for every $\mathcal{M} \in \mathfrak{F}(\mathcal{O})$. The relation \geq is called the *dependency relation* of \mathcal{O} ; it is obviously a partial order. The *atomic decomposition* (AD) of \mathcal{O} is the poset ($\mathfrak{A}(\mathcal{O}), \succ$), where $\mathfrak{a} \succ \mathfrak{b}$ iff $\mathfrak{a} \geq \mathfrak{b}$ and $\mathfrak{a} \neq \mathfrak{b}$. It can be represented using a Hasse diagram.

Although an ontology can have exponentially many modules [37], its AD can always be computed using a linear number of module extractions: it suffices to compute the genuine modules of \mathcal{O} , which are the $\mathcal{M}_{\alpha} := \text{mod}(\overline{\alpha}, \mathcal{O})$ for all $\alpha \in \mathcal{O}$, and compute the atoms and the dependency relation from only the \mathcal{M}_{α} [11]. This observation is based on several properties of the AD that follow from M1–M5, including the following.

Lemma 3 ([11]). For all $\alpha \in \mathfrak{a} \in \mathfrak{A}(\mathcal{O})$, \mathcal{M}_{α} is the smallest module of \mathcal{O} containing \mathfrak{a} .

4 Metrics for Assessing Imports

Our aim is to develop metrics that assess whether an ontology \mathcal{O}_1 imports another ontology \mathcal{O}_2 in a reasonable way. There are many possible meanings of "reasonable". We focus on the following two: *local completeness* requires that \mathcal{O}_1 does not add new knowledge about the terms from \mathcal{O}_2 ; *relevance* requires that \mathcal{O}_2 adds to the knowledge in \mathcal{O}_1 about those terms. These two conditions are orthogonal to each other, and they should also hold when the ograph contains further ontologies, as we demonstrate in Example 4 below. We thus postulate a condition that is stricter than local completeness and call it *completeness*.

A logically sound definition of "add knowledge" should arguably best be based on inseparability. Since the latter is hard to impossible to decide, approximations are needed and have been used already, e.g., locality as a qualitative approximation of local completeness [5]. Since locality is a sufficient condition for inseparability, it implies that the import is (locally) complete, but if locality is violated, we do not know and have to be cautious. Contrariwise, a necessary condition would be a useful approximation. In the following, we devise four metrics based on an arbitrary module notion that guarantees inseparability, but not necessarily minimality. By not committing to a particular module notion, we leave room for using better module notions that may be developed in the future. Each of our metrics assigns every given ograph G (e.g., import structure) a rational number between 0 and 1. This is done by comparing G with a reference ograph G' that has the same nodes as G and whose edges denote the "reasonable" import relations between the ontologies from G. For the first two measures, we base our understanding of "reasonable" on the notion of *significance*, which we will define using inseparability and approximate using modules. The second two measures will use atoms from the atomic decomposition instead of modules, thus achieving an even stronger notion of reasonableness that abstracts away from the specific signature of the imported ontology. The actual metrics will then be given by a standard notion of difference between the input and reference ographs.

In the following, let *R* be an arbitrary inseparability relation *R*. We use \equiv as a shorthand for \equiv^R . We assume that *R* is *monotone* [23], i.e., if $\mathcal{O}_1 \subseteq \mathcal{O}_2 \subseteq \mathcal{O}_3$ and $\mathcal{O}_1 \equiv_{\Sigma} \mathcal{O}_3$, then $\mathcal{O}_1 \equiv_{\Sigma} \mathcal{O}_2$. Furthermore, let *x* be an arbitrary module notion that yields unique R_{Σ} -modules, i.e., for all \mathcal{O} and Σ , we have that x-mod(Σ, \mathcal{O}) is a uniquely determined subset of \mathcal{O} with x-mod(Σ, \mathcal{O}) $\equiv_{\Sigma} \mathcal{O}$, which is guaranteed, e.g., by LBMs and MEX modules. In the following, we omit *x* where no confusion can arise.

4.1 Module-Induced Modularity

For our first two metrics, the edges of the reference ograph capture a variant of completeness between the respective nodes of G. To explain the underlying intuitions, we continue Example 2.

Example 4. Consider the ograph *G* from Example 2. Given that \mathcal{O}_2 (directly) imports \mathcal{O}_3 , as represented by *G*'s edges, this import would be "safe" if \mathcal{O}_3 were locally complete with respect to \mathcal{O}_2 , i.e., if the import into \mathcal{O}_2 did not change the meaning of the symbols in \mathcal{O}_3 , that is, $\mathcal{O}_2 \cup \mathcal{O}_3 \equiv_{\widetilde{\mathcal{O}_3}} \mathcal{O}_3$ (1). Similarly, since \mathcal{O}_1 imports the other four ontologies (directly or indirectly), local completeness would require that the meaning of the symbols in those is not changed, i.e., $\bigcup_{i=1,\dots,5} \mathcal{O}_i \equiv_{\bigcup_{i=2}} \mathcal{O}_i (2)$.

In general, (1) and (2) cannot be decided. They can be approximated using locality, as in Cuenca Grau et al.'s approach [5]. However, the authors applied their approach only to "top-level ontologies", i.e., (2) would have been tested for \mathcal{O}_G , but not (1). Furthermore, our metrics should not rely on locality, as explained above. We will therefore measure statements such as (1) and (2) in a different way, using sufficient conditions, based on the above properties of the module notion mod:

Example 5. In Example 4, the following are sufficient for (1) and (2): $\operatorname{mod}(\widetilde{\mathcal{O}_3}, \mathcal{O}_2 \cup \mathcal{O}_3) = \mathcal{O}_3$ (1') and $\operatorname{mod}(\bigcup_{i=2,\dots,5} \widetilde{\mathcal{O}_i}, \bigcup_{i=1,\dots,5} \mathcal{O}_i) = \bigcup_{i=2,\dots,5} \mathcal{O}_i$ (2'). Let *x* be the "top" version of syntactic locality, and let $\mathcal{O}_1 = \{A \sqcup B \sqsubseteq C\}, \mathcal{O}_2 = \{D \sqsubseteq B, A \sqsubseteq E\}, \mathcal{O}_3 = \{F \sqsubseteq A\}, \mathcal{O}_4 = \{B \sqsubseteq \neg A\}$ and $\mathcal{O}_5 = \emptyset$. ¹ Then both (1') and (2') hold.

¹ O₅ might still contain non-logical axioms, such as annotations or declarations. This case does occur, e.g. in DC Terms (http://purl.org/dc/elements/1.1/).

Note that we made expectation (1) implicitly based on the assumption that \mathcal{O}_1 and \mathcal{O}_4 are irrelevant for the local completeness of $\mathcal{O}_2 \cup \mathcal{O}_3$ w.r.t. \mathcal{O}_3 . However, if we take them into account too and extract the module from the whole ontology \mathcal{O}_G , then \top -mod $(\widetilde{\mathcal{O}}_3, \mathcal{O}_G)$ consists of $\mathcal{O}_3 \cup \mathcal{O}_4$ plus the first axiom of \mathcal{O}_2 . The overlap with \mathcal{O}_2 suggests that \mathcal{O}_2 does change the knowledge of the terms from \mathcal{O}_3 in the context of all of \mathcal{O}_G .

This last observation admits the following conclusions in view of our desired metrics: (1) it is not enough to consider *local* completeness; (2) for testing completeness and relevance, one needs to check edges as well as non-edges in an ograph. In order to accommodate these conclusions, we use the following notion as a basis for our metric.

Definition 6. Let Σ be a signature and $\mathcal{O}, \mathcal{O}'$ be ontologies such that $\mathcal{O}' \subseteq \mathcal{O}, \mathcal{O}'$ is Σ -significant in \mathcal{O} iff $\mathcal{O} \neq_{\Sigma} \mathcal{O} \setminus \mathcal{O}'$.

Intuitively, a Σ -significant ontology \mathcal{O}' in \mathcal{O} adds knowledge about Σ to \mathcal{O} (relevance). Contrariwise, Σ -*in*significance is similar to completeness but lets us specify a signature. Based on our considerations above and the notion of significance, we can put our expectation precisely: Given an ograph G = (V, E), for any two ontologies $\mathcal{O}_1, \mathcal{O}_2 \in V$ we expect \mathcal{O}_1 to be $\overline{\mathcal{O}_2}$ -significant in \mathcal{O}_G iff $(\mathcal{O}_1, \mathcal{O}_2) \in E^*$. That is, \mathcal{O}_2 should import \mathcal{O}_1 directly or indirectly if, and only if, \mathcal{O}_1 adds knowledge about the terms in $\overline{\mathcal{O}_2}$ to \mathcal{O}_G . In particular, if \mathcal{O}_1 and \mathcal{O}_2 do not share terms, we would not expect any path between them in G; if they do share terms and both contain knowledge about those shared terms, we would expect paths both ways.

Example 7. In Example 5, \mathcal{O}_1 is, as expected, $\widetilde{\mathcal{O}}_2$ -, $\widetilde{\mathcal{O}}_3$, $\widetilde{\mathcal{O}}_4$ - and $\widetilde{\mathcal{O}}_5$ -*in*significant in \mathcal{O}_G , but \mathcal{O}_4 is $\widetilde{\mathcal{O}}_2$ - and $\widetilde{\mathcal{O}}_3$ -significant. Analogously, \mathcal{O}_2 is $\widetilde{\mathcal{O}}_3$ - and $\widetilde{\mathcal{O}}_4$ -significant, and \mathcal{O}_3 is $\widetilde{\mathcal{O}}_2$ - and $\widetilde{\mathcal{O}}_4$ -significant. Note that \mathcal{O}_2 , \mathcal{O}_3 , \mathcal{O}_4 are all $\widetilde{\mathcal{O}}_5$ -significant but \mathcal{O}_5 is not.

Since Σ -significance is defined based on inseparability, which is undecidable already for DLs of moderate expressivity, we can only hope to find a sufficient condition for *in*significance. Indeed, due to the above properties of modules, the following holds.

Lemma 8. Let Σ be a signature and $\mathcal{O}, \mathcal{O}'$ ontologies such that $\mathcal{O}' \subseteq \mathcal{O}$.

(1) If $\mathcal{O}' \cap \operatorname{mod}(\Sigma, \mathcal{O}) = \emptyset$, then \mathcal{O}' is Σ -insignificant in \mathcal{O} .

(2) If \mathcal{O}' is Σ -insignificant in \mathcal{O} , then there is some R_{Σ} -module \mathcal{M} of \mathcal{O} with $\mathcal{O}' \cap \mathcal{M} = \emptyset$.

Proof. (1) Let $\mathcal{M} := \operatorname{mod}(\Sigma, \mathcal{O})$. Then $\mathcal{M} \equiv_{\Sigma} \mathcal{O}$. With $\mathcal{O}' \cap \mathcal{M} = \emptyset$, i.e., $\mathcal{M} = \mathcal{M} \setminus \mathcal{O}'$, we have $\mathcal{M} \setminus \mathcal{O}' \equiv_{\Sigma} \mathcal{O}$. By monotonicity of $R_{\Sigma}, \mathcal{O} \setminus \mathcal{O}' \equiv_{\Sigma} \mathcal{O}$. (2) Set $\mathcal{M} = \mathcal{O} \setminus \mathcal{O}'$. \Box

The converse of Point (1) cannot be expected to hold since mod is not required to yield minimal R_{Σ} -modules; therefore it had to be reformulated as (2).

Based on Lemma 8, we can construct an ograph that approximates our expectation and can be calculated using only |V| module extractions:

Definition 9. Let G = (V, E) be an ograph. The *module-induced dependency graph of* G is the ograph MDG(G) := (V, E') with

$$E' := \{ (\mathcal{O}_1, \mathcal{O}_2) \mid \mathcal{O}_1 \cap \mathsf{mod}(\widetilde{\mathcal{O}_2}, \mathcal{O}_G) \neq \emptyset \}.$$

(a)
$$\begin{array}{c} \bigcirc \mathcal{O}_4 \longrightarrow \mathcal{O}_5 \\ \downarrow & \swarrow & \bigcirc \mathcal{O}_2 \leftrightarrow \mathcal{O}_3 \end{array}$$
 (b) $\begin{array}{c} \mathcal{O}_4 & \overleftarrow{\leftarrow} \Rightarrow \mathcal{O}_5 \\ \downarrow & \swarrow & \frown & \bigoplus \mathsf{MDG}(G) \setminus G^* \\ \mathcal{O}_2 \longrightarrow \mathcal{O}_2 \to \mathcal{O}_3 \end{array}$ $\xrightarrow{\frown} \mathcal{O}_1 \land \mathcal{O}_2 \to \mathcal{O}_3 \end{array}$ (b) $\begin{array}{c} \mathcal{O}_1 & \bigcirc \mathcal{O}_2 \to \mathcal{O}_3 \end{array}$ $\xrightarrow{\frown} \mathcal{O} \setminus \mathsf{MDG}(G) \land \mathcal{O}_2 \to \mathcal{O}_3 \end{array}$

Fig. 2: (a) the MDG of the example ontology and (b) the visualisation of its MIC and MIR

Note that the MDG(G) is not a repair of G, but a representation of the modular dependencies given the partitioning of axioms induced by G. Therefore, rather than restructuring import statements to make the import structure match the MDG, an ontology developer should consider moving axioms responsible for unintentional dependencies from one ontology to another. In this paper, we do not investigate repairs further.

There are now two ways to compare an ograph with its MDG, leading to two measures. For capturing completeness, we determine the number of edges that are in MDG (i.e., denote significances) but not in G, relative to the overall number of edges in MDG. Since we do not want to penalise non-transitive and non-reflexive imports, we have to consider the edges in MDG $\setminus G^*$. For capturing relevance, we determine the number of edges in $G \setminus MDG$ relative to those in G. Here we have to use G rather than G^* , again to avoid penalising non-transitive and non-reflexive imports, as in the following situation.

Example 10. Assume that \mathcal{O}_a directly imports \mathcal{O}_b , and \mathcal{O}_b directly imports \mathcal{O}_c . Furthermore, \mathcal{O}_a reuses only knowledge from $\mathcal{M} \subseteq \mathcal{O}_b$ and no knowledge from \mathcal{O}_c , while $\mathcal{O}_b \setminus \mathcal{M}$ reuses knowledge from \mathcal{O}_c . Hence both direct imports satisfy relevance, but the indirect import would not.

Example 11. Consider the ograph *G* from Examples 2–5. Figure 2a shows MDG(G), and Figure 2b shows $MDG(G) \setminus G^*$ (full arrows) and $G \setminus MDG(G)$ (dashed arrows).

The actual metric is defined by dividing the size (number of edges) in one of the two differences above by the size of MDG(G) or G, respectively, and subtracting it from 1:

Definition 12. Let G = (V, E) be an ograph. We call

- 1. $MIC(G) := RSim(MDG(G), G^*)$ the module-induced completeness of G;
- 2. MIR(G) := RSim(G, MDG(G)) the module-induced relevance of G.

For the situation in Example 11 and Figure 2, we obtain MIR(G) = 0.5 and MIC(G) = 0.75. The MIR and MIC values can be considered as an "aggregated" measure for the edge-wise similarity between the actual ograph and the reference MDG. In cases where they clearly differ from the "ideal" value 1, as in the example, ontology developers can use them as an indicator for reconsidering the import structure of their ontology if that structure was meant to capture logical dependencies. The precise numerical values are of minor interest; in particular, low values can be caused by few or many "structuring errors" and do not pinpoint the precise cause. However, we will make use of the quantitative nature of the MIR and MIC values in Section 5 when we empirically analyse the extent to which adherence to completeness and relevance depend on certain ontology properties.

One might wonder whether the *global* nature of significance might cause our measures to count the same fault several times. This is not necessarily so; see Example 10.

4.2 Atom-Induced Modularity

We now additionally assume that mod satisfies (M0)–(M6) required by the AD [10].

We developed our previous two metrics extending the existing notion of local completeness to significance, which is used to define the underlying MDG. We now focus on significance. Let $\mathcal{O}_1, \mathcal{O}_2, \mathcal{O}_G$ be ontologies with $\mathcal{O}_1 \cup \mathcal{O}_2 \subseteq \mathcal{O}_G$ and $\mathcal{O}_1 \cap \operatorname{mod}(\widetilde{\mathcal{O}}_2, \mathcal{O}_G) \neq \emptyset$. Intuitively, \mathcal{O}_1 contains knowledge about the terms in $\widetilde{\mathcal{O}}_2$ and should be considered when arguing about those. This intuitive criterion can be strengthened by abstracting away from the signature of \mathcal{O}_2 : is there some signature Σ such that, whenever \mathcal{O}_2 contains knowledge about Σ , then so does \mathcal{O}_1 ? The AD allows us to verify that criterion without having to check every signature in \mathcal{O}_G . The dependency relation of the AD captures the exact same property, but between atoms: An atom \mathfrak{a} depends on an atom \mathfrak{b} ($\mathfrak{a} \geq \mathfrak{b}$) if $\mathfrak{a} \subseteq \mathcal{M}$ implies $\mathfrak{b} \subseteq \mathcal{M}$. Hence the new criterion can be approximated by checking whether or not every atom associated with \mathcal{O}_2 depends on some atom associated with \mathcal{O}_1 . Since \mathcal{O}_2 may overlap with some atoms, we need to define "associated with" as follows.

Definition 13. Let $\mathcal{O}, \mathcal{O}'$ be ontologies such that $\mathcal{O}' \subseteq \mathcal{O}$. We call the set

$$\mathsf{AC}(\mathcal{O}',\mathcal{O}) := \{ \mathfrak{a} \in \mathfrak{A}(\mathcal{O}) \mid \mathfrak{a} \cap \mathcal{O}' \neq \emptyset \}$$

the *atom cover of* \mathcal{O}' *in* \mathcal{O} . For ontologies $\mathcal{O}, \mathcal{O}_1, \mathcal{O}_2$ with $\mathcal{O}_1 \cup \mathcal{O}_2 \subseteq \mathcal{O}$, we write $AC(\mathcal{O}_2, \mathcal{O}) \ge AC(\mathcal{O}_1, \mathcal{O})$ iff there are $\mathfrak{a} \in AC(\mathcal{O}_1, \mathcal{O})$ and $\mathfrak{b} \in AC(\mathcal{O}_2, \mathcal{O})$ such that $\mathfrak{b} \ge \mathfrak{a}$.

Since $\mathcal{O} \subseteq \mathcal{O}'$ and $\mathfrak{A}(\mathcal{O})$ is a partitioning of \mathcal{O} , the atom cover of \mathcal{O}' in \mathcal{O} is the unique minimal cover of \mathcal{O}' by atoms of $\mathfrak{A}(\mathcal{O})$ in the topological sense. It is easy to see that it can be computed in polynomial time modulo the AD. Note that $\mathsf{AC}(\mathcal{O}_2, \mathcal{O}_G) \geq \mathsf{AC}(\mathcal{O}_1, \mathcal{O}_G)$ as a logical dependency between \mathcal{O}_1 and \mathcal{O}_2 is orthogonal to completeness: being stronger than significance, it would at best yield a *necessary* condition for *in*significance and thus cannot serve as a useful approximation for completeness (see above).

Based on AC and \geq , we define the atom-induced counterpart of the MDG:

Definition 14. Let G = (V, E) be an ograph. The *atom-induced dependency graph of G* is the ograph ADG(G) := (V, E') with

$$E' := \{ (\mathcal{O}_1, \mathcal{O}_2) \mid \mathsf{AC}(\mathcal{O}_2, \mathcal{O}_G) \ge \mathsf{AC}(\mathcal{O}_1, \mathcal{O}_G) \}.$$

Example 15. The ADG for the ograph G from Example 5, as shown in Figure 3a, is a proper subgraph of the MDG (Figure 2a). This is due to \mathcal{O}_5 and its atom cover being empty, while \mathcal{O}_4 is \emptyset -significant in \mathcal{O}_G .

We obtain the second two metric analogously to MIC and MIR:

Definition 16. Let G = (V, E) be an ograph. We call

- 1. $AIC(G) := RSim(ADG(G), G^*)$ the *atom-induced completeness* of G;
- 2. AIR(G) := RSim(G, ADG(G)) the *atom-induced relevance* of *G*.

For the situation in Figure 3, we obtain $AIR(G) \approx 0.62$ and AIC(G) = 0.75.

(a)
$$\subset \mathcal{O}_4 \qquad \mathcal{O}_5 \qquad \qquad \mathcal{O}_4 \leq -\mathcal{O}_5 \qquad \qquad \rightarrow \mathsf{ADG}(G) \setminus G^*$$

(b) $\mathcal{O}_1 \qquad \mathcal{O}_2 \rightarrow \mathcal{O}_3 \qquad \qquad \rightarrow G \setminus \mathsf{ADG}(G)$

Fig. 3: (a) the ADG of the example ontology and (b) the visualisation of its AIC and AIR

4.3 Relation between the metrics

The coincidence between ADG and MDG in the previous examples is not accidental:

Lemma 17. Let $\mathcal{O}_1, \mathcal{O}_2, \mathcal{O}$ be ontologies such that $\mathcal{O}_1 \cup \mathcal{O}_2 \subseteq \mathcal{O}$. If $AC(\mathcal{O}_2, \mathcal{O}) \geq AC(\mathcal{O}_1, \mathcal{O})$, then $\mathcal{O}_1 \cap mod(\widetilde{\mathcal{O}_2}, \mathcal{O}) \neq \emptyset$.

Proof. Let $AC(\mathcal{O}_2, \mathcal{O}) \ge AC(\mathcal{O}_1, \mathcal{O})$, i.e., $b \ge a$ for some $a \in AC(\mathcal{O}_1, \mathcal{O})$ and $b \in AC(\mathcal{O}_2, \mathcal{O})$. Since $b \in AC(\mathcal{O}_2, \mathcal{O})$ and by Definition 13, there is some $\beta \in b \cap \mathcal{O}_2$. By Lemma 3, $\beta \in mod(\tilde{\beta}, \mathcal{O})$. Since $\tilde{\beta} \subseteq \widetilde{\mathcal{O}}_2$ and mod is monotonic in the first argument (M3), we have $\beta \in mod(\widetilde{\mathcal{O}}_2, \mathcal{O}) := \mathcal{M}$. By the definition of atoms, we have $b \subseteq \mathcal{M}$, and $b \ge a$ implies $a \subseteq \mathcal{M}$. Since $a \in AC(\mathcal{O}_1, \mathcal{O})$ and thus $a \cap \mathcal{O}_1 \neq \emptyset$, we have $\mathcal{O}_1 \cap \mathcal{M} \neq \emptyset$. \Box

The following corollary is a direct result of Lemma 17:

Corollary 18. Let G be an ograph. ADG(G) is a subgraph of MDG(G).

As shown in Example 15, the MDG is, in general, not a subgraph of the ADG and therefore the converse of Lemma 17 does not hold.

5 Implementation and Evaluation

We implemented both the MIC, MIR, AIC and AIR based on the OWL API [35] implementation of atomic decomposition and TL^* -locality based module extraction.

We then analysed the transitive and reflexive import closure of 438 ontologies in a recent snapshot of the NCBO BioPortal ontology repository [29]. While the snapshot also provides pre-gathered ontologies as single OWL XML files, we needed the import structure and therefore used the original files. This failed for 45 ontologies, e.g., because they referenced at least one file that was not available online any more. Furthermore, we excluded 321 ontologies without import statements and 24 ontologies that violated the OWL 2 DL standard, e.g. by using punning in a prohibited way. A further 3 ontologies. Their import closures consist of 2 to 32 ontologies each, adding up to 263. Since some ontologies was 211. These multiple occurrences may have distorted our results.

We found that the median MIC and AIC was ≈ 0.75 and the median MIR and AIR was ≈ 0.89 , with a standard deviation of ≈ 0.28 and ≈ 0.22 , respectively. These medians cannot be compared directly since MIC/AIC are defined differently from MIR/AIR. 18 ontologies achieved an MIC and AIC of 1, i.e., they use imports in a "safe" way. Note that none of them contained more than four ontologies in their import closure, with PEAO

having the largest one. 21 ontologies had an MIR and AIR of 1, with COGPO having the largest import closure (size 9). The NMOBR ontology with the largest import closure (32) had both the lowest MIC and AIC, ≈ 0.09 , see [31]. The DC ontology was scored with the lowest MIR and AIR, both having the value ≈ 0.22 .

Given Lemma 17 we were not surprised to observe that ADG \subseteq MDG for all tested ontologies. In addition, the Spearman's rank correlation coefficient of MIC and AIC was as high as ≈ 0.997 with $p < 10^{-49}$ and that of MIR and AIR was ≈ 0.98 with $p < 10^{-32}$. However, in only ten cases the ADG was a *proper* subgraph of the MDG. In six cases, this was due to some axioms being non-local w.r.t. the empty signature (see Example 15). We were unable to identify the reason for the remaining four ontologies because the number of axioms in their import closure made both manual and automatic analysis infeasible.

We evaluated two more hypotheses: (A) Are larger import closures less likely to be constructed modularly? We found that MIC and AIC tended to decline with larger import closures, indicated by the correlation coefficients of \approx -0.8 and \approx -0.79 with $p < 10^{-10}$. This effect could not be observed for MIR and AIR (\approx 0.06 at p < 0.7 and \approx 0.04 at p < 0.8). A reason might be the difference between the "global" nature of completeness (considering dependencies between ontologies unrelated via the import structure) and the "local" nature of relevance (applying only to an ontology and its *direct* imports). Therefore, a more complex import closure may make completeness harder to ensure, while having no effect on relevance. (B) Do "non-modular" ontologies tend to have both a low relevance and a low completeness? We cannot confirm this hypothesis: there was no significant correlation between MIC and MIR, or AIC and AIR.

6 Conclusion and Future Work

With the MDG and the ADG we introduced two new views on the logical structure of a modular ontology. Developers may find them helpful to investigate the logical dependencies between imports in detail, while researchers may use the metrics based upon them to analyse large ontology corpora similarly to what we did above. Nevertheless, there is no precise general understanding of the terms "modularity" and "logical dependency", and our definitions capture only two of the possible variants.

While we used a generalisation of local completeness, other modularity criteria may be investigated using the same techniques, e.g., one might want to check whether ontologies reuse *all* the imported knowledge. Even more so, because, for example, ontology developers might not have control over the import structure of an imported foreign ontology, it might make sense to evaluate certain import statements a special way. Such scenarios can be taken care of by refining our approach with labelled ographs. Further questions for continuing this work in progress include: In which cases do the MDG and ADG actually differ? How are the experimental results affected by using a module notion that provides minimal modules, such as MEX [21]? Can our metrics be used in an optimisation problem for automatically calculating a "good" import structure of a given ontology with maximal values of some/all measures? The last one does not seem easy, as further parameters are needed to avoid trivial cases, such as constructing an import structure without import statements.

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