# BUILDING TAILORED ONTOLOGIES FROM VERY LARGE KNOWLEDGE RESOURCES

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Abstract: Nowadays very large domain knowledge resources are being developed in domains like Biomedicine. Users and applications can benefit enormously from these repositories in very different tasks, such as visualization, vocabulary homogenizing and classification. However, due to their large size and lack of formal semantics, they cannot be properly managed and exploited. Instead, it is necessary to provide small and useful logic-based ontologies from these large knowledge resource so that they become manageable and the user can take benefit from the semantics encoded. In this work we present a novel framework for efficiently indexing and generating ontologies according to the user requirements. Moreover, the generated ontologies are encoded using OWL logic-based axioms so that ontologies are provided with reasoning capabilities. Such a framework relies on an interval labeling scheme that efficiently manages the transitive relationships present in the domain knowledge resources. We have evaluated the proposed framework over the Unified Medical Language System (UMLS). Results show very good performance and scalability, demonstrating the applicability of the proposed framework in real scenarios.

### **1** INTRODUCTION

Ontologies are a knowledge representation formalism that capture the semantics of the real world entities by defining concepts and the relationships between them. The knowledge captured in ontologies can be used, among other things, to share common understanding of the structure of information among people and/or software agents, to enable the reuse of domain knowledge and to introduce standards to allow interoperability (Noy et al., 2001). Recently, many application domains are being represented using ontologies, one of the most prominent being the life-science fields. An example of a large repository of biomedical information is the Unified Medical Language System (UMLS). This knowledge resource is a vast and very comprehensive repository of information. However, the large amount of different terminologies it gathers makes it hard to select a relevant and manageable subset for an specific application. Moreover, UMLS is not represented in a standard interchange ontology language such as the W3C recommended OWL, which prevents the knowledge base from the benefits of logic-based formalisms.

In this paper, we tackle the evident scaling problems when dealing with very large and complex knowledge resources. Our proposal consists of a framework for building compact and customized logic-based ontologies from large knowledge resources. The proposed system allows the user to specify a query as free-text, which encapsulates the semantics the output ontology should gather. The input query goes through a process of semantic annotation and later assessment in order to obtain a set of relevant and meaningful ontology concepts. These set of concepts, called *signature*, is used by the *Ontology Extractor* to obtain a specific application-oriented ontology in OWL format. To our best knowledge, our approach is the first one on addressing the following requirements:

- *Scalability*. Knowledge resources tend to be large and complex repositories of information. We achieve scalability through the use of tools aimed at extracting customized ontologies from the knowledge resources, which just involve the necessary elements.
- Ontology Compactness. Specific application ontologies are usually subject-oriented, which means they gather semantically related concepts. The compactness of these ontologies depends greatly on the precision of the semantic annota-

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tion of the user query. Therefore, we propose an assessment step that filters the semantic annotations obtained based on the conceptual density of each selected ontology concept.

• *Logic-based Formalism.* The ontologies built from the knowledge resources are represented in OWL, which offers several advantages such as reasoning capabilities, consistency of terminology, sharing and reusing knowledge, etc.

The rest of the paper is organized as follows. Section 2 describes an application scenario that motivates the proposed approach of building OWL ontologies from large knowledge resources. Section 3 explains in detail the different components of the framework and Section 4 shows the evaluation performed. Finally, Section 5 gives some conclusions and future work.

# 2 APPLICATION SCENARIO

In the biomedical domain, the gathering and representation of knowledge have been the main concerns of researchers and domain experts for several years. Supporting evidence is the great effort made by the National Library of Medicine (US) in developing the UMLS over the past 18 years. UMLS can be thought as a large repository of biological and clinical information covering multiple domains: from genetics and celular to disease level. The version 2007AC has 1,516,299 concepts and 13,226,382 relations. UMLS includes three resources: the Metathesaurus, the Semantic Network, and the Specialist Lexicon. The first one consists of several thesauri (more than 100 different sources such as FMA, MeSH, etc.) The Semantic Network consists of 135 semantic types organised in 7 main groups - e.g. anatomical structure or biologic function - and linked by "is\_a" relationships. There are also 53 kind of non-hierarchical relationships among these semantic types, e.g. causes(Virus, Disease). A concept of the metathesaurus can be assigned at one or more semantic types in the Semantic Network. The SPECIALIST Lexicon, the third resource of UMLS, has been developed in order to provide lexical information needed for an NLP application e.g. syntactic, morphological. It includes many biomedical terms, dictionaries of abbreviations, etc.

The conceptual model of UMLS is centred on Sources (i.e. ICD-10, MesH), which contain Atoms (the distinct concepts within each source). Each Atom is assigned to one and only one Concept, whose identifier is called CUI. Concepts consist in Terms owing the same meaning. One Term can belong to several concepts but not often. Terms consist of Strings, i.e. string variants. Figure 1 shows an example of the conceptual model of UMLS. The proposed frame-work works at the level of concept identifiers (CUIs).

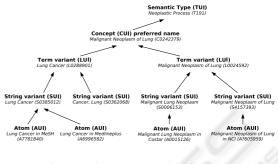


Figure 1: Conceptual model of UMLS.

UMLS can be considered a vast and complex ontology, from which is hard to select a relevant manageable subset for a specific application. Moreover, the metathesaurus gathers vocabularies that have been developed independently, resulting in a lot of inconsistencies such as cycles in hierarchies. Moreover, the UMLS knowledge resource has a proprietary format, which prevents interoperability and the use of standard languages and tools designed for the Semantic Web. One could think of translating the whole metathesaurus into OWL. However, authors such as (Cornet and Abu-Hanna, 2002) and (Kashyap and Borgida, 2003) claim this is not feasible since the semantics of the relations present in the vocabularies (e.g. ICD, MeSH) is often underspecified. Therefore, UMLS relations can be interpreted in several ways. As a result, only the Semantic Network has been translated into OWL (Kashyap and Borgida, 2003). Our proposal addresses this issue by building specific ontologies tailored to the needs of a concrete application. The output ontology should be used by knowing that it is a specific interpretation of the metathesaurus. Moreover, we put special emphasis in building ontologies in a logic-based formalism such as OWL due to the several advantages it offers. OWL brings powerful reasoning based on Description Logic (DL). In the biomedical domain, reasoning can be a very powerful tool to infer new or implicit knowledge. For example, it can serve to make relevant links between two different biomedical domains. Moreover, we can also check the consistency of the terminology and perform more meaningful queries. On the other hand, adding a description logic to a large coarse-grained conceptual model of a biomedical domain serves to disambiguate imprecise representations. Finally, by using OWL, which is a W3C standard, we can benefit from the tools made available for OWL as well as share and reuse knowledge in an easy way.

## **3 SYSTEM ARCHITECTURE**

In this section we present the framework for building tailored application ontologies from very large knowledge resources. Figure 2 shows the different components of the framework. The workflow of the framework is as follows: the user specifies a free-text query that describes the application ontology he wants to obtain. The Symbol Searcher tool performs the Semantic Annotation of the user query with the lexicon of the knowledge resource. The set of obtained concepts go through an Assessment step that filters the concepts according to their conceptual density. The output of the Symbol Searcher tool is the signature, which is composed by the knowledge resource concepts that best match the user query both syntactically and semantically. Taking as input the signature, the Ontology Extractor retrieves from the knowledge resource the sub-ontology (necessary concepts along with their taxonomic relationships) that best covers the signature. In a final step, the ontology is converted into OWL format and further enriched with additional OWL axioms.

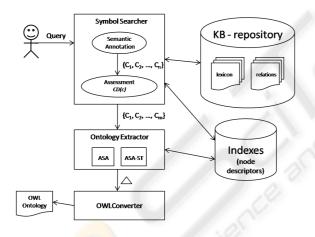


Figure 2: Framework for building logic based application ontologies from knowledge resources.

Next sections are devoted to explain with more detail the main components of the framework, which are in turn the *Symbol Searcher*, *Ontology Extractor* and *OWL Converter*.

### 3.1 Symbol Searcher

The *Symbol Searcher* is in charge of finding the appropriate set of ontology concepts that best match the user query. This process is carried out in two phases, which will be explained in turn: *Semantic Annotation* and *Assessment*.

#### 3.1.1 Semantic Annotation

The main idea behind semantic annotation is the identification of relevant terms and the linking of these terms to thesauri, databases or ontologies. In our application scenario, we are interested in finding relevant terms in the user query and linking them to UMLS concepts. One option consists of performing manual annotation. However, this process is subject to human errors and factors such as familiarity with the domain, scale of the knowledge resource, etc. An alternative to overcome these difficulties is the automatic semantic annotation of text. MetaMap (Aronson, 2001) and Whatizit (Rebholz-Schuhmann et al., 2007) are examples of automatic semantic annotators that use large terminological databases as input lexicons. MetaMap has been specifically designed to map text into concepts from the UMLS Metathesaurus while Whatizit can be used on several resources such as UniProtKb/Swiss-Prot, GO, UMLS, etc. Both semantic annotators have been tested in the context of the application scenario and, although they are effective, a supervised process is still required to complete and verify the obtained annotations. Since we want all the steps of the framework to be as automatic as possible, in the next section we propose an assessment step that filters out the concepts found by the semantic annotator.

#### 3.1.2 Assessment

The quality and compactness of the resulting application ontology is severely affected by the input signature used to generate it. As earlier mentioned, automatic semantic annotators are subject to imprecission and ambiguity. Therefore, the objective of this assessment step is to evaluate and rank the output ontology concepts found by the semantic annotator according to their conceptual density. Let *C* be the set of concepts found by the semantic annotator and *N* its size. We define the conceptual density of a concept of *C* as follows:

$$CD(c) = \sum_{c_i \in C, c_i \neq c}^{N} \frac{1}{d(c, c_i)} \frac{1}{N}$$
(1)

where  $d(c, c_i)$  is the taxonomic distance between concepts c and  $c_i$  in the knowledge resource.

Notice that CD(c) = 1 if the rest of concepts from *C* are direct neighbours of *c*. Therefore, concepts with bigger *CD* are closer one another in the knowledge resource, while concepts with smaller *CD* are far away from the rest of concepts in *C*. The latter probably correspond to incorrect or ambiguous semantic annotations. In order to filter them out the user can specify

a minimum *Threshold* as shown in Figure 2. With this procedure we remove concepts found by the semantic annotator that may introduce noise in the resulting ontology.

### 3.2 Ontology Extractor

The Ontology Extractor task consists of retrieving from the knowledge resource an application ontology (e.g. a set of concepts along with their taxonomic relationships) that fulfils the user needs. The application ontology has to provide the necessary semantics demanded by the user query while keeping a reduced size in order to achieve scalability. In order to accomplish both requirements we have developed and tested an indexing mechanism over the "is-a" relationships of the knowledge resource that enables us to efficiently retrieve a small subset that satisfies the user query. Next section describes the indexing process of the knowledge resource and then we present an ontology retrieval strategy based on the indexes created.

#### 3.2.1 Knowledge Resource Indexing Process

In most knowledge resources, as is the case of UMLS, concepts are organized into "is-a" hierarchies, which constitute the backbone of the repository. This leads to an underlying graph-like structure. In order to efficiently retrieve a sub-ontology from this graph structure guided by the signature, we need some kind of indexing scheme over the graph that encodes descendant and ancestor relationships in a compressed and efficient way. We have adopted a labeling scheme, which assigns to each node in the graph some identifier that allows the computation of relationships between nodes using simple arithmetic operations. For our purposes, we have adopted and extended Agrawal's interval scheme (Agrawal et al., 1989) but with a labeling variation from (Schubert et al., 1983), which takes preorder identifiers of nodes instead of postorders used in Agrawal's technique. The approach can be applied to directed trees and Directed Acyclic Graphs (DAGs), which will be the underlying structure of most ontologies (Christophides et al., 2003). With respect to our application scenario, we have preprocessed UMLS in order to delete cycles in the "is-a" hierarchy and obtain a DAG.

Figure 3 (left graph) shows a labeled DAG. The process is as follows: in an initial step, disjoint components can be hooked together by creating a virtual root node. The compression scheme first finds a spanning tree T for the given graph (solid edges). Then it assigns an interval to each node based on the preorder traversal of T. That is, the interval associated with a

node v is [pre(v), maxpre(v)], where pre(v) is the preorder number of v and maxpre(v) is the highest preorder number of v's descendants. Notice the preorder of each node is used as its unique identifier. Next, all nodes of the graph are examined in the reverse topological order so that for every edge from node p to q, all the intervals associated with node q are added to the intervals associated with node p, taking into account that if one interval is subsumed by another, the subsumed interval is not added. In the figure, the interval [2,7] is associated to node d when labeling the spanning tree. Then, during the reverse topological traversal, node d inherits intervals [6,6], [4,6] and [5,5] corresponding to nodes g, e and h, which come from the dashed edges not belonging to the spanning tree. Since these intervals are already subsumed by d's interval [2,7], they are not added to d. Otherwise, they would be included.

The storage requirements for trees labeled with this interval scheme is O(n), since one interval per node is enough. For DAGs, the worst case requires  $O(n^2)$  space. However, this situation is unlikely because Agrawal's approach for DAGs finds the optimum spanning tree, that is, the spanning tree that leads to minimum amount of intervals per node and thus, minimum storage requirements.

Next step consists of obtaining analogous information about ancestors of each node. The strategy applied is as follows. First, we reverse the edges of the original structure so that each node now points to its parent/s (see right graph of Figure 3). Then, a virtual root node has to be created to hook together what are leaf nodes in the original structure. Then, the same labeling scheme described previously is applied to the reversed structure. Since now the edges denote ancestor relationships, the labeling scheme will encode ancestor nodes. Notice that each node identifier is its preorder number and both the original structure and the reversed one have each own preorder system.

We finally define the *descriptor* function of a node *v* as follows:

descriptor(v) = < descpre(v), descintervals(v),ancpre(v), ancintervals(v),topo(v) >

where descpre(v) denotes the preorder number of v in the original structure, descintervals(v) denotes the set of intervals encoding v's descendants, ancpre(v) denotes the preorder number of v in the reversed structure, ancintervals(v) denotes the set of intervals encoding v's ancestors and topo(v) denotes the topological order of v.

Gathering all together, we have designed an encoding mechanism for concepts in a knowledge re-

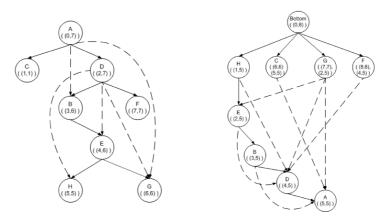


Figure 3: Compressed transitive closure of descendants (left graph) and ancestors (right graph).

source based on interval labeling schemes that is able to encapsulate in a compressed and efficient way all the descendants and ancestors of each concept. The information encapsulated in the concept descriptors can be exploited to efficiently retrieve related concepts. Therefore, we define a set of operations intended to manipulate the intervals of the descriptors. The most important operations are the next:

- The descendants of *v* is the serialization of *descintervals*(*v*).
- The ancestors of *v* is the serialization of *ancintervals*(*v*).
- The topological order of v is topo(v).
- Concept  $v_1$  subsumes  $v_2$  if:

 $descintervals(v_1) \cap descintervals(v_2) == \\ descintervals(v_2)$ 

• Common ancestors of  $v_1$  and  $v_2$  are:

 $ancintervals(v_1) \cap ancintervals(v_2).$ 

• Nearest common ancestor of  $v_1$  and  $v_2$  is:

 $max\{topo(commonAncestors(v_1, v_2))\}.$ 

#### 3.2.2 Ontology Retrieval Strategy

The aim of the strategy presented in this section is to extract ontologies with a reduced size and relevant to the user query. The output constitutes the skeleton of the application ontology ("is-a" relationships with tree-like structure). This ontology skeleton can be further enriched with additional "is-a" relationships in order to obtain a DAG structure, which has the property of preserving all the taxonomic relationships among the input signature concepts. This section is dedicated to describe the strategy followed in order to achieve such a goal.

#### Algorithm 1: Compute spanning tree.

**Require:** *L* list of output nodes sorted by preorder number Ensure: G spanning tree of the output nodes Stack *parents* =  $\emptyset$  $C = next\_node(L)$  $D = next\_node(L)$ while L do **if** subsumes(descintervals(C), descintervals(D) **then**  $add\_edge(G, edge(C, D))$ push(parents,D) C = D $D = next\_node(L)$ else *pop*(*parents*) C = top(parents)end if end while

All Signature Ancestors (ASA). The ontology retrieval strategy presented consists of extracting all ancestors from the signature concepts encoded in the descriptors. Then, Algorithm 1 computes a spanning tree with the signature and their ancestors based on their subsumption relationships encoded in the descendant intervals. The output ontology contains all concepts from the signature plus all their ancestors organized by their "is-a" relationships.

Figure 4 shows an example of the output ontologies (tree-like structure) that would be retrieved by this strategy and the refinement presented next taking as starting point the same signature. Figure 4.a shows the underlying graph-like "is-a" relationships of the original knowledge resource, in which thicker lines correspond to the spanning tree calculated by the interval labeling scheme described in Section 3.2.1. Figure 4.b including the crossed out nodes corresponds to the ontology skeleton that would be retrieved by ASA strategy, in which black nodes are the input signature.

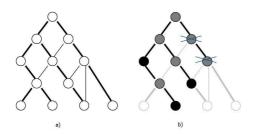


Figure 4: Output ontology skeleton. a) Original knowledge resource "is-a" relationships; b) Output ontology of ASA (all nodes) and ASA-ST (crossed out nodes not included).

Algorithm 2: Search additional edges to get a DAG.
<b>Require:</b> <i>G</i> output tree structure of ASA or ASA-ST
<b>Ensure:</b> G with DAG-structure
$sorted\_nodes = topological\_order(G)$
for all node n in sorted_nodes do
ancestors = ancestors(n)
while ancestors do
$nearest\_ancestor =$
get_nearest_ancestor(n,ancestors)
$add\_edge(G, edge(nearest\_ancestor, n)$
nodes_to_root =
get_nodes_to_root(nearest_ancestor)
delete_from(ancestors, nodes_to_root)
end while
end for

All Signature Ancestors Spanning Tree (ASA-ST). In the previous approach, retrieving all ancestors from the signature concepts can result in an excessive amount of nodes in the output ontology that are not relevant to the reconstructed hierarchy. Thus, we have introduced an enhancement by just selecting ancestor nodes that relate concepts of the signature through the spanning tree calculated (see crossed out nodes of Figure 4.b). This approach can be considered an extension of ASA strategy, since it is applied to the ASA output ontology. In this strategy, deleted nodes do not participate in the transitive closure of the signature, thus, it is not altered. The experiments performed show that ASA-ST strategy is more adequate when working with UMLS due the great amount of unrelevant ancestors pruned. Therefore, we take ASA-ST strategy as the one suitable for our application scenario.

**Obtaining a DAG.** The output ontology consists of a tree structure for simplicity, since many applications do not require all "is-a" relationships among concepts but rather a tree hierarchy (e.g. datawarehouse dimensions). However, in many cases it is necessary to get the complete DAG structure. For this purpose, the Algorithm 2 has been designed.

This algorithm adds the remaining relationships

between pairs of nodes belonging to the signature. This is accomplished by calculating nearest ancestors using the topological order of nodes.

This algorithm does not add an extra temporal complexity because all operations have a linear cost w.r.t. the number of nodes if they make use of the *descriptor* functions of each node.

#### 3.2.3 UMLS Specific Customizations

The indexing scheme and ontology retrieval strategy presented in this paper are not specific to UMLS. They can be applied to any knowledge resource with some kind of transitive relationship (e.g. "is-a", "partof", etc.). However, once the ontology skeleton is obtained one can enrich it with specific features from the knowledge resource. In the case of UMLS, concepts belong to one or more semantic types as explained in Section 2. Therefore, we enrich the graph structure obtained in the previous phase with the corresponding semantic types and "is-a" relationships.

### 3.3 OWL Converter

The final step performed by the system consists of building an interchangeable OWL file with the graphbased structure returned by the Ontology Extractor. Table 1 summarizes the patterns applied to the graph to obtain the final OWL ontology. For the sake of space, we use DL notation instead of OWL constructors. Axiom 1 converts a node, which represents a concept, into an OWL class. Then, axiom 2 adds a subClassOf axiom for each edge, which represents an "is-a" relationship. By applying the previous axioms we obtain a taxonomy where classes are primitive, i.e. without explicit definition. In order to enrich the ontology with reasoning capabilities, we need to make explicit some concept definitions using existing ones. Axioms 3 and 4 perform this task. In particular, axiom 3 defines a concept as the intersection of its parents, while axiom 4 defines a concept as the union of its children. Additionally, axiom 5 includes UMLS relationships as ObjectProperties and Restrictions over the involved concepts only if both domain and range are included in the graph so that we obtain closed ontologies. Following (Kashyap and Borgida, 2003), we only add axiom 5 if the corresponding relationship is not blocked in the Semantic Network. Finally, we can further enrich the ontology concepts and properties with annotations provided by the knowledge resource (e.g. label, comment, user-defined annotation properties, etc).

	DAG	OWL (DL)
(1)	node(C)	С
	$C \in CUIs \cup Semtypes$	
(2)	edge(D,C)	$C \sqsubseteq D$
(3)	$edge(D_1,C)$	
	•••	$C \sqsubseteq (\equiv) D_1 \sqcap \ldots \sqcap D_n$
	$edge(D_n,C)$	
(4)	$edge(C, D_1)$	
	•••	$C \equiv D_1 \sqcup \ldots \sqcup D_n$
	$edge(C,D_n)$	
(5)	node(A), node(C)	$A \sqsubseteq \exists R.C$
	R(A,C)	

Table 1: OWL conversions from	m a DAG structure.
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Table 2: UMLS statistics: # intervals per descriptor.

UMLS number of intervals per descriptor
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	<u> </u>
Number of descriptors	293041
Avg. descendants	2.28
Max. descendants	2326
Avg. ancestors	11.46
Max. ancestors	114
Depth	27

### **4 EVALUATION**

In the following, we describe the experiments performed over the UMLS to prove that our framework is both scalable and able to retrieve relatively small sized ontologies compared to the whole knowledge resource. A prototype was implemented in Python and MySql has been used as back-end storage system for the indexes.

Firstly, Table 2 shows some statistics about the size of the indexes generated by our ontology indexing system (concept descriptors) for UMLS. As we can observe, the maximum number of intervals in a concept descriptor can be quite large but this is not usual at all since the average in the descendant intervals is really low while in the ancestors' increases but not too much. Thus, we can state that our indexes are scalable when dealing with large knowledge resources. Some of these repositories have a high degree of dynamism, since they are continously evolving and growing (e.g. a new version of UMLS is made available every few months, more or less). This is not quite a problem for our framework since newer versions of repositories can be indexed in a few minutes.

The performance evaluation of the framework has been carried out over a set of 100 different signatures derived from a collection of 15000 abstracts taken from MEDLINE. These signatures have been developed in the context of the Health-e-Child<sup>1</sup> project,

where each signature represents a different perspective for the study of a given disease. We selected the diseases Juvenile Idiopathic Arthritis (JIA) and Tetralogy of Fallot (TOF). Abstracts are processed with a semantic tagger, in our case (Jimeno et al., 2008), which identifies UMLS concepts from texts. These concepts are grouped according to the target disease (JIA or TOF) and their semantic type. For the assessment phase, the conceptual density has been shown quite useful to detect both wrongly annotated strings and non-relevant concepts derived from the user's request. In the experiments, we have combined the conceptual density with the frequency in which concept strings occur in the collection. In this way, concepts with high frequency and low density are likely to be wrong annotations, whereas concepts with low frequency and relative low density are not relevant to the signature. In both cases, concepts are removed from the signature. Notice that this reduction contributes to the increase of both the compactness and the performance of the ontology construction process. In our experiments the density threshold is around 0.1, under which concepts can be potentially rejected. The resulting groups constitute the signatures for the experiments.

Figure 5 shows the size of the output ontology as the size of the signature increases for both versions of strategy ASA-ST (tree and DAG). The size of the ontology (axis Y) is measured in number of edges since both versions extract an ontology with the same amount of nodes. The increase of edges in the DAG version is due to the fact that UMLS mixes different classifications over the same concepts, and this leads to multiple inheritance. Overall, we can predict a linear tendency of the ontology size as the signature increases in both versions.

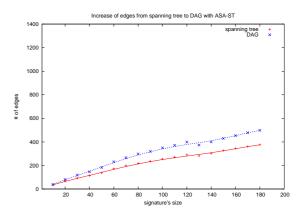


Figure 5: Signature's size vs. ontology's size.

We have also evaluated the temporal complexity of both ASA-ST versions (see Figure 6). Although

<sup>&</sup>lt;sup>1</sup>Health-e-Child Project: http://www.health-e-child.org

the time required to generate a DAG is slightly larger, the general tendency is linear in both cases.

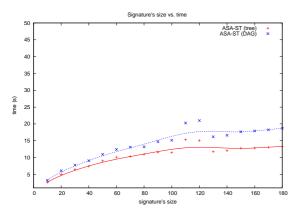


Figure 6: Signature's size vs. temporal complexity.

# **5** CONCLUSIONS

Using semantics and managing efficiently very large domain knowledge resources suffers severely from scaling problems. The framework presented in this paper is a way of overcoming these difficulties. Developers can use it to quickly create an application logic-based ontology that covers just a small part of the knowledge resource. Moreover, ontologies generated and enriched with a DAG-structure preserve the taxonomic relationships over the signature concepts.

Evaluation has shown ontologies generated with this framework keep their size relatively small and manageable according to their signature. Therefore, the framework presented achieves scalability by providing compact and logic-based OWL ontologies from very large knowledge resources.

In the future, we plan to study different relevance judgements for the assessment phase that help filtering out semantic annotations. We are also interested in finding an automatic method for the calculation of a threshold in this phase. Other future lines focus more on the relationships of the knowledge resource and in finding efficient indexing techniques that allow to efficiently manage them.

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