Enriching Semantic Relations of Basic Sciences Ontology

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ABSTRACT: Ontology is the tool for representing knowledge in the fields of knowledge organization and artificial intelligence, and in the past decade, has gained attention in the semantic web as well. The main necessity in developing an ontology is generating a hierarchical structure of the concepts and the next requirement is creating and determining the type of the semantic relations among concepts. The present article introduces a semi-automated method for enriching semantic relations in the basic sciences ontology, which was developed based on domain-specific thesauri. In the proposed method, first the hierarchical relations in the ontology are reviewed and refined in order to distinguish their different types. In the next step, the concepts in the ontology are classified and the semantic relations among the concepts, based on the associative relationships in the thesaurus and semantic relation patterns extracted from a top-level ontology, are distinguished and added to the ontology. Using this method, semantic relations in the area of chemistry in the basic sciences ontology were refined and enriched. Almost seventy percent of the associative relationships were directly converted to semantic relations in the ontology. The remaining thirty percent are the inter-concept relations that can be concluded from other relations if the other associative relationships are correctly converted to semantic relations.

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1.0 Introduction

Ontology is a branch of philosophy concerned with the study of what categories of entities exist and how each of them is related to each other (Lowe 2006). In recent decades, the word ontology has been accepted and used in other fields such as computer science and information science. In the former, ontology is used to refer both to a vocabulary expressed in a knowledge representation language, and a kind of theory where one explains phenomena using facts and rules. In the latter, ontological principles may be used to support the building of categorical structures for representation of the content of documents (Almeida 2013). In practice, an ontology is expressed as a taxonomy of concepts linked by Is-a, part-whole and attribute-value relations, sometimes enriched by other kinds of relations as well as additional rules or constraints called axioms (Khoo and Na 2006). Ontology can be classified into top-level, task, domain, and application ontologies based on its dependence on a particular task or point of view (Guarino 1997). The interdependencies between these four ontology types are shown in Figure 1. Since a top-level ontology explains general concepts which are independent of a particular issue or area, domain ontologies describe the vocabulary related to a specific area of expertise by specifying terms introduced in the top-level ontology. Similarly, in task ontologies, vocabulary of the overall task or activity is specified by assigning terms introduced in the top-level ontology. Likewise, the concepts needed for a particular application can be defined by combining concepts from both a domain and a task ontology to develop an application ontology.

However, developing domain ontologies is a time-consuming and laborious task, so many ontology developers try to facilitate and speed up this process by reusing other resources such as thesaurus. A thesaurus is a collection that contains items within a selected domain. It allows for the specification of the attributes of items as well as the definition of equivalence, hierarchical, associative and/or contrast semantic relationships between its items (Pieterse and Kourie 2014). According to Almeida (2011) a thesaurus is a tool for vocabulary control and its semantics are used by humans, in contrast to the semantics in ontology which are used by machines. The traditional aim of a thesaurus is to guide indexer and searcher to choose the same term for the same concept (ISO 2011). The major difference between an ontology and a thesaurus is the richer set of relations used in an ontology (Khoo and Na 2006).

In a thesaurus, terms stand for concepts. Each concept can be represented by one or more terms but just one term is selected as the preferred term per language for a concept. An equivalence relationship should be established between a preferred term and its corresponding non-preferred term. Hierarchical (BT/NT) and associative (RT) relationships are established only between preferred terms. Whenever the scope of one concept falls completely within the scope of other concept, hierarchical relationship should be established between them. Additionally, the associative relationship is used between terms that are conceptually or semantically related and do not belong to the same hierarchical structure.

While there is an opinion that thesauri can be simply reused as ontologies (Simprel 2009), some other authors emphasize the need to re-engineer thesauri to be used as ontology (Kless 2015). Pieterse and Kourie (2014) define ontology as an extension of a thesaurus, which contains items representing concepts, their attributes and relations in a more formal structure than required for thesauri in general. In fact, a thesaurus contains semantic information and hierarchical structure that make it an appropriate resource for ontology construction, nevertheless the semantically different kinds of relationships that are summarized as hierarchical relationships and associative relationships in thesauri have to be distinguished explicitly in ontologies (Kless 2015).

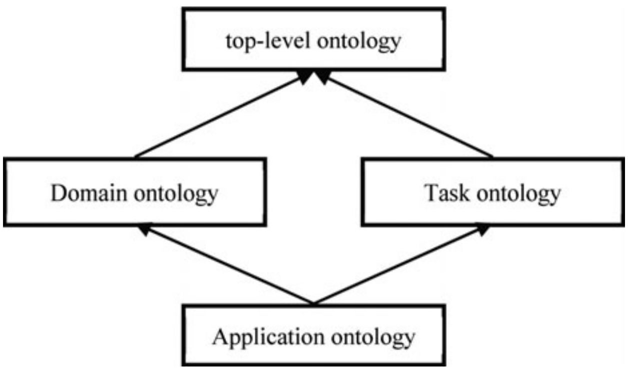

Figure 1. Ontology types according to their level of dependence on a particular task or point of view (Guarino 1997).

In particular, Soergel et al. (2004) and Kawtrakul et al. (2005) tried to reengineer AGROVOC into ontology by building the ontology on the information contained in thesaurus and refined the information as needed. Moreover, Huang et al. (2007) proposed a method in which the "Inspec" thesaurus is used to enrich core ontology in the IT domain. Research in the field of ontology in Persian language has mainly focused on Farsi WordNet and lexical ontologies (Shamsfard 2008, Montazery and Faili 2010). Moreover, Khosravi and Vazifedoost (2007) worked on re-engineering the ASFA thesaurus into ontology in the field of library and information science.

Another method in converting thesaurus to ontology is proposed by Kless et al. (2012) which includes eight different steps that guarantee the lowest rate of error and incompatibility in the resulting ontology. The method makes use of top-level ontologies and was derived from the structural differences between thesauri and ontologies. However, as the authors themselves acknowledge, when implementing this re-engineering method, only a number of steps may be done automatically and it seems that automating the rest of the steps is infeasible, and using this method for a large number of terms (one or more thesauri), is technically impossible.

Due to the need for various ontologies in the Persian language, we decided to build a domain ontology in the field of basic sciences using the domain-specific thesauri compiled in IRANDOC, to be used as a reference for developing application ontologies. By examining the steps of the method proposed by Kless et al. (2012), we found that our approach is completely consistent with the basic steps in developing ontology, and we tried to take the principles of this approach into consideration all through. In the next section, generating the ontology based on the thesaurus is briefly explained, and afterwards, the enrichment method of the semantic relations in basic science ontology, which can semi-automatically be executed by domain experts, is described.

2.0 Building basic science ontology

We used bilingual (Persian/English) thesauri of basic sciences (chemistry, physics, biology, geology, and mathematics), which were previously developed at IRANDOC, as resources for ontology construction. The thesauri contained tens of thousands of specialized terms and relationships between them that have been collected over several years by domain experts. Since the terms of each area were determined by different experts, common concepts in the thesauri had to be expressed in the same way so that they can be used in a single ontology for basic sciences. For this purpose, an application was designed to synchronize terms and using this software, common concepts in thesauri were investigated by domain experts and differences between them were resolved.

After complete and precise synchronization of concepts in thesauri according to the ISO 25964 standard (ISO 2011), all thesauri in various areas of basic sciences were integrated and a macro thesaurus was created. In the ISO 25964 standard, each concept in the thesaurus is shown by a preferred term for any language and with any number of non-preferred terms, and scope notes, annotations, and hierarchical and associative relationships are connected to a whole concept rather than the preferred term.

In the next stage, the ontology was designed based on the macro thesaurus. At this stage, the thesaurus was changed syntactically into ontology. Since ISO 25964 is concept-based, all the thesaurus concepts were considered as the ontology classes and thesaurus terminology as class labels. Definitions, scope notes, and other notes and information were transferred into comments. Hierarchical relationships in the thesaurus were considered as generic or Is-a relations in the ontology whereas associative relationships were considered as a part of formal specification of a concept as a class in ontology and not transferred into ontology relations in this stage. Finally, the macro thesaurus was converted to ontology based on the syntactic conversion defined in the OWL language. A further description of designing conceptual model of ontology and formalizing it is explained in Beheshti and Ejei (2014). A part of the developed ontology is shown in Figure 2.

3.0 Semantic relations enrichment method

After implementing the ontology, we need to distinguish the accurate meaning of its relations. These relations include hierarchical relations and also associative relationships. The difference between the applications of thesaurus and ontology and the ambiguity in existing relationships in thesaurus, make the refinement process necessary. The hierarchical relationship in thesaurus may be one of the three types: generic, hierarchical whole-part, or instance relationship. However, in practice few thesauri make the distinction between them and therefore, this kind of hierarchical relationship has insufficient precision for ontologies. Likewise, the associative relationship is very ambiguous. It is used in many different situations and it links any two related terms with non-hierarchical relationship. Thus, its semantic is unspecified and cannot be used for reasoning.

As a result, the relations of developed ontology needed to be refined and converted to more precise ones. Our proposed approach for refining and enriching ontology relations is similar to Huang's method for enriching core ontology with domain thesaurus (Huang et al. 2007). The

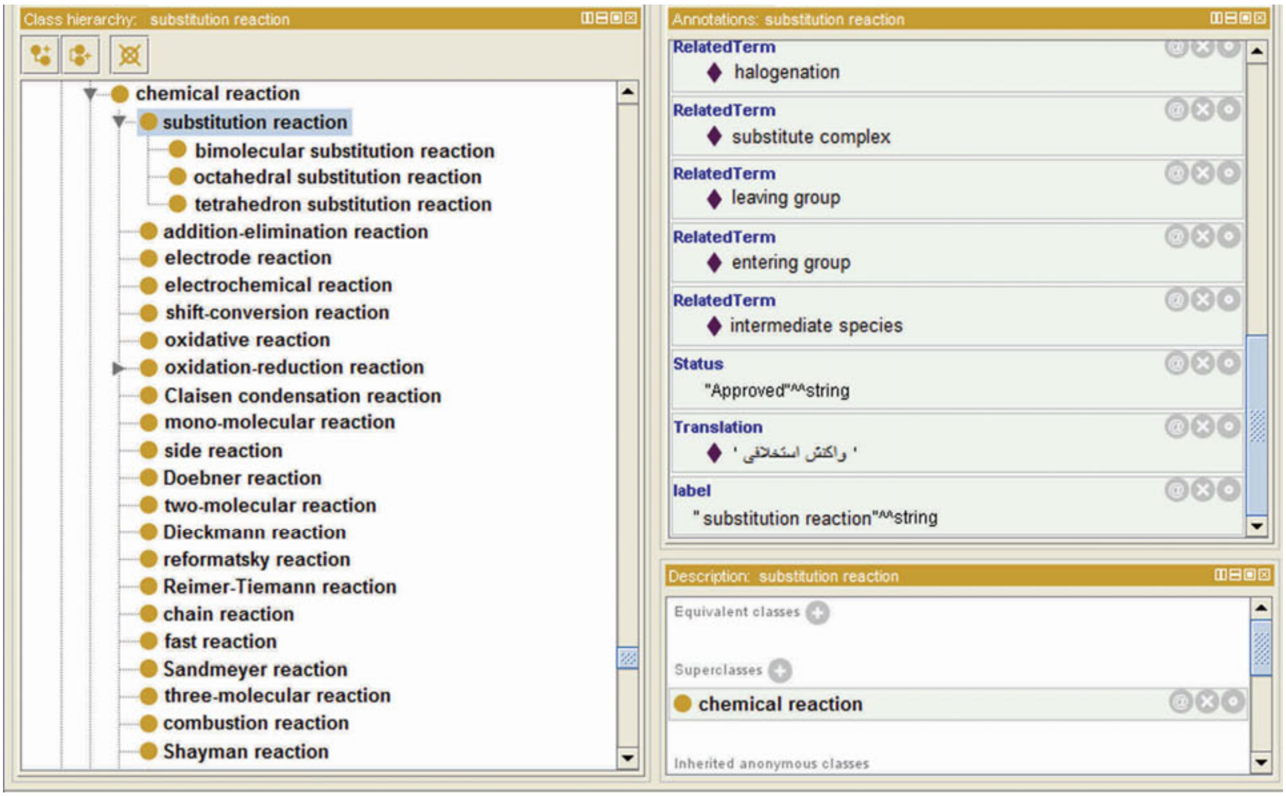

Figure 2. Part of developed ontology

enrichment process includes three main steps: First, the hierarchical relations are refined in order to differentiate the generic and whole-part ones. The second step is to align the concepts of our developed ontology to a top-level ontology. In this step, the type of each concept is determined based on the main concept categories in top-level ontology. The last step is to convert relationships into semantic relations. This is done by extracting semantic relation patterns from top-level ontology and finding the patterns which match with each relationship of our developed ontology. The appropriate pattern is selected by the domain expert based on the relationship's sematic.

3.1 Refining hierarchical relations

To develop ontology, we already transformed all of the hierarchical relationships in the thesaurus into generic relations of ontology but the semantic of some of these relations is not the same as an Is-a relation. They may show whole-part relationship between concepts and must be specified from structural relationships. If we assume each concept as a class, Is-a relations, also called generic, mean all instances of subclass are also instances of its superclass, and subclass inherits all properties of the superclass.

For example, the "اتم" (/atom/: atom) concept has some narrower terms like "اتم فلزی" (/atom-e felezi/: metallic atom), "اتم الکترونگاتیو" (/atom-e electronegative/: electronegative atom), "الکترون" (/electron/: electron) and "هسته" (/haste/: nucleon) in the thesaurus. At ontology development process, the relationships between "atom" and all these concepts were transformed into Is-a relations. However, the relationship of "atom" with two first concepts can be accepted as generic relations in ontology because "metallic atom" and "electronegative atom" are types of "atom", but the relationship of "atom" with "electron" and also with "nucleon" cannot be accepted as an Is-a relation in ontology and must be changed to a whole-part relation. The specific type of each whole-part relation is distinguished at the enrichment step.

In order to facilitate the refining process, we ought to use some rules. The main rule is that if a term has the same headword with its narrower term, their relationship is of generic relation type. So, the relations between such concepts in ontology remain unchanged. An example for this rule is "atom" and "electronegative atom" which have the same headword "atom." The second rule is defined for concepts that have a relationship with a concept which reflects a laboratory accessory or part of it. This kind of relation is often a part-whole relation and must be separated from generic relations.

Most of the concepts in the basic science ontology are functional complexes and according to Guizzardi (2009) parthood relations between functional complexes are neither transitive nor intransitive, but non-transitive, i.e., transitive in certain occasions and intransitive in others. The problem of transitivity in the refined part of the basic science ontology occur in parthood relations where different parts of laboratory accessories and also their different types exist in hierarchy. In return some others like the parthood relations between subgroups of periodic table are transitive.

3.2 Categorizing concepts

For enriching ontology relations, at first we choose a top-level ontology to align our developed ontology to it and use its set of formally defined semantic relations. These semantic relations are constrained in their domain and range with reference to the top-level ontology and can be used to determine the semantic relations corresponding with associative relationships between concepts. The alignment process has been done by classifying the developed ontology concepts into concepts in the top-level ontology which is the prerequisite for enriching relations of developed ontology by classifying them into semantic relations defined on the top-level ontology.

We start the enrichment process from chemistry domain and align the chemistry segment of our developed ontology to "ChemTop" (Stenzhorn et al. 2008), a top-domain ontology defined to describe the foundational entities needed to characterize phenomena in the domain of chemistry and to interface both top and domain ontologies. ChemTop is based on the top ontology BFO (Basic Formal Ontology) (Smith et al. 2005) and can be used as a top-level ontology for domain ontologies of chemistry area (Gomez-Perez 2013). ChemTop also uses a set of formally defined relations from RO (the Relation Ontology) (Smith et al. 2007), which can be utilized to decide the association of concepts in the chemistry domain.

For aligning the chemistry segment of the developed ontology to the top-level ontology, the concepts on the top-level of ChemTop are considered as semantic categories and the top-level concepts of developed ontology are classified into target categories. The main semantic categories are "material entity," "immaterial entity," "information entity," "process," "role," "time," "condition," "disposition," "value region" and "quality." The semantic category of other concepts in the developed ontology is assumed to be identical with the category of their top-level concept in the hierarchy. For example, "chemical reaction" is a top-level concept and is classified as "process"; so its class is set to be the subclass of the "process" concept in the top-level ontology and all concepts which have a generic relation with "chemical reaction" are categorized as "process." Therefore, concepts like "substitution reaction" and its subclasses "bimolecular substitution reaction" and "tetrahedral substitution reaction" are all of the type "process" based on their top-level concept category.

In order to facilitate the categorization of concepts, some rules are constituted. First, concepts which have the same headword are of the same category. For example, the concept category of "tetrahedral arrangement" is distinguished as "object quality" by the domain expert. We categorize "linear arrangement" as "object quality" as well, because its headword is the same as "tetrahedral arrangement." Second, a concept that its headword is showing an action like "extraction," "substitution" and "crystallization" should be categorized as "process." The label of these kinds of concepts typically ends with "-tion." Third, concepts which are parts of the same whole are commonly of the same category. One instance is "periodic table" which has two concepts as its part: "main group" and "subgroups." These two concepts are both of the same category and are classified as "information entity."

3.3 Using semantic relation patterns

The aim of this step is to generate a semantic relation between concepts that have associative relationships in the thesaurus. Associative relationships show relevance between concept pairs that are not hierarchically related, but are strongly related semantically or conceptually. This relationship is bilateral in the thesaurus. As all concepts are classified and their categories are distinguished, we can use semantic relation patterns in order to enrich existing relations between concepts in our ontology. The patterns are extracted from the top-level ontology. Each pattern includes definition, label, domain and range of relation and also inverse of it. Table 1 shows some of the patterns. The definitions of patterns are not shown in the table.

In Table 1, each semantic relation has a label which expresses the type of the semantic relation between two concepts. A pattern can be applied to decide the relation between two concepts if the type of the first concept coincides with the domain of pattern and the type of the second concept conforms to the range of pattern. Inverse relation demonstrates the relation of the second concept with the first concept. The domain and the range of inverse relation correspond to the range and the domain of the original relation respectively. Some semantic relations can have several patterns, for example, the "has outcome" relation can be defined from a concept with the "process" type to concepts with the "material entity," "immaterial entity" or "information entity" types. These

Relation Label	Relation Properties		Pattern and Example
abstract part of	**Domain**	information entity	Pattern: Information entity < *abstract part of* > information entity Example: main groups < *abstract part of* > periodic table
	Range	information entity	
	Inverse	has abstract part	
process quality of	**Domain**	process quality	Pattern: process quality < *process quality of* > process Example: trans effect < *process quality of* > ligand replacement
	Range	process	
	Inverse	has process quality	
process role of	**Domain**	process role	Pattern: process role < *process role of* > process Example: leaving group < *process role of* > substitution reaction
	Range	process	
	Inverse	has process role	
component part of	**Domain**	material entity	Pattern: material entity < *component part of* > material entity Example: hydrogen < *component part of* > acids
	Range	material entity	
	Inverse	has component part	
component part of	**Domain**	immaterial entity	Pattern: immaterial entity < *component part of* > material entity Example: hydrogen bond < *component part of* > ammonia
	Range	material entity	
	Inverse	has component part	
agent in	**Domain**	material entity	Pattern: material entity < *agent in* > process Example: ammonia < *agent* in> preparation of amines
	Range	process	
	Inverse	has agent	
patient in	**Domain**	material entity	Pattern: material entity < *patient in* > process Example: crystal < *patient in* > crystal growth
	Range	process	
	Inverse	has patient	
outcome of	**Domain**	material entity	Pattern: material entity < *outcome of* > process Example: crystal < *outcome of* > crystallization
	Range	process	
	Inverse	has outcome	
outcome of	**Domain**	immaterial entity	Pattern: immaterial entity < *outcome of* > process Example: gamma ray < *outcome of* > radioactivity
	Range	process	
	Inverse	has outcome	

Table 1. Some semantic relation patterns extracted from top-level ontology

patterns show that the outcome of a process can be any of these three entities.

Some patterns indicate the whole-part relations. The type of relations determined as whole-part in the refinement step, will be determined more specifically in this step based on these semantic relation patterns. For instance, the relation of "periodic table," which is an information entity, with the concepts of "main groups" and "sub-groups" is distinguished as a whole-part relation in the refinement step. In this step, the relation is determined as "has abstract part" type according to the patterns above. According to Table 1, for "atom" and "electron" concepts, both of which are material entities, more than one pattern can be used. In such cases, the domain expert should choose and implement the appropriate pattern based on the two concepts' association semantic. In this example, the relation between "atom" and "electron" is "has component part."

To convert the associative relationships between concepts to semantic relations, other patterns can be used. For example, the concept of "substitution reaction" has an associative relationship with the concepts of "leaving groups" and "entering groups" in the thesaurus. The type of "substitution reaction" is "process" and the other two concepts are considered "chemical role" type which is a sub-class to "role." Therefore, based on the patterns extracted, the relation between the concept of "substitution reaction" and the concepts of "leaving groups" and "entering groups" is determined as "has process role." Another example is the relationship between the concepts of "linear combination of atomic orbitals" and "molecular orbital" which are related terms in the thesaurus. The first concept is determined as the "process" type and the second as "immaterial entity." Based on the semantic relations patterns and the meaning of these two concepts' association, the domain expert determines the relation of these two concepts as the "has outcome" type.

4.0 Implementing the ontology enrichment method

Based on the proposed method, which was explained in the previous section, refining and enriching semantic relations in an ontology should be done in three steps: refining hierarchical relations and separating whole-part relations from the generic ones, categorizing concepts based on the main classes defined in a top-level ontology, and finally, refining the semantic relations in the ontology using semantic relations' patterns extracted from the top-level ontologies. According to this, the domain expert first distinguished whole-part relations through studying all the hierarchical relations defined in the ontology and another domain expert assessed and revised the relations' refinement. In the second stage, the domain expert classified all the concepts placed on top of the hierarchies in the thesaurus's tree diagrams according to the levels defined in the chosen top-level ontology. These concepts included almost one third of the ontology's concepts. Afterwards, the rest of the concepts' categories were determined based on the types identified for these concepts.

Finally, five hundred associative relationships in the area of inorganic chemistry, which were chosen according to the domain expert's main expertise, were considered for refinement. The types determined for the concepts in this field were evaluated by the second domain expert in the previous step. The semantic relations that could replace the associative relationship were determined through matching the types of the two concepts with associative relationship in thesaurus with the semantic relation patterns' domain and range extracted from top-level ontology. Finally, one semantic relation that showed the right relation between two concepts was chosen among determined relations, based on the domain expert's opinion. The selected semantic relation is the one that will be added to the ontology for enrichment.

Almost three hundred fifty semantic relations were detected between concepts through implementing this method. The unconverted relations were among concepts in which their association was definable through one or more other concepts and were not directly related. In such cases, if the relations of each concept with the intermediate concepts are correctly added to the ontology, the unconverted relations can be inference from these relations and there is no need for adding direct relations to ontology.

5.0 Conclusion

In this article, a method for enriching semantic relations in basic science ontology, which was built upon thesauri published in different areas of basic science, was introduced. A thesaurus is a set of specialized terminologies and has hierarchical relationships and also relationships that show the association between the concepts in them. These associative relationships should be determined more precisely as semantic relations in the ontology. In order to do that, the semantic relations patterns, extracted from top-level ontologies, were used and the defined relations were matched with these patterns to determine the semantic relations among concepts and to add them to the ontology.

This approach currently has been applied on only one part of the basic science ontology, which is the area of chemistry. In order to do this, after inspecting all hierarchical relations and distinguishing whole-part relations from generic relations, all of the concepts were classified and a number of associative relationships were converted to semantic relations through matching semantic relations patterns.

Our next aim is to expand this approach for it to be used in other parts of ontology and also to create tools in order to simplify concepts' classification and semantic relations determination, so that semantic relations enrichment is done easier and faster in other parts of the ontology.

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