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Instance-based Hierarchical Schema Alignment in Linked Data

링크드 데이터에 대한 인스턴스 기반 온톨로지 매핑

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Abstract

Instance-based Hierarchical Schema Alignment in Linked Data

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Along with the development of Web of documents, there is a natural need for sharing, exchanging, and merging heterogeneous data to provide more comprehensive information and answer users with more complex questions. However, the data published on the Web are raw dumps that sacrifice much of the semantics that can be used for exchanging and integrating data. Resource Description Framework (RDF) and Linked Data are designed to expose the semantics of data by interlinking data represented with well-defined relations. With the profusion of RDF resources and Linked Data, ontology alignment has gained significance in providing highly comprehensive knowledge embedded in disparate sources. Ontology alignment, however, in Linking Open Data (LOD) has traditionally focused more on the instance-level rather than the schema-level. Linked Data supports schema-level matching, provided that instance-level matching is already established. Linked Data is a hotbed for instance-based schema matching, which is
considered a better solution for matching classes with ambiguous or obscure names.

In this dissertation, the author focuses on three issues in instance-based schema alignment for Linked Data: (1) how to align schemas based on instances, (2) how to scale the schema alignment, (3) how to generate a hierarchical schema structure.

Targeting the first issue, the author has proposed an instance-based schema alignment algorithm called IUT. The IUT builds a unified taxonomy for the classes from two ontologies based on an instance-class matrix and obtains the relations of two classes by the common instances. The author tested the IUT with DBpedia and YAGO2, and compared the IUT with two state-of-the-art methods in four alignment tasks. The experiments show that the IUT outperforms the methods in terms of efficiency and effectiveness (e.g., costs 968 ms to obtain 0.810 F-score on intra-subsumption alignment in DBpedia).

Targeting the second issue, the author has proposed a scaled version of the IUT called IUT(M). The IUT(M) decreases the computations of the IUT from two aspects based on Locality Sensitive Hashing (LSH): (1) decreasing the similarity computations for each pair of classes with MinHash functions, and (2) decreasing the number of similarity computations with banding. The author tested the IUT(M) with YAGO2-YAGO2 intra-subsumption alignment task to demonstrate that the running time of IUT can be reduced by 94% with a 5% loss in F-score.

Targeting the third issue, the author has proposed a method to generate a faceted taxonomy based on object properties on Linked Data. A framework is proposed to build a sub-taxonomy in each facet with sub-data, extracted with an object property, with an Instance-based Concept Taxonomy generation algorithm.
called ICT. Two experiments demonstrate: (1) The ICT efficiently and effectively generates a sub-taxonomy with “rdf:type” in DBpedia and YAGO2 (e.g., costs 49 and 11,790 ms to build the concept taxonomies that achieve 0.917 and 0.780 on Taxonomic F-score). (2) The faceted taxonomies for Diseasome and DrugBank, efficiently generated based on multiple object properties (e.g., costs 2,032 and 2,525 ms to build the faceted taxonomies based on 6 and 16 properties), can effectively reduce the search spaces in faceted searches (e.g., obtains 1.65 and 1.03 on Maximum Resolution with 2 facets).

**Keywords:** Schema Alignment, Instance-based Matching, Linked Data, Scaling Alignment, Hierarchy Generation

**Student Number:** 2010-31375
# Contents

1  Introduction..................................................................................................................1

1.1 Background and Motivations ......................................................................................1

1.1.1 Data Integration and Schema Alignment ..............................................................1

1.1.2 From RDF to Linked Data .........................................................................................3

1.1.3 Schema Alignment in Linked Data .........................................................................5

1.2 Instance-based Schema Alignment .............................................................................9

1.3 Contributions of this Dissertation ..............................................................................13

1.4 Organization of this Dissertation ...............................................................................15

2  Preliminaries and Related Works ...............................................................................17

2.1 Preliminaries .............................................................................................................17

2.1.1 RDF and Linked Data ...........................................................................................17

2.1.2 Ontology and Schema Alignment in Linked Data .................................................20

2.2 Related Works .........................................................................................................23

2.2.1 Instance-based Schema Alignment .......................................................................23

2.2.2 Scaling Pairwise Similarity Computations .........................................................29

2.2.3 Automatic Taxonomy Generation .......................................................................32

3  Aligning Schemas with Subsumption and Equivalence Relations .......................36

3.1 Introduction .............................................................................................................36

3.2 Problem Definition ...................................................................................................38

3.3 Methods ....................................................................................................................41
Unsupervised Hierarchical Schema Structure Generation in Linked Data...

5.1 Introduction

5.2 Faceted Taxonomy for Linked Data

5.3 Framework

5.3.1 Facets Extraction

5.3.2 Instance Restriction and Redundancy Removal

5.3.3 Redundant Object Removal

5.3.4 Instance-object Matrix Generation

5.4 Generating Faceted Taxonomy

5.4.1 The Problem of Generating a Sub-taxonomy for a Facet

5.4.2 Concept Definition and Naming

5.4.3 Taxonomy Generation Algorithm

5.4.4 Instantiation and Taxonomy Refinement

5.5 Experiments

5.5.1 Task 1-Construction of Taxonomy with “rdf:type”

5.5.2 Task 2-Construction of Multiple Faceted Taxonomies

5.6 Results

5.6.1 Results of Task 1

5.6.2 Results of Task 2

5.7 Discussion

5.8 Conclusion

Future Works and Conclusion
6.1 Future Works..............................................................................................................134

6.1.1 Similarity Measures for Instance-based Schema Alignment............134

6.1.2 Ontology Evolution for Instance-based Schema Alignment ..........135

6.1.3 Combining the IUT with Structure- and Lexical-based Methods ......136

6.1.4 Scaling the IUT with Parallel Computations.............................................137

6.1.5 Faceted Navigation and Search for Linked Data.................................137

6.2 Conclusion...............................................................................................................139

Bibliography..................................................................................................................142

초 록.................................................................................................................................152
List of Tables

Table 2-1: Comparison of schema alignment methods ...........................................27
Table 3-1: Statistic information of the data sets.........................................................49
Table 3-2: Results of subsumption alignment in YAGO2-YAGO2 .........................55
Table 3-3: Results of subsumption alignment in DBpedia-DBpedia .........................59
Table 3-4: Results of subsumption alignment in YAGO2-DBpedia .............................62
Table 3-5: Results of equivalence alignment in YAGO2-DBpedia .............................65
Table 4-1: Efficiency of scaling the IUT for alignment in YAGO2-YAGO2
\((v_s = 1,000)\)........................................................................................................87
Table 4-2: Precision of scaling the IUT for alignment in YAGO2-YAGO2
\((v_s = 10,00)\).........................................................................................................88
Table 4-3: Recall of scaling the IUT for alignment in YAGO2-YAGO2
\((v_s = 1,000)\)........................................................................................................88
Table 4-4: F-score of scaling the IUT for alignment in YAGO2-YAGO2
\((v_s = 1,000)\)........................................................................................................89
Table 5-1. Statistic of the data sets originally and after pre-processed ..........113
Table 5-2. Statistic of the two data sets.................................................................115
Table 5-3. Results of conceptualizing disease and drug instances with multiple
object properties .........................................................................................................126
Table 6-1. Summarization of the conditions for the proposed methods ..............141
List of Figures

Figure 1-1: Data integration methods.................................................................2
Figure 1-2: Data format evolution of Semantic Web........................................4
Figure 1-3: Growth of LOD..............................................................................6
Figure 1-4: An example of linked data set......................................................8
Figure 1-5: Classification of schema matching approaches..........................9
Figure 1-6: Equivalent concept alignment based on instances....................12
Figure 1-7: Structure of the dissertation.......................................................15
Figure 1-8: An example of RDF/XML and N-Triples formatted RDF documents.................................................................18
Figure 2-1: De-reference a Web resource......................................................19
Figure 2-2: Two strategies for scaling pairwise computations.....................30
Figure 3-1: A data example for ontology alignment.....................................38
Figure 3-2: Workflow of instance-based schema alignment with the IUT........41
Figure 3-3: An example of instance-class matrix generation.......................42
Figure 3-4: F-score and running time of the methods..................................52
Figure 3-5: Running time of the three methods for YAGO2-YAGO2............54
Figure 3-6: Running time of the three methods of DBpedia-DBpedia............58
Figure 3-7: Running time of the three methods of YAGO2-DBpedia for inter-subsumption alignment.................................................................61
Figure 3-8: Running time of the three methods of YAGO2-DBpedia for equivalence alignment.................................................................64
Figure 3-9: $\chi_s$ and $\chi_e$ for the IUT..............................................................69
Figure 4-1: The search spaces of different algorithms in Section 3.4............76
Figure 4-2: Workflow of scaling the IUT with the LSH................................78
Figure 4-3: An example of a matrix based on the instance-class matrix used in Section 3.3.2 with a permutated order of instances ................................................................. 80

Figure 4-4: An example of computing signatures with the fast MinHashing algorithm ................................................................................................................................. 82

Figure 4-5: Signatures and buckets with two hash functions ............................................ 83

Figure 4-6: S-curves of \(1 - (1 - s^v)^v_b\) with different combinations of \(v_r\) and \(v_b\) when using 50 hash functions ........................................................................................................ 84

Figure 4-7: Efficiency comparison of the IUT and the IUT(M) that with \(v_r = 2\) and \(v_s = 1,000\) ................................................................................................................................. 91

Figure 5-1. A faceted taxonomy for a sample of Linked Data ........................................ 98

Figure 5-2. The framework of faceted taxonomy construction ..................................... 101

Figure 5-3. An ongoing example of building a sub-taxonomy with an object property “Diseasome:possibleDrug” partially extracted from Diseasome. ........ 102

Figure 5-4. TF-score and running time of the methods ................................................. 120

Figure 5-5. TP-scores of ICT for DBpedia and YAGO2 with different \(\varphi\) .......... 123

Figure 5-6. Running time of building a sub-taxonomy with a single property. ....... 124

Figure 5-7. Average running time of building faceted taxonomies with different facets (properties) .......................................................................................................... 127

Figure 5-8. Maximum Resolution scores with different facets (properties). ........... 129

Figure 5-9. Number of top 500 important concepts in each sub-taxonomy in a faceted taxonomy. ........................................................................................................... 130


1 Introduction

1.1 Background and Motivations

1.1.1 Data Integration and Schema Alignment

Information, along with our human civilization development, is the basic human need. Data that supplies users with abundant information is stored scattered in different repositories. Along with the increasing of data, there is a natural need of sharing, exchanging, and merging heterogeneous data to provide more comprehensive information and answer users with more complex questions. For example, an integration of data on diseases and genes can help users to better understand the mechanism of diseases. The data integration minimizes the inconsistency of data formats and specifications, and decreases redundant data in different sources.

Integration of heterogeneous data sources have been studied (Batini, Lenzerini, & Navathe, 1986; Doan & Halevy, 2005; Lenzerini, 2002). The first popular solution is to build a data warehouse on top of existing databases (Gardner, 1998), which is considered as a tightly coupled solution that reconciles heterogeneous data into a single repository on the physical level. The limitations, such as the invalidation of the warehouse when sources are updating, make this solution be replaced with loosening coupled solutions. A unified view of two independent but overlapped databases is used. This approach needs to build an integrated schema or sometimes a medicate schema that is recognized as Global
Schema Pattern. The object of this method is to unify data, which heavily relies on the stability of data sources. When the structures of some data sources change, the whole unified global schema needs to be redefined (L. Xu, Xu, Tjoa, & Chaudhry, 2007). Another solution is using a transformation pattern (Czarnecki & Helsen, 2006) to exchanging data instead of unifying data. The two methods both require the establishment of correspondences between schemas of different data sources. Therefore, schema alignment or schema matching is one of the fundamental tasks in realizing data integration.

Figure 1-1: Data integration methods.
1.1.2 From RDF to Linked Data

Along with the development of the Internet, more and more data are published on Web that lowers the expense of publishing and accessing information. The data published on the Web are raw dumps formatted as CSV, XML, or HTML tables, which sacrifices much of the semantics (Bizer, Heath, & Berners-Lee, 2009). The semantics behind the data defines the context or meaning of the data, and helps exchanging data in business or other areas. In traditional hypertext Web, semantics of a document is implicit. For example, “apple” can denote an information technology company or a kind of fruit in different documents. Exchanging data between documents sometimes require more man-powers to understand the semantics behind documents.

Therefore, expressing information under a description framework is needed. Resource Description Framework (RDF) supports data merging and schema evolution by explicating the semantics behind data ("Resource Description Framework (RDF),"). RDF is designed to expose the semantics of data for machines to understand. The concepts used in the schema of one data set are defined and connected with other related concepts in the same data under an RDF document. For example, the same concept “apple” used in two different data sources, can be distinguished by the definitions of the concept “apple” with two RDF documents. Even though, the semantics can be exposed with RDF, the data interlinking between different sources still not be accomplished. In order to create a global information space of both linked document and data, data (i.e., entities that are classes or instances) contained in RDF documents starts to link, which is
called Linked Data. Linked Data refers to the data set that is published on the Web with a machine-readable format (e.g., RDF) and links to external RDF data sets, and further can be linked as an external data set for other RDF data. Figure 1-2 shows the evolution of data format in Semantic Web.

![Figure 1-2: Data format evolution of Semantic Web.](image)
1.1.3 Schema Alignment in Linked Data

Linked Data describes a method for publishing structured data and has become popular for connecting distributed data sets across the Web. During the past few years, the size of Linking Open Data (LOD) ("Linked Data - Connect Distributed Data across the Web," has increased gradually as Figure 1-3 shows, reaching 32 billion triples in 2011 ("Linked Data on the Web (LDOW2012)," 2012). Different universities and institutes published their own linked data sets and ontologies in diverse domains, such as DBpedia ("DBpedia," and YAGO2 ("YAGO2s: A High-Quality Knowledge Base,")) that are domain independent, and the Gene Ontology (GO) ("Gene Ontology Consortium," 1999) that is domain dependent (biomedical). Different entities (e.g., instances or classes) can be easily connected and searched from the Web by with Linked Data. For example, a connection can be easily found by using the link

"<Diseasome:3166 (Migraine without aura, susceptibility to, 157300)> <Diseasome:possibleDrug > <DrugBank:DB01427(Amrinone)>". The overlaps of linked data sets published in different areas bridge the gaps between local knowledge and related areas, and provide users with comprehensive knowledge. In the same example, connecting Diseasome ("Diseasome," to DrugBank ("DrugBank," helps users to know that the drug “DrugBank:DB01427(Amrinone)” can be used for the disease “Diseasome:3166(Migraine without aura, susceptibility to, 157300)”, and further get more information of the drug “DrugBank:DB01427(Amrinone)” in detail.
Figure 1-3: Growth of LOD. (this figure is originated from the paper (Heath & Bizer, 2011).)
Driving by the benefits behind the interoperability and information integration, ontology alignment has been studied for years (S. Wang, Englebienne, & Schlobach, 2008), but it still lacks the study in Linked Data. The terms “alignment” and “matching” denote a process in which to find correspondences between concepts, whereas mapping can be defined as the products of alignment or matching (Bellahsene, Bonifati, & Rahm, 2011; Miller, Haas, & Hernández, 2000). Conventionally, “alignment” is frequently used for Ontology and “matching” is primarily used in Database area (Bellahsene et al., 2011). In order to avoid the ambiguities that may affect the understanding of readers, the author uses “alignment” primarily to indicate the process of finding correspondences.

The data in a linked data set normally are constituted of two parts: assertions and terminologies. The assertions in a link data set normally contain the information about instances. For example, as shown in Figure 1-4, an entity “Dbpedia:Gannys” is contained by four triples: (1) has a name “Gannys”, (2) is a type of “DBpediaOntology:General”, (3) is same as “FreeBase:m.04n2vn1”, and (4) is the commander of the entity “Dbpedia:Battle_of_Antioch(218)”. The terminologies contain the information about classes. For example in the same figure, “DBpediaOntology:General” is a sub-class of “DBpediaOntology:Person”.

Therefore, ontology alignment in Linked Data includes the alignment in A-Box (Assertion Box) and T-box (Terminology Box). The mappings for A-Box known as instance-level mapping (i.e., aligning instances from different ontologies) have received most attention in research, whereas T-Box mappings known as schema-level mapping are little studied (i.e., aligning schemas from different
ontologies) (P. Jain, Hitzler, Sheth, Verma, & Yeh, 2010; Parundekar, Knoblock, & Ambite, 2010). For example, in Linked Life Data ("Repository overview - Linked Life Data," 2009), only instances are mapped between different data resources but schema-level mappings are missing. With the schema-level mapping, a consumer can model the local data from other sources in terms of their own knowledge. Furthermore, missing ontology annotations and recommendations for possible ontology associations can be obtained (Parundekar et al., 2010). This dissertation focuses on schema alignment in Linked Data.

Figure 1-4: An example of linked data set. (this is a simplified version of DBpedia.)
1.2 Instance-Based Schema Alignment

The methods for schema matching (alignment) can be generally classified into two kinds: schema-based and instance-based schema alignment (Rahm & Bernstein, 2001). Please note that the term “instance-based alignment” in this dissertation denotes schema alignment using instances, whereas the term “instance alignment” signifies aligning instances from different ontologies. The schema-based matchers can further be classified into lexical-, structural- and background-based matchers by the methods with the similarity calculations (Rahm & Bernstein, 2001). Without globally standardized naming schemas, lexical-based matchers are incapable of finding mappings when schema elements have ambiguous or obscure names. For example, lexical-based matchers may fail to discover the equivalence mapping from

**Figure 1-5**: Classification of schema matching approaches. (this figure is originated from the paper (Rahm & Bernstein, 2001).)
“DBpediaOntology:Nerve” to “YAGO:FiberBundle”. The structural-based and background-based methods fail to find mappings when two ontologies have different granularity in the schema (Kirsten, Thor, & Rahm, 2007). For example, BLOOMS (P. Jain et al., 2010), a lexical- and structural-based matcher for Linked Data, fails to find the subsumption relations between DBpedia ontology and YAGO2 used in Section 3.4. Even though BLOOMS outperformed traditional schema alignment methods, it is still not sufficient enough in terms of running time (efficiency) and F-score (effectiveness).

A class (concept) represents a whole group of individuals sharing common attributes. In ontology, a class is defined by intension or extension ("Class (philosophy),"). The intension of a class is a set of properties (attributes) shared by instances to which they apply, whereas the extension is a collection of instances (individuals) to which they apply.

The problem of identity is a long-standing debate in philosophy, and in linked data, it is no exception. In Leibnitz’s Law ("The Identity of Indiscernibles," 2010), two objects are identical, if they have the same description on the intension, which is adapted to define class equality as well in OWL 2 (Carroll, Herman, & Patel-Schneider, 2012). Therefore, the alignment of two classes based on the intensional description (properties) is frequently used for the upper ontologies where the classes are mostly defined intensionally, such as ontologies in OBO Foundry. For those ontologies constructed by the software developers and engineers without training in ontology modeling in Linked Data, the extensional description
can stand to match classes, as the identifying characteristics for the identity conditions (Guarino & Welty, 2002).

It is difficult to keep the consistency of using identity with its logical definition in the wild, since there are diverse varieties of perceived identity, such as “identical but referential Opaque”, “identical as claims”, “matching”, and “similar” (Halpin, Hayes, McCusker, McGuinness, & Thompson, 2010). Without considering the first two issues (i.e., “identical but referential Opaque” and “identical as claims”) in the ideal knowledge representation, the “matching” and “similar” are mostly considered to model identity. In OWL 2, two classes are defined as “Owl:equivClass” if they have the same extensional definition (i.e., “matching”) (Carroll et al., 2012). For example, in Figure 1-6 (a), “class 1” and “class 1’” are considered same when the two classes have the same four instances. More practical in SKOS, the classes are defined as “Skos:exactMatch” if they have a high degree of confidence (e.g., similarity) to support themselves to be used interchangeably, or as “Skos:closeMatch” if they reach a certain level of similarity ("SKOS Simple Knowledge Organization System Reference," 2009).

Similar with the definition used in SKOS for identity in non-ideal knowledge representation, the author considers that two concepts are equivalent if they reach a certain level of similarity (i.e., $\chi_e$ used in the proposed method) in this dissertation. Similarly, instead of adapting the strict definition of the subsumption in ideal knowledge representation, the author considers two concepts have a subsumption relation if they reach a certain level of containment (i.e., $\chi_s$ used in the proposed method).
A more broadly applicable case of instance-based schema alignment is how to determine a correspondence of two classes from different ontologies (Bellahsene et al., 2011). In Linked Data, instances are linked with “Owl:sameAs”. Therefore, two classes are equal if two extensions of the classes are fully one-to-one interlinked with “Owl:sameAs”. For example, in Figure 1-6 (b), “class 1” have four instances that are same with the instances belonging to “class 1’”, and we consider “class 1” are same with “class 1’”. The classes comparison based on the extensional definition requires that the instances from different ontologies are inter-linked. Therefore, Linked Data satisfies the requirement of instance-based schema alignment.

(a) When two classes sharing common instances.

(b) When two classes sharing aligned instances.

Figure 1-6: Equivalent concept alignment based on instances.
1.3 Contributions of this Dissertation

With abundant instantiation on schema in Linked Data, the extensions of a concept can provide better interpretation for a concept, where it has ambiguous or obscure name. Therefore, the object of this thesis is to align of schema in Linked Data with the help of instances. In this dissertation, the author discusses three issues in instance-based schema alignment for Linked Data, which are (1) how to effectively design an algorithm to align schemas, (2) how to scale the schema alignment with an efficient algorithm, (3) how to generate a concept hierarchy for an ontology without hierarchical schema structure. Please note that in this dissertation, the author uses hierarchy to denote a Directed Acyclic Graph (DAG) graph that only contains subsumption relations between concepts, and uses taxonomy to denote a graph that contains multiple relations (e.g., subsumption and equivalence). The author lists the contributions as follows:

(a) The author proposes a new Instance-based Unified Taxonomy generation algorithm called IUT for aligning ontology in Linked Data. The IUT adapts the EXT (Heymann & Garcia-Molina, 2006) to build a unified graph to restrict the alignment search space, which is proved to be more efficient and effective than two state-of-the-art schema alignment methods (the Heuristic Mapper (HM) (Parundekar et al., 2010) and BLOOMS (P. Jain et al., 2010)) with four alignment tasks based on two well-known Linked Data sets, DBpedia and YAGO2 (e.g., costs 968 ms to obtain 0.810 F-score on intra-subsumption alignment in DBpedia).

(b) The author adapts a scaling method, Locality Sensitive Hashing (LSH) (Rajaraman & Ullman, 2011), to reduce the pair-wise computations in schema
alignment and call this method IUT(M). The author tests the IUT(M) with YAGO2 (YAGO2-YAGO2) in intra-subsumption task, and demonstrates that the IUT(M) can effectively reduce the 94% of the original running time with a loss of 5% F-score.

(c) The author proposes a robust method for generating a faceted taxonomy based on object properties of instances in Linked Data. The author has developed a framework that dynamically extracts data with a single object property and generates a sub-taxonomy in each facet based on an Instance-based Concept Taxonomy generation algorithm called ICT. Two experiments demonstrate: (1) The ICT efficiently and effectively generates a sub-taxonomy with “rdf:type” in DBpedia and YAGO2 (e.g., costs 49 and 11,790 ms to build the concept taxonomies that achieve 0.917 and 0.780 on Taxonomic F-score). (2) The faceted taxonomies with Diseasome ("Diseasome," ) and DrugBank ("DrugBank," ), efficiently generated based on multiple object properties (e.g., costs 2,032 and 2,525 ms to build the faceted taxonomies based on 6 and 16 properties), can effectively reduce the search spaces in faceted searches (e.g., obtains 1.65 and 1.03 on Maximum Resolution with 2 facets).
1.4 Organization of this Dissertation

**Figure 1-7:** Structure of the dissertation.

The author shows the organization of this dissertation in Figure 1-7. The focus of this dissertation is to align schemas based on instances. The author introduces the background of this dissertation in Chapter 1. In order to help readers better understand this dissertation, the author describes the preliminaries of the researches related to the dissertation in Chapter 2. Two concepts, (1) RDF and Linked Data, (2) schema alignment are introduced in detail. The author also introduces the related works in this chapter.

The precondition of this research is that schemas have a hierarchical structure. Therefore, this schema alignment problem can be separated for two scenarios: (1) when schemas satisfy the precondition (i.e., the schemas have hierarchical
structures) in Chapters 3 and 4, and (2) schemas do not satisfy the precondition in Chapter 5.

For the schemas having a hierarchical structure, the author details the methodology of instance-based schema alignment in Chapter 3. And in Chapter 4, the author presents the scaling algorithm based on the LSH.

For those do not have a hierarchical structure, the author proposes a method of generating a faceted taxonomy automatically in Chapter 5.

Finally, the author concludes the works of this dissertation, and lists several future works as the research extensions for this dissertation.
2 Preliminaries and Related Works

2.1 Preliminaries

2.1.1 RDF and Linked Data

The RDF is a metadata data model for conceptual description or information expression, which is proposed and promoted by World Wide Web Consortium (W3C) ("Resource Description Framework (RDF) Model and Syntax Specification," 1999). Similar with the classic modeling approaches, such as Entity-Relation (ER) diagrams, the RDF data models resources with statements. A resource in the RDF denotes a thing that is identified with a de-referencable URL. A resource can be anything on the Web. For example, a person named “Michael Jackson” identified with “http://dbpedia.org/page/Michael_Jackson (Dbpedia:Michael_Jackson)” is a resource. Sometimes, we also call a resource as an entity. A statement that consists of subject-predicate-object is called triple in the RDF. A subject in a triple is a resource (entity). An object can be an entity or a literal text. A predicate, also be called as attribute or property, demonstrates a relation between a subject and an object. The property can be two types: object-type and data-type. In a triple, if the object is an entity, the property is the object-type property. For example, the triple “<Dbpedia:Michael_Jackson><Rdfs:label> ’Michael Jackson’ ” contains the data-type property “Rdfs:label”. The triple “<Dbpedia:Michael_Jackson><foaf:homepage><http://www.michaeljackson.com>” contains an object-type property “foaf:homepage”. Since all resources are
described with properties, the vocabularies are defined and can be reused by other RDF documents. For example, the “rdfs:Class”, denoting that a subject is a class, is defined in “http://www.w3.org/2000/01/rdf-schema#”. The vocabularies defined by the RDF specification can be found in ("Resource Description Framework (RDF) Model and Syntax Specification," 1999).

Figure 2-1: An example of RDF/XML and N-Triples formatted RDF documents.

A RDF document can be presented with different formats, such as RDF/XML and N-Triples. RDF/XML is the first W3C serialization format historically, and it is gradually replaced with other formats that are more human-readable and less restrictions on the syntax of XML names ("Resource Description Framework
The author shows an example of RDF/XML and N-Triples formatted RDF documents of an RDF graph in Figure 2-1.

Linked Data uses RDF links to connect a subject with a de-reference URL in a local set to an object with a URL reference in an external data set. When an object is de-referenced over the HTTP protocol, a server of this URL will return an RDF document about the object to a client, which helps users to get more related information, object in this case, about a subject. The author shows the process of de-reference in Figure 2-2.

(a) De-reference a vocabulary URL

(b) De-reference a class or property URL

Figure 2-2: De-reference a Web resource. (this figure is originated from ("Best Practice Recipes for Publishing RDF Vocabularies,").)
2.1.2 Ontology and Schema Alignment in Linked Data

As the author mentioned in Section 1.2, Ontology in computer science and information science is a way of presenting knowledge. Components, such as classes, instances (i.e., individuals), properties (i.e., attributes or predicates) are used to present the semantics in an ontology. Please note that, the author only introduces the components of an ontology that are most frequently used for schema alignment, other components, such as restrictions and axioms, are not covered by this section.

Classes in ontology are hierarchical organized, which means that if a class “general” is a sub concept of a class “people”, the two classes are connected with an is_A relation. Sub-classes inherit properties from the super class. For example, if the class “people” has a property “nationality”, the class “general” also has the property “nationality”. Some ontologies allow multiple inheritance, which means a class can have multiple super classes. For example, the class “general” can be sub-class of both the class “people” and a class “job”.

Instances (individual) are used to detail a class. For example, “Gannys” is an instance of “general”. Instantiation, populating a class with instances, is supported by inheritance, which means that instances belonging to a sub-class also belong to its super class. For example, “Gannys” is an instance of the class the class “general” and its super class “people”.

Properties are used to describe a class, and an instance has specific values of a property. For example, for the property “nationality” of a class “people”, the instance of this class “Gannys” can has a value “Rome” for “nationality”. A
property can be a data-type or object-type. The property “nationality” is a data-type property, because the value of this property is literal. However, if we have an instance for “Rome” with a de-referencable URL, then the property “nationality” becomes an object-type property.

With the vocabularies in a RDF, an ontology can be defined with its syntax and vocabularies. For example, in Figure 2-1, the Is_A relations can be defined with the triple: “<subject><rdf:type><owl:Class>”. Other definitions, such as instances, data- and object-type properties can be also defined similarly with abundant vocabularies provided by RDF schema ("RDF Schema,"), OWL ("OWL."), and et cetera.

Schema alignment is to find correspondences between concepts. In Linked Data, concepts are represented within ontologies. Therefore, schema alignment is to find correspondences between classes.

The fundamental computation for schema alignment is the similarity computation between two classes. Therefore, all resources in an ontology can be used for computing similarities. For example, the information of a class can be used (Please note that this method is called as schema-based schema alignment, which uses the information, such as names, about a class). Instances of classes (called instance-based) or partial structures (called structure-based) of ontologies that contain the classes also can be used to measure the similarity.

There are different types of alignment, such as subsumption and equivalence. Subsumption alignments establish is_A relations between classes in different ontologies. The subsumption relations are directly found rather than found by
reasoning based on equivalence and intra-subsumption relations (Spiliopoulos, Vouros, & Karkaletsis, 2010). Equivalence alignments establish “Owl:equivalentClass”, “Skos:exactMatch”, or “Skos:closeMatch” relations. Normally, for a class in a source ontology, the alignment is an one-to-one mapping. However, thanks to multiple inheritance on classes, the alignments for some source classes are one-to-n mappings. Other types of alignments, such as disjointness, part-of, can also be required by users for different purposes (Shvaiko & Euzenat, 2005). In this dissertation, the author only considers the subsumption and equivalence alignment.
2.2 Related Works

2.2.1 Instance-based Schema Alignment

Along with the increasing number of ontologies, ontology integration becomes a natural need for providing more generic and comprehensive knowledge, and ontology alignment is considered as the fundamental to realize the ontology integration (Sowa, 2000). Ontology alignment is studied to provide the correspondences, such as subsumption and equivalence, between concepts from different ontologies. The subsumption relations are considered as important as equivalence and need to be separately discovered from the subsumptions deduced by a reasoning mechanism (Spiliopoulos et al., 2010). The results of ontology alignment are systematically evaluated by gold standards from diversity of workshops, such as Ontology Alignment Evaluation Initiative workshops ("Ontology Alignment Evaluation Initiative," 2004). The methods for schema alignment in ontologies can be classified into four categories, which are lexical-, structural-, background-, and instance-based (Euzenat & Shvaiko, 2007; Jean-Mary, Shironoshita, & Kabuka, 2009; Jiménez-Ruiz, Grau, Horrocks, & Berlanga, 2009; Udrea, Getoor, & Miller, 2007). However, the instinctively schema naming and diversity of granularity weaken the performance of the first three methods. Furthermore, the unique data structure of Linked Data where thousands of instances belonging to a class are linked to instances from another ontology, makes the rise of the instance-based schema mapping method attract the attention of academia (Kirsten et al., 2007).
The idea behind the instance-based schema mapping, which is inherited from the schema alignment (matching) using duplicates in Database area (Bilke & Naumann, 2005; J. Wang, Wen, Lochovsky, & Ma, 2004), is to use the statistical information of two instance sets, held separately by two classes, in discovering the relation between the classes. The overlapped instances of two classes indicate the subsumption or equivalence relation of the two classes, which is called common extension comparison (Isaac, Meij, Schlobach, & Wang, 2007; Kirsten et al., 2007). (Isaac et al., 2007) aligns concepts in two thesauri, GTT and Brinkman thesaurus, used to describe books in National Library of Netherlands. Common instances (books) are used to compute the similarity between two concepts in different thesauri with diverse measures, including various Jaccard similarity measures and standard information-theory measures. Different instance extension strategies, such as with and without inheritance based on hierarchy, are also tested with the real data set. The experiments show that the instance-based schema alignment is promising on alignment for large size ontologies (Isaac et al., 2007). Biomedical ontologies also have large-size on concepts and instances. (Kirsten et al., 2007) adapts instance-based methods on mapping Gene Ontology (GO). More similarity computing metrics, including dice similarity, minimum similarity, and kappa similarity, are used in (Kirsten et al., 2007). The experiments with large life ontologies also show satisfactory results. The data used in the above-mentioned studies have a limitation that without a consideration the scalability of these methods. The method developed in this dissertation in Chapter 4 scales pairwise
similarity computations by decreasing unnecessary computing pairs, which previous studies ignored.

Recall that there are two cases of instance-based alignment in Figure 1-6. The instance-based mapping needs the instances shared or annotated by two ontologies (common instances shared in Figure 1-6 (a)). However, some schema alignment tasks may require methods for similar but different instances when there are not existing common instances (Bellahsene et al., 2011). One solution is to use the information of the instances to compute the similarity between two classes. COMA++ uses constraints and contents to compute the similarity of two instances sets belonging to two classes (Engmann & Massmann, 2007). The names and descriptions of the instances are also tokened and put into a name set and a description set. The similarity of two classes is computed by the four similarity measures based on the TF/IDF values of tokens in the name set and description set (Massmann & Rahm, 2008). Similar with COMA++, tokens of content in instances used to form a vector space for each class in RiMOM (Li, Tang, Li, & Luo, 2009). The similarity is computed with cosine similarity based on the vector spaces of two classes. The internal structures of instances are also considered to determine the similarity of two instances for refining the schema alignment in ASMOV (Jean-Mary et al., 2009). The AgreementMaker (Cruz, Antonelli, & Stroe, 2009) also computes similarity for two classes based on the Vector Space Model that uses TF/IDF values of extract strings from instances. The machine learning approaches, such as classification, are also adapted to align the schemas. (S. Wang et al., 2008) adapts Markov Random Field, a classification algorithm, to train the
instances based on the similarity of the feature vectors for heterogeneous data sets without sharing common instances. GLUE (Doan, Madhavan, Domingos, & Halevy, 2004) uses joint probability distributions as a framework for multiple similarity measures for the classes, such as Jaccard coefficient. The joint probability distributions are estimated by the classifiers using terms learned from the names or descriptions of the instances. General schema alignment frameworks, such as SAMBO (Lambrix & Tan, 2006), merge different instance-based methods to provide comprehensive ontology alignment service.

Schema alignment for Linked Data has been studied in recent years. With the help of a third party thesauri (WordNet and Wikipedia), a lexical- and structured-based alignment method is introduced in BLOOMS (P. Jain et al., 2010). BLOOMS shows that the existing schema alignment algorithms, such as S-Match (Giunchiglia, Shvaiko, & Yatskevich, 2004), AROMA (David, Guillet, & Briand, 2006), and RiMOM (Li et al., 2009) in OAEI 2009 ("2009 Campaign - Ontology Alignment Evaluation Initiative," 2009), are not suitable for schema alignment in LOD. Linked Data has a natural advantage for instance-based alignment, which most well-known data sets are interlinked at the instance level. For instance, DBpedia has 18 million and Linked Life Data has 8 million inter-links at the instance level. Similar with BLOOMS, the HCM (Gruetze, Böhm, & Naumann, 2012) also uses Wikipedia category forest to compute the similarity between classes and without using instances. Different with BLOOMS and the HCM, the proposed method uses instance to align schemas in Linked Data. The HM (Parundekar et al., 2010) attempts to adapt instance-based schema alignment for
linked data. It uses heuristic rules to generate subsumption and equivalence relations based on a probability model. Similar with HM, (Suchanek, Abiteboul, & Senellart, 2011) also uses conditional probability to decide the relation between two classes based on instances that are aligned two probabilistic models. With instances, the proposed method proposes more comprehensive functions to decide equivalence and subsumption relations for two classes, and outperforms the HM and BLOOMS.

The author summarizes instance-based schema alignment methods in Table 2-1. Please note that, BLOOMS and the HCM are not instance-based methods. The author lists them in Table 2-1 because they are designed for Linked Data, and the author compared BLOOMS with the proposed method in Chapter 3.

Table 2-1: Comparison of schema alignment methods. (Attri.1: “year”, Attri.2: “input data”, Attri.3: “similarity metrics with instances”, Attri.4: “scaling search space”, Attri.5: “require common instances or aligned instances”, Attri.6: “GUI”, Attri.7: “data sets for testing”)

<table>
<thead>
<tr>
<th>Name</th>
<th>Attri. 1</th>
<th>Attri. 2</th>
<th>Attri. 3</th>
<th>Attri. 4</th>
<th>Attri. 5</th>
<th>Attri. 6</th>
<th>Attri. 7</th>
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<td>NO</td>
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<tr>
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<td>YES</td>
<td>OAEI</td>
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<td>Dice similarity,</td>
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<td>Minimal similarity,</td>
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<tr>
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<td>Year</td>
<td>Domain</td>
<td>Similarity Measure</td>
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<td>Books of National Library of Netherlands annotated with two thesauri</td>
<td>GO ontologies</td>
<td>Real-world ontologies</td>
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<tr>
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<td>Thesauri</td>
<td>Jaccard similarity, Standard NO YES NO</td>
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<td>Books of National Library of Netherlands annotated with two thesauri</td>
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</tr>
<tr>
<td>(Kirsten et al., 2007)</td>
<td>2007</td>
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<tr>
<td>Agreement Maker</td>
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<tr>
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<td>Linked Data</td>
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<tr>
<td>BLOOMS</td>
<td>2010</td>
<td>Linked Data</td>
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suchanek et al., 2011) | 2011 | linked data | conditional probability based similarity | no | no | no | dbpedia, yago
---|---|---|---|---|---|---|---

hcm | 2012 | linked data | - | - | no | no | oaei billion triple challenge

2.2.2 scaling pairwise similarity computations

the instance-based schema alignments compute the similarities of all class pairs based on instances, which addresses a scalability issue of alignment methods. generally, there are two ways to scale the computations as shown in figure 2-3: (1) parallel computation, (2) reduction computations of each matcher.

parallel computations are used to reduce the computation time. there are two kinds of parallel alignment: inter- and intra-matcher parallelization (gross, hartung, kirsten, & rahm, 2010). the inter-matcher realizes parallel alignment based on independent matchers with multiple processors, whereas intra-matcher enables parallel alignment based on internal decomposition of individual matchers. each intra-matcher processes alignment based on a partial data and assembles the final results with other matchers, which makes intra-alignment parallelization require fewer memories than inter-alignment parallelization and more scalable than inter-alignment parallelization. the parallel computation frameworks, such as
MapReduce (Dean & Ghemawat, 2008), are used to find duplicates over massive datasets (C. Wang et al., 2010), which can be used to decrease pair-wise similarity computations in schema alignment. (Lin, 2009) and (Y. Wang, Metwally, & Parthasarathy, 2013) use MapReduce to scale the similarity computations on documents and entities that resemble instance-based schema alignment. (Tenschert et al., 2009) introduces a workflow of ontology alignment based on MapReduce. The V-Doc+ (Zhang, Hu, & Qu, 2012), PIDGIN (Wijaya, Talukdar, & Mitchell, 2013), and Parallel Ontology Bridge (Freckleton, 2013) scale the computations of ontology alignment based on MapReduce.

Figure 2-3: Two strategies for scaling pairwise computations.

The second way is to reduce pairwise similarity computations of each matcher, which is recognized as the problem of duplicate detection. This problem is addressed by (Broder, Glassman, Manasse, & Zweig, 1997) to find duplicate
Web pages. A Sketch that is a compressed Web document vector based on min-wise independent permutations is used to represent a Web Document for similarity computations. Similarly, the dimension of document vector can be reduced by hashing functions reflecting to similarity computation functions in Locality Sensitive Hashing (LSH) (Rajaraman & Ullman, 2011). These methods are approximate duplicate detection. The LSH is adapted in (Duan et al., 2012) on scaling instance-based schema alignment. The difference between the (Duan et al., 2012) and the proposed method is that the IUT also considers the sequence for pair-wise computations and limits the candidate pairs into the buckets created by banding when using MinHash functions. The exact duplicate detection problem is known as similarity join problem in the database community. Signatures represented the original documents with a filtering phase to eliminate false positives are used to match exact sets based on Hamming and Jaccard similarities in PARTENUM and WTENUM (Arasu, Ganti, & Kaushik, 2006). The q-grams are used to represented original text document, and the candidate pairs are extracted based on prefix-filtering (Chaudhuri, Ganti, & Kaushik, 2006). For fast navigate compared document, inverted index is also used in a prefix-filtering based model in All-Pairs (Bayardo, Ma, & Srikant, 2007). For achieving better performance, the PPjoin and PPjoin+ (Xiao, Wang, Lin, & Yu, 2008) use positional and suffix filtering to eliminate candidate pairs. The PPjoin is adapted into ontology alignment for scaling pairwise computations in HCM (Gruetze et al., 2012).
2.2.3 Automatic Taxonomy Generation

With the rapid growth of large data sets in commercial, industrial, administrative and other applications, the concept hierarchy generation has been studied from 1990s (Han, Cai, & Cercone, 1992; Piatetski & Frawley, 1991). In an automatic generated taxonomy, the data are organized with the concepts extracted from three types of source data: (1) unstructured, (2) semi-structured, and (3) structured (Hazman, El-Beltagy, & Rafea, 2011; Santoso, Haw, & Abdul-Mehdi, 2011). In unstructured data, the terms are extracted based on Nature Language Processing (NLP) methods, such as POS tagging (Drymonas, Zervanou, & Petrakis, 2010; Knijff, Frasincar, & Hogenboom, 2013; Kummamuru, Lotlikar, Roy, Singal, & Krishnapuram, 2004) or syntactic dependency (Cimiano, Hotho, & Staab, 2005). The important ones are considered as the concepts with different metrics, such as C/NC-value in (Drymonas et al., 2010), conditional probability, Pointwise Mutual Information (PMI) and Resnik in (Cimiano et al., 2005), TF/IDF in (Brewster & Wilks, 2004), domain pertinence and lexical cohesion in (Knijff et al., 2013). Rather than a term, a concept can also be defined as a set of terms (Fung, Wang, & Ester, 2003; Paukkeri, García-Plaza, Fresno, Unanue, & Honkela, 2012).

In semi-structured data and structured data, concepts are extracted from schema with different transforming patterns. For example in XML, concepts can be mapped from complexType (Bedini, Matheus, Patel-Schneider, Boran, & Nguyen, 2011; Ferdinand, Zirpins, & Trastour, 2004; Ghawi & Cullot, 2009; J. Xu & Li, 2007). Similar with XML, for databases, concepts can be mapped from relations (Astrova, 2004; Cerbah, 2008; Lammari, Comyn-Wattiau, & Akoka,
In contrast with these methods above, the proposed method in Chapter 5 does not use any complex machine learning algorithms or heuristic rules targeting specific data to get concepts, but only extracts objects to form concepts, which is lightweight and robust to be applied to any Linked Data set.

With the concepts established, taxonomies can be generated either with heuristic rules based on features of data, such as extension and restriction in XML (Bedini et al., 2011; Ghawi & Cullot, 2009) or different relationships in databases (Cerbah, 2008; Lammari et al., 2007). Reference ontologies, such as WordNet (Lee, Huh, & McNiel, 2008; Zheng, Borchert, & Kim, 2008), are also used to build taxonomies. Nevertheless, the most popular methods are based on probabilistic models and can be classified into two kinds:

(a) Fill the taxonomy with the established concepts and new discovered concepts. The most traditional methods of this kind use the established concepts as leaf nodes and create stem nodes with them. The hierarchical clustering algorithms known as agglomerative UPGMA and bisecting k-means (A. K. Jain & Dubes, 1988) are frequently used. And the bisecting k-means is considered a better solution than UPGMA (Steinbach, Karypis, & Kumar, 2000). However, it is inflexible to use these methods that need to set parameters, such as the number of clusters for k-means. The established concepts are not only used as leafs but also used as stems. The Formal Concept Analysis (FCA) uses a set of terms as intensions of a concept, and builds a taxonomy with these concepts (Cimiano et al., 2005; Drymonas et al., 2010). The Self-Organizing Map (SOM) is also used to reduce the dimensions of data (instances) features into SOM neurons for clustering.
data at each level of a taxonomy (Paukkeri et al., 2012). Different with the proposed method in Chapter 5, these methods focus on building a hierarchical structure for organizing instances, but with little consideration of the concept interpretation or labeling. For example, in the experiment in Section 5.6, FCA obtains low precision for generating meaningless concepts that have common instances.

(b) Fill the taxonomy only with the established concepts.

The methods of this kind build a taxonomy only with already established concepts. The relation between two concepts is mostly defined with a similarity measure. The Subsumption (Sanderson & Croft, 1999) is used to determine a subsumption relation between two concepts, and is considered as one of the most classical methods for concept hierarchy generation. Studies, such as (Schmitz, 2006) and (Krijff et al., 2013), improve the subsumption-based approaches for different usages. Other studies are inspired to boost the precision of the subsumption-based method by using probability models. Some of them try to improve the precision by developing more advanced metrics to compute the importance of a concept, such as topicality and predictiveness in DSP (Lawrie & Croft, 2003), hierarchy coverage and concept distinctiveness in DisCover (Kummamuru et al., 2004). To build a taxonomy for social tags, the EXT (Heymann & García-Molina, 2006) is introduced as a high efficient and effective extensible greedy algorithm that places concepts ordered with importance of a similarity graph into a hierarchy based on a similarity measure. Furthermore, the EXT is improved by modifying the greedy algorithm into a Directed Acyclic Graph (DAG) allocation algorithm (Eda,
Yoshikawa, Uchiyama, & Uchiyama, 2009) or by changing the sorting algorithm and similarity measure in the IUT (Zong et al., 2015).

The proposed method in Chapter 5 combines the IUT and Subsumption to generate a taxonomy based on the concept defined. In an addition, the proposed method further decreases the computations by removing the redundant instances and objects, and refines a generated taxonomy with these removed instances and objects. These mechanism guarantees both the efficiency and effectiveness on taxonomy construction. In contrast with the existing methods, with the multiple features of Linked Data, the proposed method adapts automatic taxonomy generation methods to build diverse taxonomies in different facets. To the best of the author’s knowledge, this is the first study that realizes generation of faceted taxonomy automatically in Linked Data.
3 Aligning Schemas with Subsumption and Equivalence Relations

3.1 Introduction

In this chapter, the author proposes a new Instance-based Unified Taxonomy generation algorithm called IUT for aligning ontology in Linked Data. The taxonomy used in this chapter is defined in general, which contains two relations, subsumption and equivalence, and supports multiple inheritance. The content of this chapter is based on the author’s previous work published (Zong et al., 2015).

The IUT adapts the EXT (Heymann & Garcia-Molina, 2006), an algorithm that builds a taxonomy for social tags originally and can be used for generating ontology for RDF resources in the work (Nansu, Sungin, & Hong-Gee, 2013). The IUT uses a unified graph to restrict the alignment search space, which is proved to be capable of finding more suitable pairs to be compared instead of using all the combinations of instances. The author tests the IUT with two data sets, DBpedia and YAGO2 in LOD, and evaluates the results with gold standards. Four tasks, intra-subsumption in DBpedia (DBpedia-DBpedia), and YAGO2 (YAGO2-YAGO2), inter-subsumption and equivalence between DBpedia and YAGO2 (YAGO2-DBpedia), are designed to discover two kinds of relations, subsumption and equivalence. The author compares the IUT with two other state-of-the-art methods (the Heuristic Mapper (HM) (Parundekar et al., 2010) and BLOOMS (P. Jain et al., 2010)), and the experiments show that the IUT outperforms the existing ontology alignment algorithms. Three main reasons for failures of instance-based
ontology alignment in LOD, which are (1) insufficient taxonomic description on the instance level, (2) multi-instantiation, and (3) different taxonomic structure of ontologies, are also discussed.

The rest of this chapter is organized as follows: Section 3.2 gives a formal problem definition; Section 3.3 details on the methodology of the proposed method; in Section 3.4 and 3.5, the author demonstrates the results of the proposed method; Section 3.6 discusses limitations of this study, and the conclusions are presented in Section 3.7.
3.2 Problem Definition

In order to help readers understand this paper, the author uses an ongoing example in Figure 3-1 to explain the problem of schema alignment and the process of the proposed method. The author uses two ontologies as input data. That is the one shaped in solid line from DBpedia Ontology containing five classes ("c1:LegalActor", "c2:Person", "c3:Organization", "c4:General", and "c5:Artist") and four instances ("i1_1:Gannys", "i2_1:Bashy", "i3_1:Double_O(charity)", and "i4_1:Patrick_Huse"). And the other one shaped in dotted line from YAGO2 contains three classes ("c6:Agent", "c7:People", and "c8:Group") and three instances ("i1_2:Gannys", "i2_2:Bashy", and "i3_2:Double_O(charity)") (the author changed the original ontologies to simplify the example used). The classes belonging to the same ontology are connected with the intra-subsumption relations. For example, "c2:Person" is a sub-class of "c1:LegalActor" in the first ontology. Schema alignment is the process of discovering correspondences that include subsumption and equivalence relations between classes from multiple ontologies. The author adapts the
conditions for an instance-based schema alignment that instances are aligned with “Owl:sameAS” to other instances from different ontologies. The author defines the problem in more detail as follows:

**Input:** Given two ontologies, a source ontology $O_1(C_1, I_1)$ and a target ontology $O_2(C_2, I_2)$, where $O_1(C_1, I_1)$ contains a class set $C_1 = \{c_1, c_2, ..., c_k\}$ and an instance set $I_1 = \{i_1, i_2, ..., i_l\}$, and $O_2(C_2, I_2)$ contains a class set $C_2 = \{c_{k+1}, c_{k+2}, ..., c_m\}$ and an instance set $I_2 = \{i_{l+1}, i_{l+2}, ..., i_n\}$. The two instance sets are mapped by “Owl:sameAs”. For example, instance “$i_{1.1}: Gannys$” from $C_1$ is same with “$i_{1.2}: Gannys$” from $C_2$. Each class $c_i$ in $C_1$ or $C_2$ contains an instance set $I_{c_i}$, where each element is corresponding to the element in the instance set $I_1$ or $I_2$. The instance set $I_{c_i}$ for class $c_i$ follows the common extension (Isaac et al., 2007) to describe the taxonomic information of $c_i$ in $C_1$ or $C_2$, which is that $c_i$ contains all the instances of $c_j$ if $c_i$ is the super class of $c_j$. For example in Figure 3-1, $I_{c_2: Person} = \{"i_{2.1}: Bashy","i_{1.1}: Gannys","i_{4.1}: Patric_Huse"\}$ contains the instance “$i_{2.1}: Bashy$” because “$c_2: Person$” is the super class of “$c_5: Artist$” that has the instance set $I_{c_5: Artist} = \{"i_{2.1}: Bashy"\}$.

**Output:** A set of mappings $A = \{a_1, a_2, ..., a_k\}$ is the output of the alignment processing. Each mapping $a_i = (c_e, c_f, r_i)$ contains three elements, where $c_e \in C_1$, $c_f \in C_2$, and $r_i$ can be a subsumption or equivalence relation.

The subsumption relations are directly determined instead of being deduced by a reasoning mechanism based on equivalence relations and existing intra-subsumptions, otherwise the generated subsumption relations are not independent and can be affected by the equivalence relations (Spiliopoulos et al.,...
2010). For example, the class “\(c_1: \text{LegalActor}\)” from \(C_1\) should not be considered equivalent as the class “\(c_6: \text{Agent}\)” from \(C_2\) if the relation is deduced by the facts that (1) “\(c_1: \text{LegalActor}\)” is the super class of “\(c_2: \text{Person}\)” and (2) “\(c_6: \text{Agent}\)” is the super class of “\(c_7: \text{People}\)” and (3) a new established relation that “\(c_2: \text{Person}\)” is equivalent to “\(c_7: \text{People}\)”.
3.3 Methods

3.3.1 Workflow of Instance-based Schema Alignment

Figure 3-2: Workflow of instance-based schema alignment with the IUT.

The IUT is a unified taxonomy generation algorithm that generates alignments for a source ontology and a target ontology based on a virtual graph generated by using the common instances shared in two classes from the two ontologies. Figure 3-2 shows the workflow of the IUT. The procedure of aligning is separated into two parts: instance-class matrix generation, and subsumption and equivalence relations generation. In first part, the input data will be converted into an instance-class matrix, and the matrix will be used to build a virtual graph based on the aligned instances in the second part. The subsumption and equivalence relations are extracted from the virtual graph after the virtual graph is established.
3.3.2 Instance-class Matrix Generation

Before discovering the relations between classes from multiple ontologies, the author performs a pre-processing step on unifying the common instances from different ontologies by three steps. First, all the instances are filtered to remove the instances only used in one ontology. Second, two instances aligned with “Owl:sameAs” are merged into one common instance. Finally, an instance-class matrix will be generated based on the step 2.

Figure 3-3: An example of instance-class matrix generation.

(1) Common instances scoping

In Linked Data, some instances can be excluded by one ontology while included by another one because of the Open-World Assumption (OWA). In practice, the
reasons could be: (1) different data resources for ontology construction, (2) different purposes of ontology design, and (3) different frequencies of ontology updating. The instances only used in one ontology cannot contribute to instance-based alignment approaches. Therefore, in order to mitigate the negative effects of the asymmetric ontology update and OWA (the author will discuss it in Section 3.6), the author limits the instances used for alignment into the instances only shared in the multiple resources. For example, “i_{4,1}:Patrick_Huse” in Figure 3-3 is removed during the pre-processing stage since it is only used in DBpedia ontology (shaped in solid line) and will not contribute to the alignment.

(2) Creating common instances for aligned instances

If two instances from two different data sources, such as “i_{1,1}:Gannys” from the first ontology (shaped in solid line) and “i_{1,2}:Gannys” from the second ontology (shaped in dotted line), are aligned by “Owl:sameAs”, the two instances are considered to be the same and can be replaced with a common instance “i_{1}:Gannys”. In the ongoing example, six instances from two resources are replaced with three common instances on the right top of Figure 3-3.

(3) Generating instance-class matrix

The two steps decrease \( n' \) instances into \( n \) common instances. The author transforms the classes and common instances into an instance-class binary matrix \( M_{n \times m} \), where the columns of the matrix correspond to the class set \( C = \{c_1, c_2, ..., c_m\} \), and the rows correspond to the common instance set \( I = \{i_1, i_2, ..., i_n\} \). The value of an entry \( e_{i,j} \) is one if the class \( c_j \) contains the common instance \( i_i \), otherwise it is zero. For example, the \( c_1 = [1,1,1]^T \) is corresponding to
the fact that the class “$c_1$: LegalActor” contains three instances “$i_1$: Gannys”, “$i_2$: Bashy”, and “$i_3$: Double_O(charity)” in Figure 3-3.

### 3.3.3 Subsumption and Equivalence Relations Discovering

The alignment is processed by the following steps based on the instance-class matrix generated: first, the classes in the matrix are sorted in descending order by the degrees in a class-relation multi-graph $G(E,V)$; second, the sorted classes are put onto the right position in a virtual graph. The subsumption and equivalence relations are used to form the virtual graph.

1. **Class-relation multi-graph generation**

   For a class-relation multi-graph $G(E,V)$, all the classes $C = \{c_1, c_2, ..., c_m\}$ are put into the $G(E,V)$, and each class $c_i$ is a vertex $v_i$. For each pair of vertices $c_i$ and $c_j$, $|\text{commonInstances}(c_i, c_j)|$ number of links between $c_i$ and $c_j$ are built, where $|\text{commonInstances}(c_i, c_j)|$ is the cardinality of the common instances set of $c_i$ and $c_j$.

   For example, $|\text{commonInstances}("c_1: LegalActor", "c_j: Agent")| = 3$ in the ongoing example.

2. **Virtual graph generation**

   The vertices (classes) are sorted in descending order by the degrees and are put into a queue $Q$. In each iteration, a class is de-queued and put onto the right position by computing the relation with existing classes in the virtual graph using the following definitions:
**Definition 3-1. Subsumption:** For a pair of vertices $c_i$ and $c_j$, where $c_i$ originates from either one of the two ontologies (source and target) and $c_j$ from the other ontology, if $\text{sub}(c_i, c_j) \geq \chi_s$, then $c_i$ is considered as the subclass of $c_j$. The $\text{sub}(c_i, c_j)$ is computed by:

$$\text{sub}(c_i, c_j) = \frac{|\text{commonInstance}(c_i, c_j)|}{|c_i|} \quad (3.1)$$

**Definition 3-2. Equivalence:** For a pair of vertices $c_i$ and $c_j$, where $c_i$ originates from either one of the two ontologies (source and target) and $c_j$ from the other ontology, if $\text{sub}(c_i, c_j) \geq \chi_s$ and $\text{sub}(c_j, c_i) \geq \chi_s$, then $c_i$ is considered equivalent to $c_j$.

In practice, if the above mentioned two definitions are not satisfied, the author will further compute a supplementary definition for equivalence by Jaccard similarity.

**Definition 3-3. Equivalence (supplementary):** For a pair of vertices $c_i$ and $c_j$, where $c_i$ originates from either one of the two ontologies (source and target) and $c_j$ from the other ontology, if $\text{sim}(c_i, c_j) \geq \chi_e$, then $c_i$ is considered equivalent to $c_j$.

The $\text{sim}(c_i, c_j)$ is computed by Jaccard similarity shown as follows:

$$\text{sim}(c_i, c_j) = \frac{|\text{commonInstance}(c_i, c_j)|}{|c_i|+|c_j|-|\text{commonInstance}(c_i, c_j)|} \quad (3.2)$$

For a new added vertex, if the relation with an existing vertex is equivalence, an inbound edge and outbound edge of the vertex will be added to the existing vertex.

If a new added vertex has multiple subsumption relations with the existing vertices (ancestors), the outbound edges of the vertex will be added to the super-vertices that is an ancestor without a path from any other ancestor. The relations between classes in the unified graph contain the new discovered relations and the original
existing relations. We return the new discovered relations as the alignments. The
details of the process of the IUT are shown in Algorithm 3-1.
Algorithm 3-1: The IUT for schema alignment.

**Input:** a source ontology $O_1(C_1, I_1)$, a target ontology $O_2(C_2, I_2)$, $\chi_s$, $\chi_e$

**Output:** subsumption and equivalence alignments $A$

1. Instance-class matrix $M :=$ generate from $O_1$ and $O_2$

2. Put all classes into a class relation graph $G$ and initiate an empty virtual graph $H$

3. **For** each class $c_i$ in $M$ **do**

4. **For** each class $c_j$ in $M$ **do**

5. Let $\#links(c_i, c_j) := |commonInstance(c_i, c_j)|$

6. Queue $Q :=$ all the classes sorted by the descending order of degree in $G$

7. **While** $size(Q) > 0$ **do**

8. $c_i := dequeue(Q)$

9. Add $c_i$ into $H$

10. Initiate an ancestor list $S$ and an equivalence list $E$

11. **For** $c_j$ in $H$ **do**

12. **If** $c_i$ originates from either one of the two ontologies (source and target) and $c_j$ from the other ontology **then**

13. **If** $(sub(c_i, c_j) \geq \chi_s$ and $sub(c_j, c_i) \geq \chi_s) \text{ put } c_j \text{ into } E$

14. **Else if** $(sub(c_i, c_j) \geq \chi_s) \text{ put } c_j \text{ into } S$

15. **Else if** $(sim(c_i, c_j) \geq \chi_e) \text{ put } c_j \text{ into } E$

16. **Else** put $c_j$ into $E$ or $S$ based on the original existing relation of $c_i$ and $c_j$

17. Add inbound and outbound edges from $c_i$ to the vertices in $E$

18. Add outbound edges from $c_i$ to the sup-vertices in $S$

19. Return new discovered relations as the alignments $A$ in $H$
3.4 Experiments

The author implemented the proposed method based on JDK 1.6 using an Intel I7-2600 CPU with 16 GB RAM on Windows 8 64 bit version.

3.4.1 Schema Alignment Algorithms in Comparison

The author compared the IUT with two state-of-the-art methods: the HM (Parundekar et al., 2010) that is an instance-based alignment method and BLOOMS (P. Jain et al., 2010) that is a lexical- and structure-based method.

For the HM, the author used the threshold (min=0.01 max=0.90) as mentioned in (Parundekar et al., 2010). For BLOOMS, the author downloaded the source code from the website ("BLOOMS," ) and used the WordNet 2.1 ("WordNet," ) as the thesauri. (The reason why the author did not use Wikipedia is that too much time is spent to send the request to the server, which makes the computation not feasible).

3.4.2 Data and Experiment Design

In ontology alignment, comparison of alignment methods should be based on an identical evaluation scenario, a standardized set of tests serving as a basis for comparison (Bellahsene et al., 2011). However, as far as we know, there lacks benchmarks for measuring the efficiency and effectiveness of the LOD schema alignment methods. The author decided to build the test data sets based on the most famous ontology in LOD that supplies both taxonomic structure and rich instances. Furthermore, the author chose the gold standards either used in the existing schema-matching projects or created manually as the expected mappings for the tests. The author gained the study population, with instance size ranged from 0 to
10,000, which contains 368,870 classes from YAGO2 ("Downloads - YAGO2," and 299 classes from DBpedia ("Downloads - Dbpedia."). In order to detect the effects of number of instances, the author divided the classes into three groups by the number of instance contained (0-100), [100-500), [500-10,000) in DBpedia and YAGO2. The statistics of the data the author used are shown in Table 3-1.

**Table 3-1: Statistic information of the data sets.**

<table>
<thead>
<tr>
<th></th>
<th>YAGO2</th>
<th></th>
<th></th>
<th></th>
<th>DBpedia</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>#instances</td>
<td>#instances</td>
<td>#instances</td>
<td>#instances</td>
<td>#instances</td>
</tr>
<tr>
<td>(0-100)</td>
<td>(0-10,000)</td>
<td>(100-500)</td>
<td>(500-10,000)</td>
<td>(0-10,000)</td>
<td>(0-10,000)</td>
</tr>
<tr>
<td>#classes</td>
<td>352,452</td>
<td>13,705</td>
<td>2,713</td>
<td>368,870</td>
<td>50</td>
</tr>
<tr>
<td>#avg. ins.</td>
<td>11</td>
<td>198</td>
<td>1553</td>
<td>30</td>
<td>28</td>
</tr>
</tbody>
</table>

The author performed intra- and inter-alignment missions as the schema alignment tests performed in (Kirsten et al., 2007; Parundekar et al., 2010). The experiment is separated into four parts: discovering intra-subsumption relations for YAGO2-YAGO2, intra-subsumption relations for DBpedia-DBpedia, inter-subsumption and inter-equivalence relations for YAGO2-DBpedia. Each
alignment method is measured for each task in terms of its running time (efficiency) and F-measure (effectiveness) (Bellahsene et al., 2011).

(1) For YAGO2-YAGO2, the classes with the cardinality of the instances set ranging from 0 to 10,000 in the YAGO2 are used to generate intra-subsumption relations between classes, and the relations are evaluated by the YAGO Taxonomy ("Downloads - YAGO2.").

(2) Similar to YAGO2-YAGO2, intra-subsumption relations in DBpedia-DBpedia are generated based on the DBpedia classes with the same cardinality range (0-10,000) and are evaluated by DBpedia Ontology ("Downloads - Dbpedia.").

(3) For YAGO2-DBpedia, the same DBpedia and YAGO2 classes used in the previous two experiments are adopted. In order to create common instances shared by the classes from DBpedia and YAGO2, the YAGO2-DBpedia instances-mapping file downloaded from DBpedia 3.9 was used. For example, through the “Owl:sameAs” mapping for the instance “YAGO:ESF_Men's_Championship” contained by a YAGO2 class “YAGO:SoftballChampionships” and the instance “DBpedia:ESF_Men's_Championship” contained by a DBpedia class “DBPedia:SoftballLeague”, can consider that “YAGO:SoftballChampionships” and “DBPedia:SoftballLeague” contain a same instance “ESF_Men's_Championship” that represents “YAGO:ESF_Men's_Championship” and “DBpedia:ESF_Men's_Championship”. The subsumption relations are evaluated by the gold standard used in the PARIS ("Subsumption alignment of YAGO2 and Dbpedia."). The equivalence relations are evaluated by the gold standard that is
manually created in NetEstate ("Ontology matching for classes in YAGO and DBpedia ontologies," 2014). In order to compute the recall, the classes needed to be aligned are limited into the classes existing in the gold standard instead of using all the classes in two data sets.
3.5 Results

Figure 3-4: F-score and running time of the methods. The IUT uses the parameter setting $\chi_s = 1$ and $\chi_e = 0.6$. The HM uses the parameter setting $\min = 0.01$ and $\max = 0.9$. BLOOMS uses the WordNet as the thesauri and the parameter setting confidence = 0.95. All the experiments in Section 3.5 use the same settings.
Figure 3-4 shows the overall (0-10,000) results of the three methods for four alignment experiments. The IUT is the fastest algorithm for two intra-alignment tasks (968 (ms) for DBpedia-DBpedia intra-subsumption and 3,981,676 (ms) for YAGO2-YAGO2 intra-subsumption), since an instance-based approach is more efficient for large classes. BLOOMS is the fastest algorithm for the two inter-alignment tasks (1,197 (ms) for YAGO2-DBpedia inter-subsumption and 1,205 (ms) for YAGO2-DBpedia inter-equivalence), since BLOOMS ignores the comparison of the instance sets, which is very expensive. However, BLOOMS fails inter-subsumption alignment but achieves a good result for inter-equivalence alignment (0.599). The IUT achieves the best F-score for all the alignment tasks (0.666 for YAGO2-YAGO2 subsumption, 0.810 for DBpedia-DBpedia subsumption, 0.388 for YAGO2-DBpedia subsumption, and 0.641 for YAGO2-DBpedia equivalence) within a relatively reasonable time. The author introduces the experiments results in detail in the next sub-sections.
3.5.1 Intra-subsumption Relations for YAGO2-YAGO2

![Intra-subsumption Relations for YAGO2-YAGO2](image)

**Figure 3-5**: Running time of the three methods for YAGO2-YAGO2.

Figure 3-5 shows the running time for different algorithms for aligning YAGO2 intra-classes. The IUT is the fastest methods for aligning the classes having small- and medium-scale size of instances (0-100) and [100-500), but the second fastest method for the large-scale size of instances [500-10,000). BLOOMS aligns classes based on labels of classes and WordNet, thus the running time of BLOOMS only relates to the number of classes instead of the number of instances. YAGO2 has much more classes that have a small-scale size of instances than medium- and large-scale size, which makes the running time of BLOOMS decrease along with the number of instances.
Table 3-2: Results of subsumption alignment in YAGO2-YAGO2.

<table>
<thead>
<tr>
<th></th>
<th>#instances(0-100)</th>
<th>#instances [100-500)</th>
<th>#instances [500-10,000)</th>
<th>Overall (0-10,000)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Precision</td>
<td>Recall</td>
<td>F-score</td>
<td>Precision</td>
</tr>
<tr>
<td>IUT</td>
<td>0.680</td>
<td>0.677</td>
<td>0.678</td>
<td>0.813</td>
</tr>
<tr>
<td>HM</td>
<td>0.741</td>
<td>0.455</td>
<td>0.564</td>
<td>0.763</td>
</tr>
<tr>
<td>BLOOMS</td>
<td>0.010</td>
<td>0.003</td>
<td>0.004</td>
<td>0.039</td>
</tr>
<tr>
<td></td>
<td>0.606</td>
<td>0.740</td>
<td>0.667</td>
<td>0.596</td>
</tr>
</tbody>
</table>
Table 3-2 shows that the IUT obtains the most satisfactory F-score compared with the other two approaches (0.678, 0.773, and 0.898). The results show the lexical- and structure-based approach (BLOOMS) is unsuitable for discovering the subsumption relations (0.004, 0.022, and 0.041). The subsumption relations are more likely to be found by using instances than using lexical or structure information. For example, the “YAGO:Hog110179649” contains eight instances (“Russ Grimm”, “Jeff Bostic”, “Joe Jacoby”, “Rick Walker”, “Ken Huff”, “Don Warren”, “George Starke”, “The Hogs (American football)”) and “YAGO:SelfishPerson110576962” contains nine instances (“Russ Grimm”, “Jeff Bostic”, “Joe Jacoby”, “Rick Walker”, “Ken Huff”, “Don Warren”, “George Starke”, “The Hogs (American football)”, “Tulillo Triviño Tulio”). The instance-based methods successfully discovered the subsumption relation between “YAGO:Hog110179649” and “YAGO:SelfishPerson110576962”, but the BLOOMS failed to find this relation since a hog can mean a greedy person but can also mean a domesticated pig. However, some relations built are wrong by using instance-based approaches, which are false positives and false negatives in F-score. The author noticed two main reasons caused the false positives and false negatives for intra-subsumption discovery: (1) insufficient description of taxonomy on the instance level. A super class may have the same instances as its sub-class. For example, “YAGO:Saber104121511” contains eight instances (“Swiss saber”, “Szabla”, “Sabre de cavalerie légère modèle An IX”, “Sabre (fencing)”, “Sabre de cuirassier modèle An IX”, “The French Connection (ice hockey)”, “Shashka”, “Curved saber of San Martín”), and “YAGO:FencingSword103327691” contains
the exact same eight instances. The instance-based method got a wrong relation (equivalence) since the two classes are same at the instance level. (2) multiple instantiation. Instances may be assigned to multiple classes that have no relations between each other. For example, “YAGO:ItalianBasses” containing one instance (“Franco Calabrese”) has no connection with “YAGO:OperaticBasses” containing three instances (“Charles Manners (bass)”, “Franco Calabrese”, “Alexandrov Ensemble soloists”). However, the instance-based methods may discover a wrong subsumption relation that “YAGO:ItalianBasses” is a sub-class of “YAGO:OperaticBasses”. The author noticed that the 76.9% false positives and false negatives are caused by the first reason.

Another phenomenon the author observed is that the F-score increases along with the cardinality of instances sets of classes. Both the HM and the IUT get the best F-score when using “500-10,000” data (0.666, 0.898). The author believes that the more instances used for describing a class, the better the instances used can represent the hierarchical structure of the class, which decreases the effects of the first reason.
### 3.5.2 Intra-subsumption Relations for DBpedia-DBpedia

![Bar Chart](image)

**Figure 3-6**: Running time of the three methods of DBpedia-DBpedia.

The DBpedia ontology has a small size of classes with a big number of instances. As Figure 3-6 shows, the IUT works more efficient than the HM. Figure 3-6 also shows the small number of classes with large-scale size of instances that underutilizes the advantages of BLOOMS.
Table 3-3: Results of subsumption alignment in DBpedia-DBpedia.

<table>
<thead>
<tr>
<th></th>
<th>#instances (0-100)</th>
<th>#instances [100-500]</th>
<th>#instances [500-10,000]</th>
<th>Overall (0-10,000)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Precision</td>
<td>Recall</td>
<td>F-score</td>
<td>Precision</td>
</tr>
<tr>
<td>IUT</td>
<td>1.0</td>
<td>0.80</td>
<td>0.889</td>
<td>1.0</td>
</tr>
<tr>
<td>HM</td>
<td>1.0</td>
<td>0.40</td>
<td>0.571</td>
<td>1.0</td>
</tr>
<tr>
<td>BLOOMS</td>
<td>NaN</td>
<td>0.0</td>
<td>NaN</td>
<td>NaN</td>
</tr>
</tbody>
</table>
Table 3-3 shows that the IUT obtains the most satisfactory F-score compared with the other two approaches (0.889, 0.750, and 0.821). The HM gets fewer F-score than the IUT because the HM finds less alignments than the IUT does. The author also notices that BLOOMS fails to find the alignments for the classes with small- and medium-scale size of instances, which is different with the YAGO2 data sets. The author considers the reason is that the WordNet used as the reference knowledge base has a different hierarchical structure with DBpedia ontology.

The author studied that the multi-instantiation does not cause failure of subsumption discovery and all the failures are caused by the insufficient description of taxonomy on the instance level. For example, “DBpedia:Racecourse” and its super class “DBpedia:RaceTrack” both contain the exactly same 300 instances, which makes the IUT discover a wrong relation that “DBpedia:Racecourse” is equivalent to “DBpedia:RaceTrack”. This mistake further be transited to make another wrong judgment that “DBpedia:Racecourse” is the sub-class of “DBpedia:SportFacility” rather than the correct assertions that “DBpedia:Racecourse” is the sub-class of “DBpedia:RaceTrack” and “DBpedia:RaceTrack” is the sub-class of “DBpedia:SportFacility”.

The author also noticed that the instance-based methods can achieve better F-score for classes with a large instance set.
3.5.3 Inter-Subsumption and Equivalence Relations for YAGO2-DBpedia

The author tries to align 358 classes from YAGO2 knowledge base to 358 classes from DBpedia ontology using subsumption relation. Same as the two previous experiments, the author separated classes into three instance-range groups. Figure 3-7 shows that the IUT is the fastest method for aligning the classes in all the instance-ranges.
<table>
<thead>
<tr>
<th>#instances (0-100)</th>
<th>Precision</th>
<th>Recall</th>
<th>F-score</th>
</tr>
</thead>
<tbody>
<tr>
<td>IUT</td>
<td>0.0</td>
<td>0.0</td>
<td>NaN</td>
</tr>
<tr>
<td>HM</td>
<td>NaN</td>
<td>0.0</td>
<td>NaN</td>
</tr>
<tr>
<td>BLOOMS</td>
<td>NaN</td>
<td>0.0</td>
<td>NaN</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>#instances [100-500)</th>
<th>Precision</th>
<th>Recall</th>
<th>F-score</th>
</tr>
</thead>
<tbody>
<tr>
<td>IUT</td>
<td>1.0</td>
<td>0.50</td>
<td>0.667</td>
</tr>
<tr>
<td>HM</td>
<td>0.250</td>
<td>0.250</td>
<td>0.250</td>
</tr>
<tr>
<td>BLOOMS</td>
<td>NaN</td>
<td>0.0</td>
<td>NaN</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>#instances [500-10,000)</th>
<th>Precision</th>
<th>Recall</th>
<th>F-score</th>
</tr>
</thead>
<tbody>
<tr>
<td>IUT</td>
<td>0.0</td>
<td>0.0</td>
<td>NaN</td>
</tr>
<tr>
<td>HM</td>
<td>1.0</td>
<td>0.40</td>
<td>0.571</td>
</tr>
<tr>
<td>BLOOMS</td>
<td>0.053</td>
<td>0.034</td>
<td>0.041</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Overall (0-10,000)</th>
<th>Precision</th>
<th>Recall</th>
<th>F-score</th>
</tr>
</thead>
<tbody>
<tr>
<td>IUT</td>
<td>0.301</td>
<td>0.546</td>
<td>0.388</td>
</tr>
<tr>
<td>HM</td>
<td>0.189</td>
<td>0.162</td>
<td>0.175</td>
</tr>
<tr>
<td>BLOOMS</td>
<td>0</td>
<td>0</td>
<td>NaN</td>
</tr>
</tbody>
</table>
Unlike the performance of the methods for intra-subsumptions in YAGO2 and DBpedia, the methods perform variously shown in Table 3-4. The IUT gets the best F-score in the overall data set (0.388), in medium-scale (0.667), and the HM gets the best F-score in large-scale (0.571). The reasons that cause the failures of the IUT to find the inter-subsumption relations are different with the reasons for intra-subsumption relations discovery. Different taxonomic systems are designed for different purposes, which make the scope of the class definitions different and distinctly instantiate the classes. Therefore, the classes having equivalence relation may not strictly satisfy the Definition 3-1 on the instance-level. More specifically, (1) two classes without subsumption relation from different ontologies share all instances from the class with a smaller cardinality, which is known as a false positive. For example, “YAGO:Ballplayer109835506” has 20,299 instances that are all included by “DBpedia:Person”. However, “YAGO:Ballplayer109835506” and “DBpedia:Person” are not connected by subsumption relation. (2) two classes with subsumption relation from different ontologies share the common instances that are only part of each instance set from the classes, which is known as a false negative. For example, “DBpediaOntology:SpaceMission” contains five instances ("Ares I-X", “Ares V-X”, “Apollo–Soyuz Test Project”, “Ares I-Y”, “Hypersonic Flight Experiment”) and only the first four instances are contained by “YAGO:Mission108403225”, which makes the instance-based methods fail to establish a subsumption relation. The taxonomic system in YAGO2 has more appropriate classes ("YAGO:Spaceflight100313502", “YAGO:Travel100295701”,
“YAGO:Voyage100312553”) to instantiate the fifth instance “Hypersonic Flight Experiment” than “YAGO:Mission108403225” does.

The author separated 326 classes belonging to YAGO2 knowledge base and DBpedia ontology into three instance-range groups using equivalence relation. As Figure 3-8 shows, the IUT runs faster than the HM but only slower than BLOOMS in large-scale instances.

**Figure 3-8:** Running time of the three methods of YAGO2-DBpedia for equivalence alignment.
Table 3-5: Results of equivalence alignment in YAGO2-DBpedia.

<table>
<thead>
<tr>
<th></th>
<th>#instances(0-100)</th>
<th>#instances [100-500)</th>
<th>#instances [500-10,000)</th>
<th>Overall (0-10,000)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Precision</td>
<td>Recall</td>
<td>F-score</td>
<td>Precision</td>
</tr>
<tr>
<td>IUT</td>
<td>1.0</td>
<td>0.20</td>
<td>0.333</td>
<td>1.0</td>
</tr>
<tr>
<td>HM</td>
<td>1.0</td>
<td>0.267</td>
<td>0.421</td>
<td>1.0</td>
</tr>
<tr>
<td>BLOOMS</td>
<td>1.0</td>
<td>0.067</td>
<td>0.125</td>
<td>0.773</td>
</tr>
</tbody>
</table>
Table 3-5 shows that the IUT gets the best F-score (0.641) for the equivalence alignment. In different data sets, BLOOMS gets the best F-score in the medium- and large-scale sized of instances (0.739, 0.756), and the HM gets the best F-score in the small-scale size of instances (0.421). Similar with the reasons for failure of inter-subsumption discovery, there are also two reasons (false negatives and false positives) for failure of equivalence discovery, which can be also considered as the cause of different taxonomy purposes. (1) distinct classes described by instances that are overlapped in majority, which is known as a false positive. Since the two different ontologies are designed to describe the different knowledge system, two distinct classes that are likely to share same instances can be considered as an equivalent pair by the IUT. For example, “DBpedia:Person” contains 511,484 instances and “YAGO:LivingThing100004258” contains 574,634 instances. “DBpedia:Person” and “YAGO:LivingThing100004258” share 501,311 instances, which the Jaccard similarity of “DBpedia:Person” and “YAGO:LivingThing100004258” is 0.8724. (2) equivalent classes described by distinct instances, which is known as a false negative. For example, “DBpedia:Protein” contains 1,620 instances and “YAGO:Protein114728724” contains 2,965 instances, and “YAGO:Protein114728724” and “YAGO:Protein114728724” only share 690 common instances.

The author also notices that the F-score of equivalence alignment is better than subsumption alignment, which indicates that the equivalent classes are more likely to have the same instances in contrast to the classes aligned with subsumption which are less likely to have the fully overlapped instances.
3.5.4 Effects of $\chi_s$ and $\chi_e$ for the IUT

The experiments demonstrate that the instance-based methods are better at discovering subsumption and equivalence relations than the state-of-the-art lexical- and structure-based method. However, the author also noticed that the performances of the instance-based approaches are affected by several reasons the author mentioned. In the IUT, there are two parameters ($\chi_s$ and $\chi_e$, where $\{\chi_s | 0 \leq \chi_s \leq 1.0\} $ and $\{\chi_e | 0 \leq \chi_e \leq \chi_s\}$) to control the confidence whether two classes have a subsumption or equivalence relation. Adjusting $\chi_s$ and $\chi_e$ directly changes the numbers of False Negative (FN) and False Positive (FP), which further affects the F-score. The author changed $\chi_s$ and $\chi_e$ to see the effects on the F-score as shown in Figure 3-9.
(a) \( \chi_s \) for intra-subsumption (YAGO2-YAGO2)

(b) \( \chi_s \) for intra-subsumption (DBpedia-DBpedia)
As Figure 3-9 (a, b, and c) show, decreasing $\chi_s$ hurts the F-score as the number of FN and FP increases. The main reason for failures of inter-subsumption discovery is FP that increases along with the decrease of $\chi_s$. The lower $\chi_s$ allows more candidate pairs to be considered as positives, which increases the recall but decreases the precision. Different with inter-subsumption discovery, FN is the main
reason for failures of intra-subsumption discovery in DBpedia-DBpedia, which increases along with the decreases of $\chi_s$. The insufficient description of the intra-taxonomy on the instance level is the main reason of alignment failures for DBpedia ontology, lowering $\chi_s$ allows more classes to establish subsumption relations, which amplifies the errors caused by the effects of insufficient taxonomic description on the instance level. The amplification decreases the recall and further decreases the F-score. The intra-subsumption in YAGO2-YAGO2 is affected by two reasons (insufficient taxonomic description on the instance level and multi-instantiation). Lowering the threshold of subsumption establishing, which is caused by decreasing of $\chi_s$, amplifies both FN and FP hence decreases the recall and the precision.

Figure 3-9 (d) shows that $\chi_e$ gets the best F-score when $\chi_e = 0.25$. The author observes that increasing $\chi_e$ boosts the F-score before the F-score reaching the summit, and hurts the F-score after overpassing the summit. Before $\chi_e$ arriving 0.25, increases of $\chi_e$ raises threshold that traps more non-equivalent classes, which decrease FN and FP. Along with $\chi_e$ increases and overpasses 0.25, fewer candidate pairs are considered to be equivalent, which increases FN and FP.

From the Figure 3-9, the author gets two important hints for setting $\chi_s$ and $\chi_e$ where $\{\chi_s | 0 \leq \chi_s \leq 1.0\}$ and $\{\chi_e | 0 \leq \chi_e \leq \chi_s\}$, that is, the higher $\chi_s$ is the better it is for subsumption discovery, and the lower $\chi_e$ is the better it is for equivalence discovery before $\chi_e = 0.25$. 


3.6 Discussions

The IUT is an instance-based schema alignment algorithm, which heavily depends on the description of ontology on the instance level. The results of the alignment of the IUT can be affected by two reasons as the author discussed in Section 3.5, which are insufficient taxonomic description on the instance level and multi-instantiation. The motley instantiation strategies for diversity ontologies weaken the subsumption and equivalence detections.

Another problem what instance-based methods should care is the issue caused by the asymmetric ontology update. The alignment of two classes from two ontologies changes if the updating speeds of two ontologies are different. For example, updating DBpedia 3.9 that uses the Wikipedia data in April 2013 from DBpedia 3.8 that uses the Wikipedia data in June 2012 costs nine months, but updating YAGO2 2.5 that uses the Wikipedia data in December 2012 from YAGO2 2.4 that uses the Wikipedia data in August 2010 costs more than two years. The imbalanced updating speed can change the original alignment results. For instance, the “DBpedia: Artery” in DBpedia 3.9 contains all the instances in “YAGO:Artery105333777” in YAGO2 2.4, which the IUT considers a subsumption relation between the two classes. However, the “DBpedia:Artery” in DBpedia 3.9 shares part of all instances (303) in “YAGO:Artery105333777” in YAGO2 2.5, which increase the Jaccard similarity into 0.75 and defines the relation as equivalence. In this study, the author simply removes the instances only used in one data resource to reduce the effects of the asymmetric ontology update. However, the added or deleted instances in an updated version can more precisely describe a class
and correct some errors in the alignments for the previous version that is poorly designed. A comprehensive solution is a new research direction for the future work.

There are two assumptions for instance-based methods: (1) instance-level alignment is established. (2) ontology has a hierarchical structure on the schema-level. Linked Data creates links to connect data in different sources based on the Web (Bizer et al., 2009). Therefore, links are one of the most important factors to evaluate the quality of a linked data set. Most famous linked data sets already have abundant links. For example, DBpedia has 39,012,034 links connected with a variety of databases, including BBC music, DailyMed, New York Times, etc. For those are not connected with other linked data sets, one solution is to establish instance alignments with existing instance alignment algorithms, which is proposed by PARIS (Suchanek et al., 2011), and use existing link discovery frameworks, such as Silk (Volz, Bizer, Gaedke, & Kobilarov, 2009). For the second assumption, some ontologies in LOD lack the hierarchical structure, which will fail the proposed approach. One solution is to build taxonomy automatically with the help of probability models, logic rules or thesauri (Bedini & Nguyen, 2007). The author has proposed a solution in Chapter 5 that introduces the methods to automatically generate hierarchical schema structure for Linked Data in detail.

In the proposed method, only inter-linked instances are used. There raises a discussion on the meaning of using of inter-linked instances in our data pre-processing.

In Semantic Web, an ontology is constructed based on Open-World Assumption (OWA), which admits incompleteness of instances at a given time.
This incompleteness in describing a concept is due to many reasons, such as unintentional omission of instances though they are exposed to the ontology developer, and lack of awareness of the existence of instances that deem the status of being included in the concept. Therefore, even for the same concept, two ontologies may have different instance sets attached to the concept, since the different instance spaces are deemed as legitimate within their sphere of known explored world.

In concept comparison, the incompleteness of concept extensions (i.e., instances) weakens the usefulness of instances as the description of understanding, or definition, of concepts, because the incompleteness itself may be the cause of varying instantiations of the concepts. In short, the instances the author gathered are just one possible representation of a concept - there may be many more such cases. In order to come up with a way that produces a convincing measure for similarity between concepts, one has to rely on truth, which in this study is links. Links are created externally, and the author has no control over, or rather should not have control over. Hence, links are taken as the sole truth statements that prove the legitimacy of similarity between two concepts. As for unlinked instances, the author takes them as neither untrue nor true, since it is beyond the scope of this study. In case a new link is created in the future between two instances which did not have a link between them, the author’s method will take it as a new truth statement and proceeds as it is designed to.

Therefore, unlinked instances are removed, and the remaining instances are conflated into one instance space. For example, to align two different versions of
DBpedia Ontology, DBpedia 3.9 and DBpedia 2014, removing the instances only existing in DBpedia 2014 can eliminate the mismatched concepts because of the new added instances (from April 2013 to May 2014) that are not acknowledged by DBpedia 3.9.
3.7 Conclusion

In this chapter, the author proposed the IUT that is an instance-based schema alignment algorithm. The IUT builds a unified taxonomy for all the classes from two ontologies to obtain the alignments. The position of each class is decided by the common instances shared with other classes in the unified taxonomy. The author tested the IUT with DBpedia and YAGO2, and compared the IUT with two state-of-the-art methods for schema alignments in LOD. The experiments show the IUT outperforms the methods in F-score. The experiments also illustrate that ontology with a larger number of instances is more likely to have a good F-score of the IUT. The author also observed the reasons of aligning failures for the IUT, that is, insufficient taxonomic description on the instance level and multi-instantiation in the intra-subsumption alignment, and different taxonomic structure of ontologies for diversity purposes in the inter-subsumption and equivalence alignment. Two parameters for the IUT are tested to control the alignment failures. The author discussed limitations of proposed method and gives several solutions to improve the works.
4 Scaling Pair-wise Computations Using the Locality Sensitive Hashing

4.1 Introduction

Figure 4-1: The search spaces of different algorithms in Section 3.4.

Comparing large number of classes based on instances will easily bring a scalability issue. If we have $k$ classes in the source ontology, the schema alignment algorithms (the HM and BLOOMS used in Section 3.4) need $k$ iterations to find the alignments for all the classes in the source ontology, and each iteration needs to search $t$ classes in the target (the source ontology is the same with the target ontology, we consider $k = t = m$). The search space (Korf, Yandell, & Bedell, 2003) is $k \times t$ as shown on the left of Figure 4-1. For a pair of classes sharing $n$ instances, the time complexity of the similarity computing needs $O(n)$ operations. The computation of the whole pairs of classes needs $O(n \times k \times t)$ operations, which makes all the pair-wise computations not efficient if the sizes of ontologies.
are too large. The IUT decreases the search space with the unified graph (the search space at the center of Figure 4-1) but could still meet a scalability issue.

The Locality Sensitive Hashing (LSH) (Rajaraman & Ullman, 2011) is a probabilistic dimension reduction algorithm. The basic idea of LSH is to map sets of values into hash values with reduced dimensions, and put similar sets into buckets with a high probability. LSH can be used to reduce large pair-wise computations, and is further adapted in instance-based schema mapping (Duan et al., 2012). The author adapts the basic idea of the LSH that uses MinHash to estimate the probability of subsumption (Definition 3-1) and equivalence (Definitions 3-2 and 3-3) in Section 3.3.3 to decrease the time complexity of a similarity computation, and use bandings to reduce the search space (on the right of Figure 4-1) used in Algorithm 3-1. The author performs an experiment of scaling the IUT based on LSH for YAGO2-YAGO2 intra-subsumption alignment task performed in Section 3.5.1. The experiment demonstrates that the running time of the original IUT can be reduced by 94% with a 5% loss in F-score using the proposed scaling method.

The content of this chapter is mainly based on the author’s previous work published (Zong et al., 2015). The rest of this chapter is organized as follows: Section 4.2 introduces MinHash and banding method of the LSH, and details on the IUT(M), an IUT-based schema algorithm with the LSH; Section 4.3 introduces the scaling results of the IUT(M) for YAGO2-YAGO2 intra-subsumption alignment task. Section 4.4 discusses limitations of this chapter, and Section 4.5 concludes this study.
4.2 Methods

For a class that is de-queued from the class-relation multi-graph generated in Section 3.3.2, the IUT has to compute the similarities with all the classes that are already in the virtual graph. The IUT(M) reduces the computations of the original IUT with an LSH-based MinHash index and a set of buckets by two steps as shown in Figure 4-2. First, after the instance-class matrix is constructed, a set of MinHash functions are used to map the values of each class in the matrix into the values in a smaller dimension in a MinHash index. Second, all the similar classes are input into a same bucket. With the MinHash index and buckets, the IUT(M) decreases the computations of the IUT from two aspects: (1) for a similarity computation on each pair of classes, the computation is decreased with the values of a smaller dimension mapped with MinHash functions, and (2) for choosing a most similar class out of
the classes in the virtual graph, the number of similarity computations is decreased by using the buckets.

In the following sections, the author will introduce the basic idea of using MinHash functions and buckets to decrease the pairwise similarity computations, and how the author applies these methods to the instance-based schema alignment.

### 4.2.1 MinHash and Signatures

Assuming $sim(c_i, c_j)$ measuring the similarity of the class $c_i$ and $c_j$, where $c_i$ and $c_j$ belong to $C = \{c_1, c_2, \ldots, c_m\}$, a family $F$ of hash functions maps all $c_i$ to a set $Z$ of integers that makes the probability $Pr(f(c_i) = f(c_j))$ of two hash values of $c_i$ and $c_j$ equal with $sim(c_i, c_j)$, that is, in another word $Pr(f(c_i) = f(c_j)) = sim(c_i, c_j)$, where $f \in F$. The principle of the LSH is to choose adequate hash functions belonging to one hash family to map two similar classes into a same value as much as possible. The hash functions are said to be $(d_1, d_2, p_1, p_2) - sensitive$ if for every $f$ in $F$ satisfies two conditions:

**Condition 1:** if $1 - sim(c_i, c_j) \leq d_1$, then $Pr(f(c_i) = f(c_j)) \geq p_1$

**Condition 2:** if $1 - sim(c_i, c_j) \geq d_2$, then $Pr(f(c_i) = f(c_j)) \leq p_2$

A MinHash (Rajaraman & Ullman, 2011) maps the $C$ to the set $Z$ by computing the minimum value of a universal hash function for $C$ and follows $Pr(f^{min}(c_i) = f^{min}(c_j)) = jaccardSim(c_i, c_j)$. In practice, for two class vectors $c_i = [i_1, i_2, \ldots, i_n]^T$ and $c_j = [i_1, i_2, \ldots, i_n]^T$, a MinHash function has a probability, equaling with the Jaccard similarity of the two classes, to produce the same values of two class vectors with a random permutation of instances.
Figure 4-3: An example of a matrix based on the instance-class matrix used in Section 3.3.2 with a permutated order of instances.

With a permutation of the rows, the min value of a column for this permutation is the number of the first row, in this permuted order, in which the column has a 1. For example, with the instance-class matrix used in Section 3.3.2, we have a permutation \( \{i_1, i_3, i_2\} \). The matrix with the permutated order of the instances is shown in Figure 4-3. Therefore, we get min value \( p_1(c_1) = i_1 \) because \( i_1 \) is the first instance that exists in this order. Similarly, we can get \( p_1(c_3) = i_3 \) and \( p_1(c_5) = i_2 \). A permutation of instances can be considered as a result of a hash function for the instances. Thus, for the hash function \( h_1 \), which reflects to the permutation \( \{i_1, i_3, i_2\} \), the value of each class for \( h_1 \) is the same value as we got for the permutation. Therefore, we get \( h_1(c_1) = i_1 \), \( h_1(c_3) = i_3 \), and \( h_1(c_5) = i_2 \).
With limited number of $v_s$ permutations, a set of the minimum values in all the permutations for a class $c_i$, which can be represented as $F_{c_i} = \{f_1^{min}, f_2^{min}, ..., f_{v_s}^{min}\}$, is called the signatures for the class $c_i$. The signatures are used to estimate the Jaccard similarity, which decreases the computation of $sim(c_i, c_j)$ from $O(N)$ to $O(v_s)$. With a fast MinHashing algorithm (Rajaraman & Ullman, 2011), we can easily get the signatures for classes in the instance-class matrix. The fast MinHashing algorithm obtains the minimum value of each function in all the rows where the values are 1.

For example, consider we have two hash functions that are $h_1 = mod(x + 1, 3)$ and $h_2 = mod(2x + 1, 3)$, where $x$ is the row of the instance-class matrix as shown in Figure 4-4. Therefore, we get $h_1 = [1,2,0]$ for the permutation of $\{i_3, i_1, i_2\}$ and $h_2 = [1,0,2]$ for the permutation of $\{i_2, i_1, i_3\}$. The fast MinHashing algorithm uses three iterations to get the signatures of all the classes. For $c_1$, since the values of row 0 to 2 are all 1s, the minimum values of the two hash functions are [0,0].
Figure 4.4: An example of computing signatures with the fast MinHashing algorithm.
4.2.2 Banding Technique

For $v_s$ MinHash signatures, each $c_i$ is represented as $c_i = \{f_1^{\text{min}}(c_i), f_2^{\text{min}}(c_i), ..., f_{v_s}^{\text{min}}(c_i)\}$. For two classes $c_i$ and $c_j$, the more elements of two vectors $c_i = \{f_1^{\text{min}}(c_i), f_2^{\text{min}}(c_i), ..., f_{v_s}^{\text{min}}(c_i)\}$ and $c_j = \{f_1^{\text{min}}(c_i), f_2^{\text{min}}(c_i), ..., f_{v_s}^{\text{min}}(c_i)\}$ are identical, the more likely that the two classes are equal. The banding technique divides each class vector into $v_b$ number of bands with length of $v_r$, where $v_r \times v_b = v_s$. For each band $b$, if two sub-vectors of $c_i$ and $c_j$ are identical, $c_i$ and $c_j$ are assigned into a same bucket for $b$.

![Instance-class Matrix](image)

![Signature Matrix](image)

**Figure 4-5:** Signatures and buckets with two hash functions.
In the same ongoing example shown in Figure 4-5, \( c_1 = [0, 0]^T \) and \( c_2 = [1, 0]^T \) have identical sub-vector \([1]^T\) in the second band. Therefore, the two classes are put into a same bucket.

![Figure 4-6: S-curves of \( 1 - (1 - s^{vr})^{vb} \) with different combinations of \( vr \) and \( vb \) when using 50 hash functions.](image)

If the Jaccard similarity of \( c_i \) and \( c_j \) is \( s \), the probability, which the corresponding elements of the signatures of \( c_i \) and \( c_j \) agree in all indices of at least one band and becomes a similar candidate pair, is \( 1 - (1 - s^{vr})^{vb} \) (Rajaraman & Ullman, 2011). For example, for the pair of classes \( c_1 \) and \( c_2 \) with Jaccard similarity \( sim(c_1, c_2) = 0.75 \), we have confidence \( 1 - (1 - 0.75^1)^2 = 0.9375 \) that \( c_1 \) and \( c_2 \) are in a similar candidate pair with \( v_b = 2 \) and \( v_r = 1 \). \( 1 - (1 - s^{vr})^{vb} \) follows an S-curve as shown in Figure 4-6. Smaller \( v_r \) and greater \( v_b \) indicate bigger chance of class pairs with small Jaccard similarities to be considered as a similar pair, and greater \( v_r \) and smaller \( v_b \) indicate less chance of class pairs.
with large Jaccard similarities to be considered as a similar pair. With good tuning of the two parameters, the computations of choosing the most similar class in a virtual graph for a de-queued class from the class-relation multi-graph can be dramatically decreased.

4.2.3 Scaling the IUT with MinHash and Banding

The author scales the IUT with MinHash and banding techniques that are used to reduce the pair-wise similar computation of Jaccard similarity, and the author calls it IUT(M). The IUT(M) builds $v_s$ MinHash functions and bands the signature matrix with $v_r$ rows and $\frac{v_s}{v_r}$ bands (line 2 in Algorithm 4-1). The similar candidate pairs are used to restrict the search space for discovering a relation for a class in the graph (line 7 in Algorithm 4-1). In practice, the IUT(M) discards the multi-graph that is used to sort the important classes and simply sorts classes by the number of instances (line 3 in Algorithm 4-1).

In order to accommodate the subsumption relation discovering using Equation 3-1, the IUT(M) computes the $\text{sim}'(c_i, c_j)$ with existing estimated Jaccard similarity $\text{jaccard}'(c_i, c_j)$ by MinHash as follows:

$$\text{sub}'(c_i, c_j) = \frac{\text{jaccard}'(c_i, c_j)}{\text{jaccard}'(c_i, c_j) + 1} \times (1 + \frac{|c_j|}{|c_i|})$$

(4.1)

The process of the IUT(M) is shown in Algorithm 4-1.
Algorithm 4-1: Scaling the IUT with MinHash and Banding (IUT(M)).

**Input:** a source ontology $O_1(C_1, I_1)$, a target ontology $O_2(C_2, I_2)$, $\chi_s$, $\chi_e$, $\nu_s$, $\nu_r$

**Output:** subsumption and equivalence alignments $A$

1: Instance-class matrix $M := \text{generate from } O_1$ and $O_2$

2: Similar candidate pairs $P = \{p_1, p_2, ..., p_k\} := \text{MinHash.banding}(\nu_s, \nu_r, M)$

3: Queue $Q := \text{all the classes sorted by the descending order of number of instances}$

4: Initiate an empty virtual graph $H$

5: While $\text{size}(Q) > 0$ do

6: $c_i := \text{dequeue}(Q)$

7: Add $c_i$ into $H$

8: Initiate an ancestor list $S$ and an equivalence list $E$

9: For $c_j$ in $H$ do

10: If $c_i$ originates from either one of the two ontologies (source and target) and $c_j$ from the other ontology then

11: If $(p = \{c_i, c_j\} \in P)$ then

12: If $(\text{sub}'(c_i, c_j) \geq \chi_s$ and $\text{sub}'(c_j, c_i) \geq \chi_s)$ put $c_j$ into $E$

13: Else if $(\text{sub}'(c_i, c_j) \geq \chi_s)$ put $c_j$ into $S$

14: Else if $(\text{sim}'(c_i, c_j) \geq \chi_e)$ put $c_j$ into $E$

15: Else put $c_j$ into $E$ or $S$ based on the original existing relation of $c_i$ and $c_j$

16: Add inbound and outbound edges from $c_i$ to the vertices in $E$

17: Add outbound edges from $c_i$ to the sup-vertices in $S$

18: Return new discovered relations as the alignments $A$ in $H$
4.3 Experiment

As Section 3.5.1 shows, big size data (YAGO2-YAGO2) addresses the scalability problem in schema alignment. The author scales the IUT by using the LSH and MinHash function. The banding technology makes the possibility of a similar candidate pair follow $1 - (1 - s^\frac{v_s}{v_r})^\frac{v_s}{v_r}$. Adjusting $\frac{v_s}{v_r}$ can change the number of candidate pairs to be compared. For example, if $v_s = 1,000$, decreasing $v_r$ from “10” to “5” makes the possibility, which one pair with similarity “0.6” to be considered as a candidate pair, increase from 0.455 to 0.999.

The author tested the scaling algorithm the IUT(M) and compared it with the baseline (the IUT) for YAGO2-YAGO2 that needs to be scaled (3,981,676 ms).

Table 4-1: Efficiency of scaling the IUT for alignment in YAGO2-YAGO2 ($v_s = 1,000$).

<table>
<thead>
<tr>
<th>$v_r$</th>
<th>Time (ms)</th>
<th>$\frac{T_{IUT(M)}}{T_B}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>245,233</td>
<td>0.06159</td>
</tr>
<tr>
<td>20</td>
<td>231,484</td>
<td>0.058137</td>
</tr>
<tr>
<td>10</td>
<td>228,938</td>
<td>0.057498</td>
</tr>
<tr>
<td>5</td>
<td>226,824</td>
<td>0.056967</td>
</tr>
<tr>
<td>3</td>
<td>228,099</td>
<td>0.057287</td>
</tr>
<tr>
<td>2</td>
<td>232,039</td>
<td>0.058277</td>
</tr>
<tr>
<td>Baseline(B)</td>
<td>3,981,676</td>
<td></td>
</tr>
</tbody>
</table>
Table 4-2: Precision of scaling the IUT for alignment in YAGO2-YAGO2 ($v_s = 10,000$).

<table>
<thead>
<tr>
<th>$v_r$</th>
<th>Precision</th>
<th>$P_{IUT(M)} - P_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>0.809322</td>
<td>+0.203712</td>
</tr>
<tr>
<td>20</td>
<td>0.778471</td>
<td>+0.172861</td>
</tr>
<tr>
<td>10</td>
<td>0.752852</td>
<td>+0.147242</td>
</tr>
<tr>
<td>5</td>
<td>0.704648</td>
<td>+0.099038</td>
</tr>
<tr>
<td>3</td>
<td>0.690829</td>
<td>+0.085219</td>
</tr>
<tr>
<td>2</td>
<td>0.681948</td>
<td>+0.076338</td>
</tr>
<tr>
<td>Baseline(B)</td>
<td>0.60561</td>
<td></td>
</tr>
</tbody>
</table>

Table 4-3: Recall of scaling the IUT for alignment in YAGO2-YAGO2 ($v_s = 1,000$).

<table>
<thead>
<tr>
<th>$v_r$</th>
<th>Recall</th>
<th>$R_{IUT(M)} - R_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>0.022538</td>
<td>-0.71756</td>
</tr>
<tr>
<td>20</td>
<td>0.058883</td>
<td>-0.68122</td>
</tr>
<tr>
<td>10</td>
<td>0.116821</td>
<td>-0.62328</td>
</tr>
<tr>
<td>5</td>
<td>0.229866</td>
<td>-0.51024</td>
</tr>
<tr>
<td>3</td>
<td>0.398667</td>
<td>-0.34144</td>
</tr>
<tr>
<td>2</td>
<td>0.563455</td>
<td>-0.17665</td>
</tr>
<tr>
<td>Baseline(B)</td>
<td>0.740103</td>
<td></td>
</tr>
</tbody>
</table>
Table 4-4: F-score of scaling the IUT for alignment in YAGO2-YAGO2 ($\nu_s = 1,000$).

<table>
<thead>
<tr>
<th>$\nu_r$</th>
<th>F-score</th>
<th>$F_{IUT(M)} - F_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.043855</td>
<td>-0.62228</td>
</tr>
<tr>
<td>10</td>
<td>0.109484</td>
<td>-0.55665</td>
</tr>
<tr>
<td>5</td>
<td>0.202258</td>
<td>-0.46388</td>
</tr>
<tr>
<td>3</td>
<td>0.34665</td>
<td>-0.31949</td>
</tr>
<tr>
<td>2</td>
<td>0.505574</td>
<td>-0.16056</td>
</tr>
<tr>
<td>50</td>
<td>0.617065</td>
<td>-0.04907</td>
</tr>
<tr>
<td>Baseline(B)</td>
<td>0.666136</td>
<td></td>
</tr>
</tbody>
</table>

Table 4-1 to Table 4-4 show that the scaling algorithm (the IUT(M)) dramatically decreases the running time ($Mean_{\frac{T_{IUT(M)}}{TB}} = 0.058293$) and keeps a good F-score ($F_{IUT(M)} - F_B = 0.04907$). The precision of the IUT(M) decreases along with the decreases of the $\nu_r$ in Table 4-2, and the recall and F-score increase along with the decrease of the $\nu_r$ in Table 4-3 and Table 4-4. In the IUT(M), raising value of $\nu_r$ keeps the pairs with higher Jaccard similarity, which increases precision. However, some pairs, having low Jaccard similarity but connected with subsumption relations, are ignored when $\nu_r$ is high. For example, “YAGO:Pen103906997” has 35 instances and “YAGO:WatermanPens” has 2 instances that are also included in “YAGO:Pen103906997”. The Jaccard similarity of “YAGO:Pen103906997” and “YAGO:WatermanPens” is 0.057. According to $1 - (1 - s^{\nu_r})^{\nu_s}$, the possibility of “YAGO:Pen103906997” and
“YAGO: WatermanPens” pair to be a candidate pair is 0.0001 when $\nu_r = 5$, but increase to 0.8035 when we decease $\nu_r$ to 2. The lower $\nu_r$ extracts more candidate pairs that have subsumption relations but with low Jaccard similarity, which increases the recall but decreases the precision.

The IUT(M) decreases the sizes of the search space for each iteration, hence it decreases the running time (Figure 4-7 (b)). As Figure 4-7 (a) shows, the IUT(M) only compares a few number of classes (less than 10 classes for most of the iterations) as compared with the IUT where the number of classes linearly increases along with the number of iterations (notice that the y axis in Figure 4-7 (a) is logarithmic scaled).
Figure 4-7: Efficiency comparison of the IUT and the IUT(M) that with $\nu_r = 2$ and $\nu_s = 1,000$. 

(a) Number of the classes compared in each iteration

(b) Running time of each iteration
4.4 Discussions

The IUT uses Jaccard similarity to calculate the similarity between two classes. Therefore, the IUT(M) scales the computations of IUT based on MinHash functions in LSH. However, there are other similarity calculation methods with corresponding scaling algorithms in LSH. (Duan et al., 2012) applied MinHash and Random Hyperplane to scale the Jaccard and Cosine similarities used in class similarity computations. The future work will try to apply Cosine similarity and Random Hyperplane to the IUT for similarity computations and scaling. The author also noticed that scaling pair-wise similarity computations in other domains can also potentially be adapted into schema alignment. These methods, such as parallel computing based on MapReduce (Lin, 2009; Y. Wang et al., 2013), and index-based method (Bayardo et al., 2007), are capable of being generalized to other similarity measures, including Jaccard, Cosine, Overlap, and Dice similarities, and can be used to improve the IUT in the future works.
4.5 Conclusion

Scaling pair-wise similarity computations for classes is vital for schema alignment in Linked Data that has a large number of instances for classes. In this chapter, the author introduced a scaling method for the IUT based on LSH to handle the scalability problem in schema alignment. The proposed method called IUT(M), which decreases the computations of the IUT when it generates the virtual graph from two aspects: (1) the similarity computation for each pair of classes is decreased with MinHash functions, and (2) the number of similarity computations that find the most similar class for a de-queued class from the class-relation multi-graph are decreased by using the banding method in LSH. The author performed the IUT(M) with YAGO2-YAGO2 intra-subsumption alignment task. The experiment shows that the running time of IUT can be reduced by 94% with a 5% loss in F-score.
5 Unsupervised Hierarchical Schema Structure Generation in Linked Data

5.1 Introduction

The growing needs of RDF resources push organizations to publish their own RDF format data by transforming their legacy data, such as relational database or Web pages, with transformation programs (Bizer, 2011; Blum & Cohen, 2010; Ding et al., 2010; Martín & Gutierrez, 2009). Lacking domain experts to build ontologies, these data, containing a limited schema but abundant relationships between instances, are incomplete (Zhu et al., 2015). Without expressive T-Box of an ontology to describe the relations between concepts, Linked Data suffers in knowledge acquisition (Zhu et al., 2015).

There are two ways to solve the problem: (1) map instances to an existing ontology (Bizer et al., 2009; Sahoo et al., 2009); and (2) generate an ontology directly from data sources (Alani et al., 2003; Mitchell, Betteridge, Carlson, Hruschka, & Wang, 2009; Pivk, 2006; Tho, Hui, Fong, & Cao, 2006; Tijerino, Embley, Lonsdale, Ding, & Nagy, 2005). However, it is not desirable to squeeze every RDF repository under a single ontology, nor for unwilling data providers to make their Linked Data adhere to any published ontology. The T-Box learned from the A-box can fully describe the local data set and better represents the knowledge induced from the instances (Völker & Niepert, 2011). Therefore, learning T-box from A-box for Linked Data has been studied in the past few years,
such as the methods in (Lehmann & Voelker, 2014; Tiddi, Mustapha, Vanrompay, & Aufaure, 2012; Völker & Niepert, 2011; Zhu et al., 2015).

These methods generate a single taxonomy for a given linked data set, which reflects an implicit perspective of viewing or understanding the data. However, it is often difficult for users to agree on a particular manner to categorize compound instances with multiple properties. (Brewster & Wilks, 2004; Han & Fu, 1994). For example, DBpedia ("DBpedia,"), and YAGO2 ("YAGO2s: A High-Quality Knowledge Base,"), have developed different ontologies for categorizing Wikipedia pages ("Wikipedia,"). Taxonomies are generated based on different ways of viewing the same data.

For example, ethic and occupation are both used to classify the concept “person” in YAGO2, which causes “YAGO:wordnet_bad_person_109831962” and “YAGO:wordnet_dancer_109990415” to be both sub-concepts of “YAGO:wordnet_person_100007846”, whereas only occupation is considered in the DBpedia Ontology. In Linked Data, instances have values of diverse properties, each of which can be viewed as a facet in faceted browsing or navigation (Sacco & Tzitzikas, 2009). Therefore, a faceted taxonomy that classifies data from multiple angles draws the attention of the Semantic Web community (Oren, Delbru, & Decker, 2006). However, though faceted navigation or search based on faceted taxonomies has received most attention in research (Erling & Mikhailov, 2009; Rodriguez-Castro, Glaser, & Carr, 2010), automatic construction of faceted taxonomy is little studied.
Consequently, in order to meet different needs arising from various uses of taxonomies, the author proposes a robust method for generating faceted taxonomies based on object properties of instances in Linked Data. Please note, different with the taxonomy defined in Chapter 3 and Chapter 4, the taxonomy used in this chapter has hierarchical structure that only contains the subsumption relation. There are three benefits of using faceted taxonomy:

(1). Faceted view of the taxonomy facilitates user experience of taxonomy navigation, since it provides guided navigation of the data organized as a taxonomy. Other taxonomy generation methods may have such views implicitly built into their taxonomies, leaving users with no direct exposure to such guidance.

(2). Update of taxonomy is modular in that when an object property is added, a new sub-taxonomy in a new facet needs to be added into the existing faceted taxonomy without disrupting existing sub-taxonomies in other facets.

(3). Flexibility in facet combination. Facets can be assembled easily, invoking rapid filtering of instances. Classifications based on facets can cope with high-stress tasks, due to its flexibility, especially so when compared with taxonomies built in a single linear hierarchy.

The author has developed a framework that dynamically extracts data with a single object property to generate a sub-taxonomy in each facet. Each sub-taxonomy is generated with an Instance-based Concept Taxonomy generation algorithm called ICT, adapted from an instance-based ontology alignment algorithm (Zong et al., 2015). In an addition, the strategies of instantiation and refinement are also proposed. The experiment comprises two tasks: (1) the construction performance
of a sub-taxonomy is tested by comparing the generated taxonomy based on “rdf:type” with two gold standards, DBpedia and YAGO2, and (2) the construction performance of a faceted taxonomy with multiple facets is evaluated by the running time and search effectiveness of the taxonomies based on two biomedical linked data sets, Diseasome ("Diseasome,")) and DrugBank ("DrugBank,"). The two tasks demonstrate the capability of the proposed method to generate a faceted taxonomy efficiently and effectively.

The rest of the chapter is organized as follows: Section 5.2 gives the basic principle of the proposed solution; Section 5.3 details on the framework of the proposed solution; Section 5.4 presents the method of faceted taxonomy generation; in Sections 5.5 and 5.6, the author demonstrates the results of the experiments; Section 5.7 discusses limitations of this study and the conclusions are presented in Section 5.8.
5.2 Faceted Taxonomy for Linked Data

The object of this study is to automatically construct a concept taxonomy that fully describes instances. Considering that different instances in the same topic may have same values of properties, the author is trying to use the property values to cluster the instances and formalize a concept hierarchy structure. There are two types of properties in Linked Data sets: data-type and object-type. Object-type properties link instances with objects, and data-type properties link instance with literal values (Bechhofer et al., 2004). Please note, given a subject-property-object (SPO) triple in an A-box, the subject is considered as an instance. If the object is a literal value, the property is a data-type property. If the object is a de-referenceable URL, the property is an object-type property, and the URL is called an object entity or object for short. The author uses the object-type instead of using data-type property with following reasons. First, instances belonging to the same concepts may share the same objects and inherit some objects from the super concept, which is hardly observed on the values of data-type properties. Second, clustering of instances based on the semantic similarities rather than on lexical
similarities is in accordance with the human habit of building a concept taxonomy. Therefore, the author only considers using object-type properties to generate a concept taxonomy for Linked Data.

Given a linked data set containing an A-box \( A = \{ I, P, O \} \) that consists of a set instances \( I \), a set of object properties \( P \) and a set of objects \( O \), where each instance \( i_u \in I \) is described with a set of property \( P_u = \{ p_1, ..., p_k \} \), each of which has a set of objects \( O_{i_u p_v} = \{ o_1, ..., o_t \} \) and \( t \geq 1 \), The author proposes a solution of building a faceted taxonomy as shown in Figure 5-1 based on the object properties, where each property can be considered as a facet. Please note that the facet differs with the facet used in OWL 2 in the context respective datatypes (Carroll et al., 2012). The author adapts the concept of facet in (Sacco & Tzitzikas, 2009) and defines a facet as:

**Definition 5-1:** a facet \( f_u \) for a linked data set is an object property \( p_u \) in the data set.

For example in Figure 5-1, there are two facets called “cause” and “symptom” that are the object properties for the linked data set about diseases.

**Definition 5-2:** a sub-taxonomy \( F_u \) in a facet \( f_u \) is a hierarchical concept taxonomy with the triples extracted with the property \( p_u \). The sub-taxonomy \( F_u(C_u, R_u) \) consists of a set of concepts \( C_u = \{ c_1, c_2, ..., c_l \} \) and a set of subsumption relations \( R_{S_u} = \{ r_{S_{u1}}, r_{S_{u2}}, ..., r_{S_{ux}} \} \). A subsumption relation \( r_{S}(c_i, c_j) \) is a subsumption relation between two concepts \( c_i \) and \( c_j \), where \( c_i \) and \( c_j \in C_u \).
For example in Figure 5-1, a sub-taxonomy about the facet “cause” is constructed with the sub-data related to “cause”. There are six concepts and five subsumption relations in this sub-taxonomy.

**Definition 5-3**: a faceted taxonomy $F$ includes a set of sub-taxonomies $\{F_1, F_2, ... F_k\}$, where each sub-taxonomy $F_u$ organizes the concepts in a facet $f_u$.

For example in Figure 5-1, a faceted taxonomy has two sub-taxonomies about the facets “cause” and “symptom”, and each taxonomy uses different concepts that are organized with a different hierarchy.

**Definition 5-4**: a materialized faceted taxonomy $\mathcal{F}(F, R)$ includes a set of sub-taxonomies $F = \{F_1, F_2, ... F_k\}$ and a set of “instance of” relations $R_I = \{r_{i_1}, r_{i_2}, ... r_{i_e}\}$. An “instance of” relation $r_I(i_u, c_v)$ is a classification of instance $i_u$ to a concept $c_v$, where $i_u \in I$ and $c_v \in C_u$.

For example in Figure 5-1, the materialized faceted taxonomy has the three instances to instantiate the concepts in two sub-taxonomies, such as “Translocation Down syndrome” is an instance of “Hereditary” and “Speech disturbance”. Please note that the statement, “Translocation Down syndrome” is an instance of “Hereditary”, is a classification for “Translocation Down syndrome”. The semantical meaning of the statement needs to be interpreted with the consideration of the semantic of a facet, and the author will discuss it further in Section 5.7.

The author has developed a framework to generate a faceted taxonomy based on multiple object properties, and the author introduces the framework in the following section.
5.3 Framework

The author separates the procedure of generating a faceted taxonomy into two stages as shown in Figure 5-2: pre-processing and taxonomical relationship generation.

The pre-processing is to generate a set of instance-object matrices, each of which represents the relations between instances in one facet (object property). Four steps, (1) facets extraction, (2) instance restriction and redundancy removal, (3) redundant object removal, and (4) instance-object matrix generation, are used at this stage in order to remove redundant instances and objects for reducing the computations of sub-taxonomy generation.

The taxonomical relationship generation is to construct sub-taxonomies based on instance-object matrices generated from multiple facets. For each matrix, the author proposes an algorithm to build a hierarchical taxonomy. An instantiation and concept taxonomy refinement strategies are also proposed to get a materialized faced taxonomy in Section 5.4.
Figure 5.3. An ongoing example of building a sub-taxonomy with an object property “Diseasome:possibleDrug” partially extracted from Diseasome.

5.3.1 Facets Extraction

In the author’s definition, each object property is considered as a facet, and object properties $P$ are identified from all the properties. Any triple that contains an object property is extracted, and the entire instances (subjects) of the extracted triples are used to build a $|P|$ faceted taxonomy. In order to help readers understand this paper, the author uses an ongoing example in Figure 5-3 to explain the procedure of generating a sub-taxonomy in one facet. The ongoing data is about the disease instances that partially extracted from Diseasome with the facet “Diseasome:possibleDrug”.

5.3.2 Instance Restriction and Redundancy Removal

First, for each facet, instances are restricted into the domain that contains an object property. For example, 1,456 disease instances of Diseasome are extracted for an
object property “Diseasome:possibleDrug”. Second, the instances that have the same property values (objects) are removed and kept only one instance as a representative instance for those removed ones. Therefore, after the first step, the unique instances that have different object sets are extracted for the next step in each facet. As Figure 5-3 (a) shows, the instances “Disease:2949” and “Disease:146” have the same objects “DB00170”, “DB00266”, and “DB02395”. Therefore, “Disease:146” is removed and only “Disease:2949” is kept as a representative for the two instances. In Figure 5-3 (a), two instances “Disease:146” and “Disease:2210” are removed during this step.

5.3.3 Redundant Object Removal

After removing the redundant instances that have the same property values (objects) in each facet, the author removes the redundant objects that are contained by the same instances and keeps only one object as a representative object for those removed ones. In another word, only the unique objects are kept for generating an instance-object matrix in a facet. For example in Figure 5-3 (b), the objects “DB00036” and “DB00682” are contained by the same instance “Disease:1175”. Therefore, “DB00682” is removed, and only “DB00036” is kept as a representative for the two objects.

5.3.4 Instance-object Matrix Generation

Based on above three steps, the instances with objects in a facet will form a binary matrix $A_{m \times n}$ with each instance is saved as row and each object as a column, and the matrix will be used to generate a sub-taxonomy for this facet. For each entry of
the matrix, $a_{uv} = 1$ if the instance $u$ contains the object $v$. There are $|P|$ matrices for all object properties $P$, and each matrix has different number of instances and objects. In the example of Figure 5-3 (c), for the facet “Diseasome:possibleDrug”, the instance-object matrix that has a five (instances) by eight (objects) matrix is generated.
5.4 Generating Faceted Taxonomy

5.4.1 The Problem of Generating a Sub-taxonomy for a facet

The author’s object is to obtain a faceted taxonomy that contains sub-taxonomies generated with instance-object matrices. Therefore, for each facet, the author defines the basic problem of building a hierarchical taxonomy in one facet as follows:

**Input:** Given an instance-object matrix $A_{m \times n}$ that contains the instances with multiple values (objects), we obtain an instance set $I = \{i_1, i_2, ..., i_m\}$ that have $m$ instances and an object set $O = \{o_1, o_2, ..., o_n\}$ that have $n$ objects. For each instance $i_k$, an instance contains by a set of objects $\{o_1, o_2, ..., o_u\}$. For example in Figure 5-3 (c), the instance “Disease:2949” contains the objects “DB00170”, “DB00266”, and “DB02395”.

**Output:** A hierarchical concept taxonomy $F(C, R_s)$, where $C = \{c_1, c_2, ..., c_k\}$ is a concept set containing $k$ concepts, $R_s = \{r_{s_1}, r_{s_2}, ..., r_{s_i}\}$ a subsumption relation set for the concepts.

5.4.2 Concept Definition and Naming

Classes (concepts) provide an abstraction mechanism to generalize the characteristics of a group of similar instances. The instances in a class are extensions that can be used to define the class (Bechhofer et al., 2004). The author defines a class with extensions (i.e., a set of instance) as :
**Definition 5-5**: A concept in a facet taxonomy that contains the extensions, a set of instance, is a binary vector \( \bar{c} = [i_1, i_2, ..., i_m] \), where \( i_m = 1 \) when the concept contains \( i_m \).

In a taxonomical class-based system, e.g. ontology, concepts comply with the class axiom (Bechhofer et al., 2004) on instances, where the extensions of a sub-concept is a subset of the extensions of its super concept. Therefore, we can formalize a concept with the extensions of sub-concepts, if the sub-concepts have common objects as:

\[
\bar{c} = \text{sub}_1 \text{OR} \text{sub}_2 \text{OR} ... \text{OR} \text{sub}_l
\]  

(5.1)

, where \( \text{sub}_l \) is a sub-concept vector. For example in Figure 5-3 (c), a concept \( \bar{c} = [1,1,0,0,0] \) with the extensions “Disease:2949” and “Disease:4161” can be formed with two concept \( \bar{c}_1 = [1,0,0,0,0] \) with the extension “Disease:2949” and \( \bar{c}_2 = [0,1,0,0,0] \) with the extension “Disease:4161”.

The intensions of a concept are the features and follows inheritance axiom in (Taivalsaari, 1996) and class axiom in (Bechhofer et al., 2004). Therefore, given a class, we have Axiom 5-1 for its sub-classes:

**Axiom 5-1**: A sub-concept inherits all the intensions from its super concepts and has new intensions that are used to differentiate its super concept.

For each instance in a facet, the objects contained in an instance are overlapped with the objects of other instances. The objects that can be used to classify instances are considered as the intensions (Sacco & Tzitzikas, 2009) in the facet. The author defines the intensions of a concept in a faceted taxonomy as follows:
**Definition 5-6:** Given an instance-object matrix $A_{m \times n}$ in a facet, the intensions $c$ of a concept $\vec{c}$ are the objects in a set $O = \{o_1, o_2, ..., o_k\}$.

With Axiom 5-1 and Definition 5-2, for a concept $\vec{c}$, the author obtains the intentions of the concept $c = \{o_1, o_2, ..., o_m\}$ as the intersection of the intentions for each sub-concept:

$$c = c_1 \cap c_2 \cap ... \cap c_i$$  \hspace{1cm} (5.2)

According to the concept axiom in OWL 2 (Carroll et al., 2012), a concept can be considered as its own instances. Therefore, with the instances, a super concept can be formed from the concepts in the bottom, i.e., the concepts only contains a representative instance as the extension.

In order to improve the readability of a concept, the author uses the reduced labeling strategy in FCA-based method (Cimiano et al., 2005) based on intensions to name the concept. The name of a concept is the objects obtained from the concept in intension that excludes the intensions of its super concepts. The naming function is defined as:

$$name(c) = c \not\supset (sup_1 \cup sup_2 \cup ... \cup sup_i)$$  \hspace{1cm} (5.3)

where $\not\supset$ is the material nonimplication or abjunction of the intension $c$ of the concept $\vec{c}$ and all intensions of its super concepts $\vec{sup_1}$ to $\vec{sup_i}$. The name can be determined with the set $name(c)$. For example, the concept $\vec{c} = [1,1,0,0,0]$, with the intensions “DB00170” and “DB00266”, has a super concept $\vec{sup} = [1,1,1,1,1]$ with the intension “DB00170”.

Therefore, with the reduced labeling strategy, we can obtain the name of $\vec{c} = [1,1,0,0,0]$ as “DB00266”. In addition, the author validates the name with a following definition:
**Definition 5-7**: A concept $\vec{c}$ is valid only if $|\text{name}(c)| = 1$.

This definition makes the proposed method differ with other taxonomy generation algorithms, such as the FCA. With Definition 5-7, the proposed taxonomy generation algorithm is more efficient and more effective than the FCA, which will be discussed in Section 5.6.1.

### 5.4.3 Taxonomy Generation Algorithm

With the concept definition and the naming strategy, the author adapts the IUT (Zong et al., 2015) that can be used to generate a taxonomy based on instance-concept matrix, and call the variation ICT (a.k.a., Instance-based hierarchical Concept Taxonomy generation). There are two steps to generate the concept taxonomy: first, the objects in the matrix $A_{m \times n}$ are sorted in descending order by the number of instances contained by the object, and are put into a queue $Q$ (line 1 in Algorithm 5-1); second, in each iteration, a concept is de-queued and put onto the right position in a graph by computing the subsumption relation with existing concepts (lines 3-9 in Algorithm 5-1). The author adapts the equation in (Sanderson & Croft, 1999) to determine a subsumption relation between two concepts $\vec{c}_u$ and $\vec{c}_v$ ($\vec{c}_u$ is a sub-concept of $\vec{c}_v$) as follows:

$$
\text{sub}(\vec{c}_u, \vec{c}_v) = \frac{|\vec{c}_u \cap \vec{c}_v|}{|\vec{c}_u|} \geq \varphi , \quad \text{sub}(\vec{c}_v, \vec{c}_u) = \frac{|\vec{c}_v \cap \vec{c}_u|}{|\vec{c}_v|} < 1 \quad (5.4)
$$

where $\varphi$ is used to adjust the effectiveness of subsumption determination for the two concepts.

If a concept $\vec{c}_u$ has two super concepts, where exists a path from one concept to the other (i.e., one concept is the ancestor of the other), the concept will be
assigned to the leaf concept (i.e., descendant). For example, if “DB02395” is found to have two super concepts “DB00266” and “DB00170”, where “DB00266” is a sub-concept of “DB00170”, “DB02395” is going to be assigned to the sub-concept “DB00266”. The details of the process of the ICT are shown in Algorithm 5.1.

**Algorithm 5.1.** Instance-based Concept Taxonomy generation algorithm (ICT).

**Input:** an instance-object matrix $A_{m \times n}$, $\varphi$

**Output:** A concept taxonomy $T(C,R_c)$

1: Queue $Q$ = all the objects by descending order of the number of instances contained

2: Initiate an empty graph $H$ with a root concept $r$

3: While size($Q$) > 0 do

4: $c_i :=$ dequeue($Q$)

5: Initiate a super concepts set sup($c_i$)

6: For $c_j$ in $H$ do

7: If ($\text{sub}(c_i,c_j) \geq \varphi$ & $\text{sub}(c_j,c_i) < 1$) sup($c_i$) $\leftarrow$ $c_j$

8: If sup($c_i$) $\neq \emptyset$, put $c_i$ onto the sub-concept of the leaf concepts of sup($c_i$)

9: Else put $c_i$ onto the sub-concept of $r$

10: Return $H$
5.4.4 Instantiation and Taxonomy Refinement

In this step, the author needs to materialize the faceted taxonomy based on multiple sub-taxonomies generated. First, the author instantiates the concepts in each sub-taxonomy. The author defines a following instantiation rule based on an instance-object matrix.

**Rule 5-1**: If an instance belongs to two concepts \( \tilde{c}_u \) and \( \tilde{c}_v \), where \( \tilde{c}_u \) is the super concept of \( \tilde{c}_v \), the instance will be used to populate \( \tilde{c}_v \).

Rule 5-1 makes an instance populate leaf nodes in a sub-taxonomy. For example, the instance “Disease:1175” belongs to two concepts “DB00036” and “DB00170” in Figure 5-3, and “Disease:1175” will be assigned to the concept “DB00036” since “DB00036” is the sub-concept of “DB00170”. Notice that Rule 5-1 supports multiple instantiation, because if an instance belongs to two concepts that are not connected with a subsumption relation, the instance will be assigned equally to the two concepts.

Second, the removed redundant instances and objects in the pre-processing stage are used to refine the taxonomy. The redundant instances are used to populate the same concepts instantiated with the representative instances. For example, “Disease:146” is assigned to the concept “DB02395” as well since “DB02395” is instantiated with “Disease:2949”. The redundant objects are considered equivalent with the representative objects in the taxonomy. For example, the concept “DB00682” is also considered as a sub-concept of the concept “DB00170” since “DB00036” is the sub-concept of “DB00170”.

110
Third, assemble all sub-taxonomies with renamed concepts. Each sub-taxonomy should be independent and contains different concepts. However, there are cases that objects in the same topic may be used in different object properties. For example, the objects typed “DrugBank:references” are used in both object properties “DrugBank:drugReference” and “DrugBank:generalReference” for the instances typed “DrugBank:targets”. Therefore, in order to disjoint all the facet concepts, the author prefixes each concept name with the name of the property in a facet (Sacco & Tzitzikas, 2009). Finally, the author puts all the sub-taxonomies under the concept “Owl:Thing” to get the faceted taxonomy.
5.5 Experiments

The author has implemented the proposed method based on JDK 1.6 using an Intel(R) Xeon CPU E5-2630 with 130 GB RAM on Windows 8 64 bit version. Since the object is to construct faceted taxonomies for Linked Data, the tests are separated into two parts that target two problems the author mentioned in Sections 5.4.1 and 5.2.2: (1) the performance of generating a sub-taxonomy in one facet. (2) the performance of generating multiple faceted taxonomies with different object properties.

5.5.1 Task 1-Construction of Taxonomy with “rdf:type”

5.5.1.1 Data Sets and Experiment Design

In Linked Data, some data sets that contain ontologies with concept taxonomies publish the classification of instances with “rdf:type”. Generating taxonomies with “rdf:type” can be viewed as the reverse engineering of this RDF publishing. Therefore, in order to evaluate the performance of the proposed method to build a sub-taxonomy with one object property, the author used the values of “rdf:type” in the RDF dumping file to construct a taxonomy. The taxonomy will be evaluated by comparing with the taxonomy of the gold standard ontology. The author chose two most well-known sets in LOD, DBpedia ("Downloads - Dbpedia," ) and YAGO2 ("Downloads - YAGO2," ) that provide the mature concept taxonomies reflecting on the values of “rdf:type”. The concept taxonomies are DBpedia ontology and YAGO-WordNet, which are extracted from DBpedia and YAGO2 respectively. The author gained the study population, with 2,885,951 instance and
8,674 concepts from YAGO2 2.5.3, and 3,243,477 instances and 389 concepts from DBpedia 3.9. The author removed the redundant instances and objects, and only kept the unique instances and objects to construct the instance-object matrix during the pre-processing stage as introduced in Section 5.3. The statistics of the data originally and after pre-processing are shown in Table 5-1.

<table>
<thead>
<tr>
<th></th>
<th>original data</th>
<th>after pre-processing</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td># instances</td>
<td># objects (concepts)</td>
</tr>
<tr>
<td>YAGO2</td>
<td>2,885,951</td>
<td>8,674</td>
</tr>
<tr>
<td>DBpedia</td>
<td>3,243,477</td>
<td>389</td>
</tr>
</tbody>
</table>

**5.5.1.2 Algorithms in comparison**

The author compared the ICT with two classic concept taxonomy construction algorithms based on an instance-object matrix: Subsumption (Sanderson & Croft, 1999) and FCA (Cimiano et al., 2005; Drymonas et al., 2010).

For the Subsumption, the author iterated all the concept pairs and established a subsumption relation of a pair of two concepts $c_1$ and $c_2$ if the two concepts satisfy the condition $P(c_1|c_2) = 1, P(c_2|c_1) < 1$. For the FCA, the author used the Colibri ("Colibri-Java,"') that implements the Next-Closure algorithm to compute the formal concept lattice (Ganter & Reuter, 1991). A concept in the lattice is used to build a taxonomy if the concept contains at least one instance, and named by the reduced labeling with the extensional interpretation of the concept (Cimiano et al., 2005).
5.5.1.3 Evaluation Criteria

The author tested all the algorithms with two criteria: efficiency and effectiveness. For evaluating the effectiveness, the author compared a generated taxonomy with the hierarchical schema structure of the ontology already exist in a linked data set. The author adopted the Taxonomic Precision (TP), Taxonomic Recall (TR), and Taxonomic F-measure (Dellschaft & Staab, 2006; Paukkeri et al., 2012) to measure the quality of the generated taxonomy.

TP and TR are based on the Semantic Cotopy (SC) (Dellschaft & Staab, 2006) that considers ancestor and descendant relation to calculate the similarity of two concepts. The Semantic Cotopy of a concept \( c \) in an ontology \( O \) is defined as:

\[
SC(c, O) = \{c_i | c_i \in C \land (c_i \leq c \lor c \geq c_i)\}
\]  \hspace{1cm} (5.5)

, where \( C \) is the concept set of \( O \), and \( c_i \leq c \lor c \geq c_i \) is an ancestor and descendant of \( c \). Therefore, the semantic cotopy of two concepts can be used to compute the local taxonomic precision of the two concepts as follows:

\[
Tp_{sc}(c_1, c_2, O_1, O_2) = \frac{\|sc(c_1, O_1) \cap sc(c_2, O_2)\|}{\|sc(c_1, O_1)\|} \hspace{1cm} (5.6)
\]

The \( TP_{SC} \) and \( TR_{SC} \) are computed based on the local taxonomic precisions and recalls as follows:

\[
TP_{SC}(O_1, O_2) = \frac{1}{|C_{O_1}|} \sum_{c_i \in C_{O_1}} \left\{ \begin{array}{ll}
Tp_{sc}(c_i, O_1, O_2) & \text{if } c_i \in C_{O_2} \\
0 & \text{if } c_i \notin C_{O_2}
\end{array} \right. \hspace{1cm} (5.7)
\]

, where \( TR_{SC}(O_1, O_2) = TP_{CSC}(O_2, O_1) \).

The Taxonomic F-measure (TF) calculates the harmonic mean of \( TP_{SC} \) and \( TR_{SC} \) as:

\[
TF(O_1, O_2) = \frac{2 \times TR_{SC}(O_1, O_2) \times TP_{SC}(O_1, O_2)}{TR_{SC}(O_1, O_2) + TP_{SC}(O_1, O_2)} \hspace{1cm} (5.8)
\]
The author uses Semantic Cotopy instead of using Common Semantic Cotopy (CSC) because some approaches, such as FCA, will generate new concepts rather than the existing concepts (value of object property “\texttt{rdf:type}”) provided in the data. The using of the Common Semantic Cotopy ignores the new generated concepts of these approaches and over-measures the precision.

5.5.2 Task 2-Construction of Multiple Faceted Taxonomies

5.5.2.1 Data Sets and Experiment Design

The author tested the multiple faceted taxonomies with different facets (i.e., object properties) in two biomedical linked data sets, DrugBank ("DrugBank,")) and Diseasome ("Diseasome,"), which do not have ontologies to organize instances. The DrugBank contains 4,772 drug instances, and the Diseasome contains 4,213 disease instances. The author used 5 and 16 object properties from Diseasome and DrugBank to generate faceted taxonomies for the disease and drug instances. Please note that not all the instances have a specific object property. For example, there are 4,213 disease instances in Diseasome, and only 1,456 of them have values of the object property “\texttt{Diseasome:possibleDrug}”. The author lists the statistic information of the two data sets in Table 5-2.

<table>
<thead>
<tr>
<th>Object Properties</th>
<th># instance</th>
<th># object</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diseasome:omim (P1)</td>
<td>2,929</td>
<td>1,778</td>
</tr>
<tr>
<td>Diseasome:associatedGene (P2)</td>
<td>4,213</td>
<td>3,919</td>
</tr>
<tr>
<td>Diseasome:chromosomalLocation (P3)</td>
<td>2,929</td>
<td>915</td>
</tr>
<tr>
<td>Diseasome:possibleDrug (P4)</td>
<td>1,456</td>
<td>2,235</td>
</tr>
<tr>
<td>Diseasome:class (P5)</td>
<td>4,213</td>
<td>24</td>
</tr>
<tr>
<td>Diseasome:diseaseSubtypeOf (P6)</td>
<td>2,929</td>
<td>1,284</td>
</tr>
</tbody>
</table>
### DrugBank

<table>
<thead>
<tr>
<th>Property</th>
<th>Value1</th>
<th>Value2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drugbank:keggCompoundId</td>
<td>1,331</td>
<td>1,316</td>
</tr>
<tr>
<td>Drugbank:pdrhealthLink</td>
<td>280</td>
<td>273</td>
</tr>
<tr>
<td>Drugbank:brandedDrug</td>
<td>524</td>
<td>1,593</td>
</tr>
<tr>
<td>Drugbank:drugCategory</td>
<td>1,879</td>
<td>584</td>
</tr>
<tr>
<td>Drugbank:chebiId</td>
<td>736</td>
<td>721</td>
</tr>
<tr>
<td>Drugbank:contraindicationInsert</td>
<td>1,112</td>
<td>1,112</td>
</tr>
<tr>
<td>Drugbank:target</td>
<td>4,408</td>
<td>4,553</td>
</tr>
<tr>
<td>Drugbank:keggDrugId</td>
<td>913</td>
<td>910</td>
</tr>
<tr>
<td>Drugbank:interactionInsert</td>
<td>1,036</td>
<td>1,036</td>
</tr>
<tr>
<td>Drugbank:rxlistLink</td>
<td>998</td>
<td>994</td>
</tr>
<tr>
<td>Drugbank:dosageForm</td>
<td>1,209</td>
<td>215</td>
</tr>
<tr>
<td>Drugbank:swissprotPage</td>
<td>74</td>
<td>48</td>
</tr>
<tr>
<td>Drugbank:drugType</td>
<td>4,772</td>
<td>8</td>
</tr>
<tr>
<td>Drugbank:patientInformationInsert</td>
<td>762</td>
<td>762</td>
</tr>
<tr>
<td>Drugbank:possibleDiseaseTarget</td>
<td>1,362</td>
<td>1,456</td>
</tr>
<tr>
<td>Drugbank:casRegistryNumber</td>
<td>2,240</td>
<td>2,218</td>
</tr>
</tbody>
</table>

#### 5.5.2.2 Evaluation Criteria

Since there lacks ontologies as gold standards to evaluate the facet concept taxonomies generated with Diseasome and DrugBank, the author adopted evaluation criteria used for the scenarios without a gold standard (Dasgupta, Dinakarpandian, & Lee, 2007). The author used, (1) Inheritance Richness (IR) (Dasgupta et al., 2007) to check the shape of a sub-taxonomy, (2) Maximum Resolution (MR) (Sacco & Tzitzikas, 2009) to check the retrieval effectiveness in faceted searches based on a faceted taxonomy, and (3) Class Importance (CI) (Dasgupta et al., 2007) to obtain the most important concepts in a faceted taxonomy.

(a) Inheritance Richness (IR)

The Inheritance Richness describes the distribution of concepts that are across different levels of a taxonomy. The Inheritance Richness can be used to detect the
shape of the concept taxonomy. A low value of Inheritance Richness indicates a horizontal hierarchy (flat structure) that has a low degree of inheritance level where each concept has a large number of sub-concepts. A high value of Inheritance Richness indicates a vertical hierarchy that has a high degree of inheritance level where each concept has a small number of sub-concepts.

The Inheritance Richness is computed as follows:

\[ IR = \frac{\sum_{c_i \in C}|\text{descend}(c_i)|}{|C|} \]  

(5.9)

, where \(|\text{Sub}(c_i)|\) is the cardinality of the set of the descendants a concept \(c_i\).

(b) Maximum Resolution (MR)

Maximum Resolution is used to measure the retrieval effectiveness with a faceted taxonomy. A Maximum Resolution measures the average minimum number of instances to be manually inspected after a refinement through operations on the faceted taxonomy. A small value of Maximum Resolution illustrates a good classification of a concept taxonomy for reducing the search space. The Maximum Resolution is computed as the average number of instances of \(k\) concept intersections in a \(k\) facets taxonomy:

\[ MR = \frac{\sum_{i=1}^{k} \bigcap_{i=1}^{k} c_i}{\left| \sum_{i=1}^{k} c_i \right|} \]  

(5.10)

, where \(\left| \sum_{i=1}^{k} c_i \right|\) is total intersection numbers of \(k\) concepts, each of which is a leaf concept from a sub-taxonomy.

(c) Class Importance (CI)

In order to obtain the important classes, the author adapts Class Importance to show the focused concepts with the consideration of instance distribution and help
users to identify where to get data if the intentions of users’ are to get consistent coverages of all concepts.

The importance of a concept $c_i$ is computed as follows:

$$CI(c_i) = \frac{|I_{c_i}|}{|\mathcal{C}|}$$

(5.11)

where $I_{c_i}$ is the instance set of $c_i$. Please note that the instances belonged to $c_i$ contain all the instances belonged to each sub-concept of the $c_i$. 
5.6 Results

5.6.1 Results of Task 1

The author has run three methods over two data sets (YAGO2 and DBpedia) respectively, and show the running time of all the methods in Figure 5-4 (b). As Figure 5-4 (b) shows, the ICT is the fastest methods (49 ms for DBpedia and 11,790 ms for YAGO2) comparing with other two methods. The ICT and Subsumption reduce the search space into the concepts already existing in the concept taxonomy with Definition 5-7, and the ICT does not need to calculate Equation 5.4 with all the combinations of the concept pairs that are needed for the Subsumption (118 ms for DBpedia and 2,597,424 ms for YAGO2). The FCA (184 ms for DBpedia and 92,656,444 ms for YAGO2) is the slowest method since it calculates all the possible pairs of concepts sharing common instances. The huge amount of discovered relations from the FCA makes the extraction of subsumption relations very expensive. In the two tests, over than 55% of the running time is spent on the extraction of the subsumption relations from all the discovered relations (103/184 for DBpedia and 90,942,222/92,656,444 for YAGO2).
The concept taxonomies generated by the three methods are compared with the gold standards of the two data sets (DBpedia ontology and YAGO-WordNet), and the effectiveness is evaluated with the Taxonomic F-measure shown in Figure 5-4 (a). As Figure 5-4 (a) shows, the ICT obtains the best f-scores for two data sets (0.917 for DBpedia and 0.780 for YAGO2). Equation 5.4 can successfully
establish a subsumption relation between two concepts. For example, “DBpedia:FloweringPlant” contains two instances “Dinka_(grape)” and “Miconia_laxa”, and “DBpedia:Grape” contains one instance “Dinka_(grape)”. Therefore, the subsumption relation can be easily built with this equation. (Please note that the instances contained by a concept are the representative instances that have a unique concept set. In this example, “Dinka_(grape)” is used as the representative instance for other 349, and all the 350 instances have a same concept set including 6 concepts: “DBpedia:Grape”, “DBpedia:Plant”, “DBpedia:Species”, “DBpedia:Eukaryote”, “DBpedia:FloweringPlant”, and “Owl:Thing”, and “Dinka_(grape)”).

However, there are two kinds of failures to affect the precision and recall known as false negative and false positive:

(1) two concepts A and B, having a subsumption relation but containing a same instance set, can cause a false negative. For example, “YAGO:Wordnet_art_school_102746978” and “YAGO:Wordnet_school_104146050” have the same instance set “St._Martin's_Lane_Academy”, “Cranbrook_Educational_Community”, “Faculty_of_Theatre_(Prague)”. This problem is recognized as insufficient taxonomic description on the instance level (Zong et al., 2015), which means the ICT is incapable of building a concept taxonomy if there does not exist taxonomic relations for concepts at the instance level. In YAGO2 and DBpedia, there are 1,634 and 16 pairs of concepts that cause false negatives.
two concepts A and B, not having a subsumption relation but containing two instance sets that one subsumes the other, can cause a false positive. For example, the concept “YAGO:Wordnet_Television106277280” has 68 instances that includes the only instance “Plats_bruts” contained by concept “YAGO:Wordnet_TeachingAid104397261”, where there does not exists a subsumption relation between the two concepts. This problem is recognized as multi-instantiation whereby one instance can be used to populate multiple concepts (Zong et al., 2015). In DBpedia, there exists none false positives, but in YAGO2, there are 1,769 pairs of concepts cause false positives. The ICT performs same with the Subsumption on DBpedia (0.917) but better on YAGO2 (0.775). The $\varphi$ controls the level of tolerance for detecting a subsumption relation. The precision decreases along with the decrease of $\varphi$ if there is multi-instantiation in the data set, as the YAGO2 shown in Figure 5-5. In Figure 5-5, DBpedia does not have multi-instantiation, so the precision is not affected by $\varphi$.

The FCA achieves good results on DBpedia (0.911) but fails on YAGO2 (0.00058). The FCA exploits every possible concept (1,397,220 on YAGO2) containing common instances, and creates abundant subsumption relations (5,825,144 on YAGO2). However, most of the created concepts and subsumption relations are not existing in the gold standard ontology (8,674 concepts and 74,897 subsumption relations on YAGO2), which causes high recall (0.679 on YAGO2) but extreme low taxonomic precision (0.00029 on YAGO2). For example, a concept that has the intensions {“YAGO:Wordnet_Abstraction100002137”, “YAGO:Wordnet_PhysicalEntity100001930”, “Owl#Thing”} (i.e., a sub-concept
of both concepts “YAGO:Wordnet_Abstraction100002137” and “YAGO:Wordnet_PhysicalEntity100001930”) is created by the FCA. However, even this concept contains 3,887 common instances of both super concepts, it does not exist in YAGO2. The ICT solves this issue with Definition 5-7, which ignores the concepts that cannot obtain meaningful names after reducing labels.

Figure 5-5. TP-scores of ICT for DBpedia and YAGO2 with different $\varphi$. 
5.6.2 Results of Task 2

![Graphs showing running times for sub-taxonomy building](image)

(a) Diseasome

(b) DrugBank

**Figure 5-6.** Running time of building a sub-taxonomy with a single property.

The author has measured the running time for each sub-taxonomy with a single property in Diseasome and DrugBank. As Figure 5-6 shows, “Diseasome:associatedGene” (1,202 ms) and “Drugbank:target” (1,453 ms)
spend the longest time on constructing a sub-taxonomy in one facet for the two data sets. The author learned that the time spent is related to the number of objects contained in an object property, and the more objects contained the longer it costs for a property. For example, “Diseasome:class” has 24 objects and spends 16 ms on creating a sub-taxonomy comparing with “Diseasome:possibleDrug” that spends 206 ms on creating a sub-taxonomy with 2,235 objects.

The author used Inheritance Richness (IR) to pry into the structure of each sub-taxonomy. As Table 5-3 shows, the “Diseasome:possibleDrug” and “Drugbank:target” get the highest IR scores on Diseasome (15.22) and DrugBank (17.72). The concept taxonomies generated with these two properties have 5 levels and 7 levels of inheritance. Therefore, the author can obtain a vertical shaped concept taxonomies with “Diseasome:possibleDrug” and “Drugbank:target” comparing with the horizontal concept taxonomies generated with “Diseasome:omim” and “Drugbank:keggCompoundId” that have only 2 levels of inheritance.

The Maximum Resolution shows the effectiveness of classification of a sub-taxonomy. The best scores obtained by “Diseasome:omim” (1.65) with Diseasome, and six properties (1.0) with DrugBank. The effectiveness of classification is contrary to the ability of generalizing instance properties in a taxonomy. A high effective classification may result in a weak ability of generalizing instance properties. For example, “Diseasome:class” get the highest MR score (175.54) and can best generalize the characteristic of the instances.
Table 5-3. Results of conceptualizing disease and drug instances with multiple object properties. The highest IR and lowest MR scores are in bold.

<table>
<thead>
<tr>
<th>Object Properties</th>
<th>Inheritance Richness</th>
<th>Maximum Resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>(P1) Diseasome:omim</td>
<td>1.00</td>
<td>1.65</td>
</tr>
<tr>
<td>(P2) Diseasome:associatedGene</td>
<td>1.66</td>
<td>2.05</td>
</tr>
<tr>
<td>(P3) Diseasome:chromosomalLocation</td>
<td>1.00</td>
<td>3.20</td>
</tr>
<tr>
<td>(P4) Diseasome:possibleDrug</td>
<td><strong>15.22</strong></td>
<td>3.96</td>
</tr>
<tr>
<td>(P5) Diseasome:class</td>
<td>0.96</td>
<td>175.54</td>
</tr>
<tr>
<td>(P6) Diseasome:diseaseSubtypeOf</td>
<td>1.00</td>
<td>2.28</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Object Properties</th>
<th>Inheritance Richness</th>
<th>Maximum Resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>(P1) Drugbank:keggCompoundId</td>
<td>1.00</td>
<td>1.01</td>
</tr>
<tr>
<td>(P2) Drugbank:pdrhealthLink</td>
<td>1.00</td>
<td>1.03</td>
</tr>
<tr>
<td>(P3) Drugbank:brandedDrug</td>
<td>1.00</td>
<td><strong>1.00</strong></td>
</tr>
<tr>
<td>(P4) Drugbank:drugCategory</td>
<td>1.76</td>
<td>3.53</td>
</tr>
<tr>
<td>(P5) Drugbank:chebiId</td>
<td>1.00</td>
<td>1.02</td>
</tr>
<tr>
<td>(P6) Drugbank:contraindicationInsert</td>
<td>1.00</td>
<td><strong>1.00</strong></td>
</tr>
<tr>
<td>(P7) Drugbank:target</td>
<td><strong>17.72</strong></td>
<td>1.27</td>
</tr>
<tr>
<td>(P8) Drugbank:keggDrugId</td>
<td>1.00</td>
<td><strong>1.00</strong></td>
</tr>
<tr>
<td>(P9) Drugbank:interactionInsert</td>
<td>1.00</td>
<td><strong>1.00</strong></td>
</tr>
<tr>
<td>(P10) Drugbank:rxlistLink</td>
<td>1.00</td>
<td><strong>1.00</strong></td>
</tr>
<tr>
<td>(P11) Drugbank:dosageForm</td>
<td>3.24</td>
<td>1.82</td>
</tr>
<tr>
<td>(P12) Drugbank:swissprotPage</td>
<td>0.98</td>
<td>1.54</td>
</tr>
<tr>
<td>(P13) Drugbank:drugType</td>
<td>1.33</td>
<td>676.33</td>
</tr>
<tr>
<td>(P14) Drugbank:patientInformationInsert</td>
<td>1.00</td>
<td><strong>1.00</strong></td>
</tr>
<tr>
<td>(P15) Drugbank:possibleDiseaseTarget</td>
<td>7.56</td>
<td>2.45</td>
</tr>
<tr>
<td>(P16) Drugbank:casRegistryNumber</td>
<td>1.00</td>
<td>1.01</td>
</tr>
</tbody>
</table>

The author tested the two data sets with different combinations of multiple object properties. The author separates all combinations with different numbers of properties used. For example, choosing two properties of Diseasome may use “Diseasome:omim” and “Diseasome:possibleDrug”, or “Diseasome:possibleDrug” and “Diseasome:diseaseSubtypeOf”. The author has measured the average running
times of creating a faceted taxonomy with a different number of properties and show in Figure 5-7.

![Graph showing average running time of building faceted taxonomies with different facets (properties).](image)

(a) Diseasome

(b) DrugBank

**Figure 5-7.** Average running time of building faceted taxonomies with different facets (properties).

As Figure 5-7 shows, the running time increases along with the increment of the number of properties. In Diseasome, the average running time increases from
338 ms up to 2,032 ms with one property and six properties. In DrugBank, the average running time increases from 157 ms up to 2,525 ms with one property and sixteen properties. The author learned that, along with increment of the number of properties, more sub-taxonomies are constructed, which can cost more time for the proposed algorithm to generate a faceted taxonomy. The more facets a taxonomy contains, the better classification of the taxonomy has. As Figure 5-8 shows, the Maximum Resolution dramatically decreases when two sub-taxonomies are used. For example, the Maximum Resolution decreases from 31.45 to 1.65 with Diseasome, and decreases from 43.56 to 1.03 with DrugBank. When the number of facet used increases up to three, the Maximum Resolution decreases slightly. The author learned that for most browsing cases, using two facets is sufficient enough to meet users’ needs of narrowing down the search space.

(a) Diseasome
Figure 5-8. Maximum Resolution scores with different facets (properties).

The author has counted the top 500 important concepts in the generated faceted taxonomies with two data sets, and shows the number of important concepts of each property in Figure 5-9. As Figure 5-9 shows, “Diseasome:possibleDrug” contains the 380 out of 500 important concepts in Diseasome, “Drugbank:possibleDiseaseTarget”, “Drugbank:target”, and “Drugbank:drugCategory” contain the important concepts in Drugbank at the most (186, 146, and 123 out of 1,000). Figure 5-9 illustrates the most important sub-taxonomies that contain important concepts. These sub-taxonomies that cover a large number of instances are recommended to the users who are unfamiliar with the data sets but want to get the most information.
Figure 5-9. Number of top 500 important concepts in each sub-taxonomy in a faceted taxonomy.
5.7 Discussion

The sub-taxonomies in each facet are constructed based on the concepts defined by the author in Section 5.4.2. This definition leaves two issues to be discussed when a faceted taxonomy is generated:

First, the concepts are removed when the concepts are unrecognizable with reduced labeling strategy in Definition 5-7. The definition has two benefits: (1) reduces unnecessary computations and decreases running time when the proposed method constructs a sub-taxonomy, and (2) reduces multiple inheritance when the concepts have multiple super concepts, and increases Taxonomic F-measure scores. However, the concept reducing strategy used in Definition 5-7 is still insufficient enough to prevent multiple inheritance, which the author has observed in the first task with YAGO2 in Section 5.6.1. To remove the meaningless concepts by judging the concept name is too simple and primitive, and the method only considers the semantics of the intension rather than the extension of a concept. There can be a more sophisticated method to decide the validity of a concept by balancing both the extensions and intensions of a concept, which leaves a potential improvement for future.

Second, the concepts are defined with the extensions (i.e., instances) and recognized with intensions (i.e., objects of properties). The concept definition and naming strategy the author applied has the advantages of improving efficiency and effectiveness, but leaves a difficulty of understanding the concepts. For example in the taxonomy in the facet “Diseasome: possibleDrug” for Diseasome in Section 5.6.2, the author found that the concept labeled as “Drug:DB00898” (Ethanol) is
the super concept of the concept labeled as “Drug:DB03929” (D-Serine), and it is hard to interpret the two concepts having a “is_A” relation semantically. However, the two concepts can be understood as having a subsumption relation in extension, since “Drug:DB03929” can treat “Disease:2666” (Hyperekplexia and spastic paraparesis), and “Drug:DB00898” can treat “Disease:2666”, “Disease:372” (Epilepsy), and “Disease:2312” (Epilepsy, juvenile myoclonic, 606904). In addition, viewing from the instance level, the ancestors of a concept are those contained by its instances in a facet. In the same example, “Disease:2666” can be treat by the possible drugs “Drug:DB00898” and “Drug:DB03929”. Therefore, the concepts in a sub-taxonomy can be understood easily to classify instances and efficiently reduce the browsing space in a navigation (Sacco & Tzitzikas, 2009). For example in a faceted search, if a user wants to find the diseases that can be cured by “Drug:DB03929”, zooming “Drug:DB00898” (i.e., zoom-in point (Sacco & Tzitzikas, 2009)) into “Drug:DB03929” can reduce three diseases into only one disease.
5.8 Conclusion

The increasing popularity of publishing Linked Data sets addresses an issue of constructing concept taxonomies for those data without ontologies. Instead of building a taxonomy to classify instances from one dimension, a faceted taxonomy that classifies instances from multiple dimensions brings the attention of academia. However, researches focus on utilizing a faceted taxonomy with an assumption that those taxonomies already exist. In order to provide faceted taxonomies for faceted navigation and search in Linked Data, this study proposed a solution of automatic construction of faceted taxonomy based on object properties. The author has developed a framework that extracts sub data for each facet and builds a sub-taxonomy with an instance-based Concept Taxonomy generation algorithm called ICT based on the concept defined by the author. The author also proposed the strategies to materialize and refine sub-taxonomies in order to get a faceted taxonomy. The author has proven that the proposed method can achieve encouraging results in terms of efficiency and effectiveness with two experiments. Finally, two issues of this study are discussed to leave further improvements in the future work.
6 Future Works and Conclusion

6.1 Future Works

6.1.1 Similarity Measures for Instance-based Schema Alignment

There are diverse similarity measures for instance-based schema alignment. A concept can be represented with a set of instances. Therefore, similarity measures used for sets can be applied, such as Jaccard similarity and standard information-theory measures (e.g., Pointwise Mutual Information, Log Likelihood ratio, and Information Gain). The performances of these metrics are discussed in (Isaac et al., 2007), which shows that the Jaccard similarity outperforms other similarity measures. Performance of other measures, such as Dice similarity, Minimum similarity, and Kappa similarity, however, varies depending on the link data used (Kirsten et al., 2007). So far, there is no direct guideline in selecting a measure for instance-based schema alignment. However, we can easily calculate that for two concepts $c_1$ and $c_2$, $sim_{dice}(c_1, c_2) \leq sim_{min}(c_1, c_2)$ and $sim_{jaccard}(c_1, c_2) \leq sim_{min}(c_1, c_2)$. Therefore, with the same threshold for determining equivalence, there are more equivalence alignments by using Minimum similarity than using Dice similarity and Jaccard similarity, which causes high recall but low precision for Minimum similarity-based method, and low recall but high precision for Dice similarity- and Jaccard similarity-based methods. A more detailed experiment could illustrate the performances of these similarity metrics with different data in my future work.
With the Vector Space Model, a concept can be represented as a vector with the values corresponding to the instance set of the concept. The vector values can be weighted by term (instance) frequency measures, such as TF/IDF. Therefore, similarity measures for vectors can be applied, such as cosine similarity. An interesting attempt is to compare the alignments generated with the same cosine similarity measure using the vectors with TF/IDF values and binary values (a.k.a., Ochiai coefficient for computing two instance sets). The cosine similarity measure can be estimated with Radom Hyperplane in LSH. Therefore, replacing Jaccard similarity with Cosine similarity can be a meaningful extension for our proposed method in Section 3.

6.1.2 Ontology Evolution for Instance-based Schema Alignment

Along with the development of linked data, Ontologies representing knowledge of the data also evolve continuously. For example, new classes are added or removed from the original ontology along with the adding of new domain data or deleting of old domain data. Not only instances belonging to a class could vary (add or delete) but also relations between classes can change.

The ontology evolution affects schema alignment results, especially for instance-based methods (Hartung, Kirsten, & Rahm, 2008; Thor, Hartung, Gross, Kirsten, & Rahm, 2009). The author has observed the different alignment results caused by evolution of DBpedia and YAGO2 in Section 3.6. The evolution of life science ontologies has been discussed in (Hartung et al., 2008; Thor et al., 2009), However, there still lacks the study of the affections in Linked Data evolution on
schema alignment. The future work will focus on answering three questions on this issue: (1) how to analyze affections of ontology evolution on schema alignment, (2) how to evaluate alignments from the perspective of ontology evolution, and (3) how to align schemas with considering ontology evolutions (several versions of the same ontology).

6.1.3 Combining the IUT with Structure- and Lexical-based Methods

The author has proposed the IUT that aligns schemas based on instances. Instance-based method is considered as a better solution for aligning schemas with ambiguous names. However, lexical- (or linguistic) and structure-based methods are frequently used in schema alignment. Lexical-based similarities are used in pre-matching to select candidate matched pairs for other sophisticated matchers (Bellahsene et al., 2011). The lexical-based methods are more efficient than instance-based methods for classes with a huge number of instances. Structure-based method is considered to align two classes with a more comprehensive view. For example, Similarity Flooding (Melnik, Garcia-Molina, & Rahm, 2002) is used to reassign similarities to matched pairs based on the schema structure. The IUT can adapt the two kinds of methods to give a hybrid solution for schema alignment to: (1) improve the efficiency with lexical-based methods, and (2) improve the effectiveness with structure-based methods.
6.1.4 Scaling the IUT with Parallel Computations

There are two ways generally to scale schema alignment as the author introduced in Section 2.2.2. In Chapter 4, the author scales the IUT based on decreasing similarity computations for classes. However, there is another solution to scale matching with parallel computations, such as MapReduce. In parallel computation based scaling methods, matchers should be independent. In the IUT, the classes de-queued from the class-relation multi-graph should compare all the classes already in the virtual graph to find an appropriate position with a matcher. Even though, similarity computations in a matcher are independent and can be computed in parallel, it is still not sufficient enough. Matchers with the input de-queued classes are sequenced and not independent. Therefore, MapReduce cannot be directly adapted to the matchers in the IUT. The future work is to change the IUT to allow using MapReduce to improve the efficiency.

6.1.5 Faceted Navigation and Search for Linked Data

The author has proposed a method to automatically generate a faceted taxonomy based on object properties. The taxonomy generated is the foundation of realizing faceted navigation and search. However, several issues still remain and are needed to be further studied: (1) how to decide the object properties to generate a faceted taxonomy that satisfies users search intension; (2) how to efficiently expand concepts dynamically in a faceted taxonomy to provide a comprehensive view of data sets; (3) how to apply ontology alignment method introduced in Chapter 3 to align the faceted taxonomy with existing ontologies to improve the experience of
navigation and search for Linked Data consumers. The future work is to develop a faceted navigation and search system that answers these questions addressed by the author.
6.2 Conclusion

This thesis solves three issues in instance-based schema alignment in Linked Data, (1) how to align schemas based on instances, (2) how to scale the schema alignment, and (3) how to generate hierarchical schema structure, with three proposed methods introduced in Chapters 3, 4, and 5.

There many types of ontologies in Linked Data, and the alignments of the ontologies have been performed diversely in our proposed method demonstrated in Section 3. Therefore, in the end of the thesis, the author wants to category the features of the ontologies targeted by the proposed methods. The sufficient feature of the targeted ontologies for the proposed method is the establishment of “Owl:sameAs” alignments between instances.

(1) Alignment on instances (with “Owl:sameAs”)

The instance-based alignment methods measure the similarity of two concepts with common instances. Therefore, in Linked Data, ontologies have to be aligned with “Owl:sameAs” or other links that provide similar functions.

There are other three features would cause the better alignments for the targeted ontologies by the proposed method than other methods, which are (1) ambiguous or without naming, (2) rich instantiation, and (3) keen hierarchical taxonomy and instantiation.

(1) Ambiguous naming or even without naming

The lexical-based matchers are incapable of finding mappings when schema elements have ambiguous or obscure names, or even without names (e.g., blank
nodes). Therefore, ontologies with ambiguous names or without names are suggested to be aligned with instance.

(2) Rich instances

As Section 3.5 shows, ontology alignment on the concepts with a large number of instances works better than on those with a limited number of instances. Therefore, the author recommends to align the ontologies with a large number of instances. However, the author still lacks a guideline on determine a threshold for the instance number contained by a concept. According to the study in (Isaac et al., 2007), a threshold improves precision but hurts recall. A practical threshold should be decided based on a user’s requirement on alignment in a real application.

(3) Keen hierarchical taxonomy and instantiation.

An ontology aligned based on instances should have a hierarchical taxonomy for the schema. However, if this condition is not satisfied, a taxonomy can be automatically generated with the ICT proposed in Chapter 5. According to the experiment results in Section 3.5, three facts can affect the performance of the alignment, which are insufficient taxonomy, multiple inheritance, and multiple instantiation.

Sufficient taxonomy means that a concept is sufficiently classified by multiple sub-concepts (i.e., one concept has more than one sub-concept). Non-multiple inheritance means that a concept cannot have multiple super concepts. Non-multiple instantiation means an instance cannot be used to populate multiple concepts. Please note that multiple inheritance can cause multiple instantiation but not vice versa.
The author summarizes these conditions for the proposed methods in this thesis in Table 6-1 as a closure for this study.

Table 6-1. Summarization of the conditions for the proposed methods. (Attri.1: Purpose, Attri.2: Concept taxonomy, Attri.3: Alignment on instances, Attri.4: Ambiguous naming, Attri.5: Rich instances, Attri.6: Insufficient taxonomy, Attri.7: Multiple inheritance, Attri.8: Multiple instantiation)

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초록

링크드 데이터에 대한 인스턴스 기반 온톨로지 매핑

웹이 발전함에 따라 사용자는 복잡한 질의에 대해서도 웹이 알기 쉽게 정보를 찾아주길 원하고 있다. 이를 위해서는 다양한 형태의 데이터를 공유, 교환 그리고 통합하는 수단이 필요하다. 하지만, 웹에 공개된 데이터들은 관련된 데이터들과 통합하기 위한 의미정보가 결여된 경우가 많다. RDF와 링크드 데이터는 잘 정의된 관계를 사용해서 데이터를 연결함으로써 의미정보를 표현하기 위해 제안됐다. RDF와 링크드 데이터가 널리 사용됨에 따라 분절된 데이터들이 가지고 있는 의미정보를 제공하기 위한 온톨로지 매핑 기술이 주목을 받고 있다. 하지만, 링크드 데이터에 대한 온톨로지 매핑 기술은 스키마 보다는 인스턴스 레벨에 초점을 맞춰왔다. 링크드 데이터에 대한 온톨로지 매핑은 인스턴스 레벨의 매핑이 존재하는 경우에만 스키마 레벨 매핑이 가능하다. 링크드 데이터는 인스턴스 기반의 스키마 매핑 기술을 적용하기에 적합한 데이터이다. 특히 모호한 이름을 가지고 있는 클래스 간의 매핑을 할 때 유용하다.
본 논문에서는 링크드 데이터에 대한 인스턴스 기반 스키마 매핑에 관한 세 가지 문제를 다뤘다. (1) 인스턴스 기반 스키마 매핑 (2) 대용량 링크드 데이터에 적용 가능하도록 알고리즘 개선 (3) 계층구조 생성

(1) 첫 번째 문제에 대해, 본 논문에서는 인스턴스 기반 스키마 매핑 알고리즘(IUT)을 제안했다. IUT 는 두 개의 대상 온톨로지에 있는 클래스들을 통합하여 하나의 계층구조를 생성한다. 이를 위해 인스턴스-클래스 매트릭스를 구축하고 인스턴스를 얼마나 공유하는지에 따라 두 개의 클래스 간의 관계를 알아낸다. DBpedia 와 YAGO2 에 대해 IUT 와 2 개의 최근 연구를 총 4 개의 매핑 종류에 대해 비교실험 하였다. 실험결과, IUT 가 매핑에 걸린 시간과 정확도 측면에서 가장 좋은 결과를 얻었다. 예를 들어, DBPedia 에 대한 intra-subsumption 매핑의 경우 968 ms 가 소모되었으며 F-score 는 0.810 이었다.

(2) 두 번째 문제에 대해, 본 논문에서는 대용량 데이터에도 적용 가능하도록 IUT 를 개선했다(IUT(M)). IUT(M)은 LSH (Locality-sensitive hashing)을 활용하여 다음과 같은 방법에 의해 계산량을 획기적으로 줄였다. (1) MinHash 함수를 사용해서 두 개의 클래스 간 유사도 계산량을 줄였고, (2) Banding 기술을 개발하여 유사도 계산의 횟수를 줄였다. YAGO-YAGO2 intra subsumption 매핑에 대해 IUT 와 IUT(M)을 비교했다. IUT(M)이 매핑에 소모된 시간을 94% 절약했는데 F-score 는 단지 5% 만 나빠졌다.

(3) 세 번째 문제에 대해, 본 논문에서는 object property 기반으로 Faceted 계층구조를 생성하는 방법을 제안했다. 인스턴스 기반의 계층구조 생성 알고리즘(ICT)을 사용하여 object property 를 추출하고 각 object property 에
대한 하부 계층구조를 생성한다. 세 번째 문제에 대해서는 2 가지 실험을 진행했다. (a) ICT를 사용해 DBpedia 와 YAGO2에 대해 “rdf:type”에 대한 하부 계층구조를 생성하는 실험 (소모된 시간은 각각 49와 11,790ms, F-score는 각각 0.917과 0.780) (b) Diseasome과 DrugBank에 대해서 multiple object properties 기반 faceted 계층구조를 얼마나 빠르게 생성하는지에 대한 실험 (6개 property의 경우 2,032 ms, 16 property의 경우 2,525 ms) 또한 얼마나 정확한 매핑을 하는지에 대한 실험 (2개 facet 기준으로 각각 1.65와 1.03 Maximum Resolution 수치) 

Keywords: 스키마 매핑, 인스턴스 기반 매핑, 링크드 데이터, 대용량 데이터 매핑, 계층구조 생성

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