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# Chapter 1

# Introduction

This research develops ***BayesOWL***, a probabilistic framework for representing and reasoning with uncertainty in semantic web. Specifically, ***BayesOWL*** provides a set of structural translation rules to map an OWL taxonomy ontology into a Bayesian network (BN) [121] directed acyclic graph (DAG) and a computational process called ***SD-IPFP*** to construct conditional probability tables (CPTs) for concept nodes in the DAG. ***SD-IPFP***, a special case of the "iterative proportional fitting procedure" (***IPFP***), is further developed to ***D-IPFP***, a more generalized method to modify BNs by probabilistic constraints in arbitrary forms, which itself can be regarded as an independent research.

With the development of the semantic web [1], ontologies have become widely used to capture the knowledge about concepts and their relations defined in a domain for information exchange and knowledge sharing. A number of ontology definition languages (e.g. SHOE [2], OIL [3], DAML [4], DMAL+OIL [5], RDF [6]/RDFS [7], and OWL [8], etc.) have been developed over the past few years. As with traditional crisp logic, any sentences in these languages, being asserted facts, domain knowledge, or reasoning results, must be either **true** or **false** and nothing in between. None of these existing ontology languages, including OWL [9], an emerging standard recommended by W3C

[1] `http://www.w3.org/DesignIssues/Semantic.html`
[2] `http://www.cs.umd.edu/projects/plus/SHOE/`
[3] `http://www.ontoknowledge.org/oil/`
[4] `http://www.daml.org/`
[5] `http://www.daml.org/2001/03/daml+oil-index`
[6] `http://www.w3.org/RDF/`
[7] `http://www.w3.org/TR/2004/REC-rdf-schema-20040210/`
[8] `http://www.w3.org/2001/sw/WebOnt/`
[9] OWL is based on description logics, a subset of first-order logic that provides sound and decidable reasoning support.

[10], provides a means to capture uncertainty about the concepts, properties and instances in a domain. However, most real world domains contain uncertain knowledge because of incomplete or partial information that is **true** only to a certain degree. Probability theory is a natural choice for dealing with this kind of uncertainty. Incorporating probability theory into existing ontology languages will strengthen these languages with additional expressive power to quantify the degree of overlap or inclusion between concepts, to support probabilistic queries such as finding the most similar concept that a given description belongs to, and to make more accurate semantic integration possible. These motivated my research in this dissertation.

## 1.1 The Motivations

As mentioned above, ontology languages in the semantic web, such as OWL and RDF(S), are based on crisp logic and thus can not handle incomplete or partial knowledge about an application domain. However, uncertainty exists in almost every aspect of ontology engineering. For example, in *domain modeling*, besides knowing that "$A$ is a subclass of $B$", which means any instance of $A$ will also be an instance of $B$, one may also know and wish to express the probability that an instance of $B$ belongs to $A$ (e.g., when a probability value of 0.1 is used to quantify the degree of inclusion of $A$ in $B$, it means by a chance of one out of ten an instance of $B$ will also be an instance of $A$, as shown in Fig. 1.1 [11]); or, in the case that $A$ and $B$ are not logically related, one may still wish to express how much is $A$ overlapped with $B$ (e.g., when a probability value of 0.9 is used to quantify the degree of overlap between $A$ and $B$, it means by 90 percent chance an instance of $A$ will also be an instance of $B$, as shown in Fig. 1.2). In *ontology reasoning*, one may want to know not only if $A$ is a subsumer of $B$, but also the degree of closeness of $A$ to $B$; or, one may want to know

[10] `http://www.w3.org/`

[11] In our context, for a concept class $C$, we use $c$ to denote that an instance belongs to this class, and $\bar{c}$ to denote that an instance does not belong to this class.

the degree of similarity between $A$ and $B$ even if $A$ and $B$ are not subsumed by each other. Moreover, a description (of a class or an individual) one wishes to input to an ontology reasoner may be noisy and uncertain, which often leads to over-generalized conclusions in logic based reasoning. Uncertainty becomes more prevalent in *concept mapping* between two ontologies where it is often the case that a concept defined in one ontology can only find partial matches to one or more concepts in another ontology with different degrees of similarity.

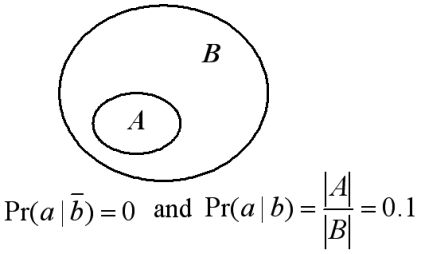



Fig. 1.1: **Concept Inclusion**

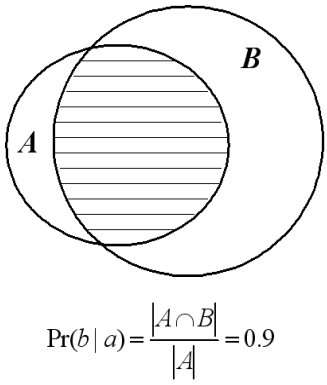



Fig. 1.2: **Concept Overlap**

Bayesian networks (BNs) [121] have been well established as an effective and principled general probabilistic framework for knowledge representation and inference under uncertainty. In the BN framework, the interdependence relationships among random variables in a domain are represented by the network structure of a directed acyclic graph (DAG), and the uncertainty of such relationships by the conditional probability table (CPT) associated with each variable. These local CPTs collectively and compactly encode the joint probability distribution of all variables in the network.

Developing a framework which augments and supplements OWL for representing and reasoning with uncertainty based on BNs may provide OWL with additional expressive power to support probabilistic queries and more accurate semantic integration. If ontologies are translated to BNs, then concept mapping between ontologies can be accomplished by evidential reasoning across the translated BNs. This ap-

proach to ontology mapping is seen to be advantageous to many existing methods in handling uncertainty in the mapping and will be discussed at the end of Chapter 5.

Besides the expressive power and the rigorous and efficient probabilistic reasoning capability, the structural similarity between the DAG of a BN and the RDF graph of an OWL ontology is also one of the reasons to choose BNs as the underlying inference mechanism for ***BayesOWL***: both of them are directed graphs, and direct correspondence exists between many nodes and arcs in the two graphs.

One thing to clarify here is the subtle differences between the three different mathematical theories in handling different kinds of uncertainties: probability theory [12], Dempster-Shafer theory [13], and fuzzy logic [14]. Although controversies still exist among mathematicians and statisticians about their philosophical meaning, in our context, we treat a probability as the chance of an instance belonging to a particular concept class (note that, the definition of the concept class itself, is precise) given the current knowledge, while viewing fuzzy logic as the mechanism used to deal with the imprecision (or vagueness) of the defined knowledge (i.e., the defined concept does not have a certain extension in semantics, and fuzzy logic can be used to specify how well an object satisfies such a vague description [133]). Dempster-Shafter theory, on the other hand, is a mechanism for "ignorance", it provides two measures (*support* and *plausibility*) for beliefs about propositions, and works well only in simple rule-based systems due to its extremely high computational complexity.

## 1.2 Thesis Statement

To address the issues raised in the previous sections, this research aimed at developing a framework which augments and supplements OWL for representing and reasoning with uncertainty based on Bayesian networks (BNs) [121]. This framework, named

[12]Refer to `http://en.wikipedia.org/wiki/Probability\_theory` for a brief definition.
[13]Refer to `http://en.wikipedia.org/wiki/Dempster-Shafer\_theory` for a brief definition.
[14]Refer to `http://en.wikipedia.org/wiki/Fuzzy\_logic` for a brief definition.

***BayesOWL***, has gone through several iterations since its inception in 2003 [38, 39]. It provides 1) a set of rules and procedures for direct translation of an OWL taxonomy ontology into a BN directed acyclic graph (DAG), and 2) a method ***SD-IPFP*** based on ***IPFP*** [15] [79, 36, 33, 152, 18, 31] that incorporates available probabilistic constraints when constructing the conditional probability tables (CPTs) of the BN. The translated BN, which preserves the semantics of the original ontology and is consistent with all the given probabilistic constraints, can support ontology reasoning, both within and across ontologies as Bayesian inferences. Aside from the ***BayesOWL*** framework, this research also involves developing methods for 1) representing probabilities in OWL statements, and 2) modifying BNs to satisfy given general probabilistic constraints by changing CPTs only.

The general principle underlying the set of structural translation rules for converting an OWL taxonomy ontology into a BN DAG is that all classes (specified as "*subjects*" and "*objects*" in RDF triples of the OWL ontology) are translated into binary nodes (named **concept node**s) in BN, and an arc is drawn between two concept nodes only if the corresponding two classes are related by a "*predicate*" in the OWL ontology, with the direction from the superclass to the subclass. A special kind of nodes (named **L-Node**s) are created during the translation to facilitate modeling relations among concept nodes that are specified by OWL logical operators.

The set of all nodes $X$ in the DAG obtained from previous step can be partitioned into two disjoint subsets: concept nodes $X_C$ which denote concept classes, and L-Nodes $X_L$ for bridging concept nodes that are associated by logical relations. CPT for an L-Node can be determined by the logical relation it represents so that when its state is "True", the corresponding logical relation holds among its parents. When the states of all the L-Nodes are set to "True", the logical relations defined in the original

[15] Abbreviated from "iterative proportional fitting procedure", a well-known mathematical procedure that modifies a given distribution to meet a set of probabilistic constraints while minimizing *I-divergence* to the original distribution.

ontology will be held in the translated BN, making the BN consistent with the OWL semantics. Denoting the situation in which all the L-Nodes in the translated BN are in "True" state as $\boldsymbol{\tau}$, the CPTs for the concept nodes in $X_C$ should be constructed in such a way that $\Pr(X_C|\boldsymbol{\tau})$, the joint probability distribution of all concept nodes in the subspace of $\boldsymbol{\tau}$, is consistent with all the given prior and conditional probabilistic constraints. ***SD-IPFP*** is developed to approximate these CPTs for nodes in $X_C$.

The ***BayesOWL*** framework can support common ontology reasoning tasks as probabilistic inference in the translated BN, for example, given a concept description $e$, it can answer queries about concept satisfiability ($\Pr(e|\boldsymbol{\tau}) = 0$?), about concept overlap (measured by $\Pr(e|c, \boldsymbol{\tau})$ for a concept $C$), and about concept subsumption (i.e., find the concept that is most similar to $e$) according to similarity measures.

Although not necessary, it is beneficial to represent probabilistic constraints attached with individual concepts, properties, and relations in an ontology as OWL statements. In ***BayesOWL***, a user can encode two types of probabilities: priors such as $\Pr(C)$ and pair-wise conditionals such as $\Pr(C|P1, P2, P3)$ where $P1$, $P2$, $P3$ are parent superconcepts of $C$. These two forms of probabilities correspond naturally to classes and relations (RDF triples) in an ontology and are most likely to be available to ontology designers. It is trivial to extend our representation to other forms of probabilistic constraints if needed.

Probabilistic constraints can be in any general forms, the ***SD-IPFP*** method used in ***BayesOWL*** is further developed into ***D-IPFP*** [123], which is an extension of the global ***E-IPFP*** [123] algorithm that is based on ***IPFP*** [152] and ***C-IPFP*** [31]. ***D-IPFP*** is applicable to the general problem of modifying BNs by low-dimensional distributions beyond ***BayesOWL***, and the joint probability distribution of the resulting network will be as close as possible to that of the original network.

A prototype system named ***OWL2BN*** is implemented to automatically translate a given valid OWL taxonomy ontology, together with some user specified con-

sistent probabilistic constraints, into a BN, with reasoning services provided based on Bayesian inferences. Java APIs for the different variations (i.e., ***IPFP***, ***C-IPFP***, ***E-IPFP***, ***D-IPFP***, and ***SD-IPFP***) of ***IPFP*** algorithms are also developed, which can be used independently.

This research is the first systematic study of uncertainty in OWL ontologies in the semantic web community. The resulting theoretical framework ***BayesOWL*** allows one to translate a given OWL taxonomy ontology into a BN that is consistent with the semantics of the given ontology and with the probabilistic constraints. With this framework, ontological reasoning within and across ontologies can be treated as probabilistic inference in the translated BNs. This work thus builds a foundation for a comprehensive solution to uncertainty in semantic web. Besides its theoretical rigor, this work also addresses the practicality of the approach with careful engineering considerations, including non-intrusiveness of the approach, flexible DAG translation rules and procedures, and systematic and efficient CPT construction mechanism, making ***BayesOWL*** easy to accept and to use by ontology designers and users. In addition, this research also contributes in 1) solving more general BN modification problems by developing two mathematically well-founded algorithms ***E-IPFP*** and ***D-IPFP***, 2) representing probabilistic information using OWL statements, and 3) providing implemented APIs to be used by other researchers and practitioners in ontology engineering.

## 1.3 Dissertation Outline

This dissertation is organized as follows. In Chapter 2, Section 2.1 provides a brief introduction to semantic web, ontology, and description logics (DLs); Section 2.2 introduces some basics about Bayesian networks (BNs) [121], its definition and semantics, existing inference and learning algorithms; Section 2.3 discusses existing

works in handling uncertainties in the semantic web; Section 2.4 gives a high-level introduction to the ***IPFP*** [152] and ***C-IPFP*** [31] algorithms; Section 2.5 surveys some of the best known ontology-based semantic integration systems and database schema integration systems; and the chapter ends with a summary in Section 2.6.

Chapter 3 starts with mathematical definitions and convergence proof of ***IPFP*** in Section 3.1, followed by a precise problem statement in Section 3.2. ***E-IPFP***, ***D-IPFP***, and ***SD-IPFP***, the algorithms we developed for modifying BNs with given probabilistic constraints [123], are presented in Section 3.3, Section 3.4, and Section 3.5, respectively. Section 3.6 describes the implementation of various ***IPFP*** algorithms. Experimental results are supplied in Section 3.7. The chapter is summarized in Section 3.8.

Chapter 4 describes ***BayesOWL*** in detail. Section 4.1 proposes an OWL representation of probabilistic information concerning the entities and relations in ontologies; Section 4.2 elaborates the structural translation rules; Section 4.3 describes the CPT construction process using ***SD-IPFP***; Section 4.4 outlines the semantics of ***BayesOWL*** and Section 4.5 presents some possible ontologies reasoning tasks with ***BayesOWL***. Section 4.6 describes the implementation of the ***OWL2BN*** API for structural translation, which, together with the ***IPFP*** API described in Section 3.6, builds up an initial version of the ***BayesOWL*** framework. Section 4.7 compares ***BayesOWL*** to other related works. Section 4.8 concludes the chapter and discusses the limitations.

Discussion and suggestions for future research are included in Chapter 5. These include 1) investigating possible methods to deal with uncertainty in properties and instances, 2) developing methods in handling inconsistent probabilistic constraints provided, 3) investigating the possibility of learning probability constants from existing web data (instead of specified by domain experts), and 4) proposing a framework for ontology mapping (or translation) based on ***BayesOWL***.

# Chapter 2

# Background and Related Works

Before we present our framework, it would be helpful to first provide some background knowledge and related works. This chapter is divided into six sections. Section 2.1 gives a brief review of the semantic web activity, ontology and its representation languages, and a brief introduction to description logics, the logical foundation behind ontology languages such as DAML+OIL and OWL. Section 2.2 introduces Bayesian networks (BNs). Section 2.3 summarizes previous works on probabilistic extensions of description logics such as P-CLASSIC and P-$SHOQ$(D), and existing works on representing probabilistic information in the semantic web. Section 2.4 introduces ***IPFP***, the "**iterative proportional fitting procedure**". Section 2.5 surveys the literature on information integration systems, especially existing approaches to ontology mapping (and merging, translation, etc.) and database schema integration. A summary is provided in Section 2.6.

## 2.1 Ontology and Semantic Web

The idea of Semantic Web was started in 1998, brought up by Tim Berners-Lee [1], the inventor of the WWW and HTML. It aims to add a layer of machine-understandable information over the existing web data [2] to provide meaning or semantics to these data. The Semantic Web activity is a joint effort by World Wide Web Consortium (W3C) [3], US Defense Advanced Research Project Agency (DARPA) [4], and EU In-

[1] http://www.w3.org/People/Berners-Lee/
[2] http://www.w3.org/DesignIssues/Semantic.html
[3] http://www.w3.org/
[4] http://www.darpa.mil/

formation Society Technologies (IST) Programme [5].

The core of the Semantic Web is "ontology", which is used to capture the concepts and relations about concepts in a particular domain. Ontology engineering in the Semantic Web is primarily involved with building and using ontologies defined with languages such as RDF(S) and OWL. The web ontology language, OWL, is a standard recommended by W3C and adopts its formal semantics and decidable inferences from description logics (DLs) - a subset of first-order logic.

### 2.1.1 The Semantic Web

People can read and understand a web page easily, but machines can not. To make web pages understandable by machines, additional semantic information needs to be attached to or embedded in the existing web data. Built upon the Resource Description Framework [6] (RDF) , the Semantic Web [7] is aimed at extending the current web so that information can be given well-defined meaning using the description logic based web ontology definition language OWL, and thus enabling better cooperation between computers and humans. Semantic web can be viewed as a web of data that is similar to a globally accessible database, but with semantics provided for information exchanged over Internet. It extends the current World Wide Web (WWW) by attaching a layer of machine understandable metadata on top of it. The Semantic Web is increasing recognized as an effective tool for globalizing knowledge representation and sharing on the Web.

To create such an infrastructure, a general assertional model to represent the resources available on the web is needed, RDF is a standard designed specifically for this purpose. RDF is a framework [8] for supporting resource description, or metadata (data about data) for a variety of applications (from library catalogs and world-

[5] http://www.cordis.lu/ist/
[6] http://www.w3.org/RDF/
[7] http://www.w3.org/2001/sw/
[8] http://www.w3.org/RDF/FAQ

wide directories to syndication and aggregation of news, software, and content to personal collections of photoes, music, and events). RDF is a collaborative effort by a number of metadata communities. RDF is based on XML, it uses XML as its syntax and it uniquely identifies resources by using URI and XML namespace mechanism. The basic building blocks of RDF are called RDF triples of "*subject*", "*predicate*" and "*object*". In general, an RDF statement includes a specific resource ("*subject*") with a property ("*predicate*") / value ("*object*") pair which form the triple, and the statement can be read as "the <*subject*> has <*predicate*> <*object*>". For example [9], in the following RDF/XML document,

```
<?xml version="1.0"?\ >
<rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns\#"
         xmlns:dc="http://purl.org/dc/elements/1.1/"\ >
  <rdf:Description rdf:about="http://www.w3.org/">
    <dc:title>World Wide Web Consortium</dc:title>
  </rdf:Description>
</rdf:RDF>
```

"`http://www.w3.org/`" is the "*subject*", "`http://purl.org/dc/elements/1.1/title`" is the "*predicate*" and "World Wide Web Consortium" is the "*object*", and it can be read as: "`http://www.w3.org/`" has a title "World Wide Web Consortium". Each RDF triple can be encoded in XML as shown in the above example. It can also be represented as the "RDF graph" in which nodes correspond to "*subject*" and "*object*" and the directed arc corresponds to the "*predicate*" as show in Fig. 2.1. RDF is only an assertional language, each triple makes a distinct assertion, adding any other triples will not change the meaning of the existing triples.

Just as the role of XML Schema to XML, a simple datatyping model of RDF called

[9]Example comes from: `http://www.w3.org/RDF/Validator/`.

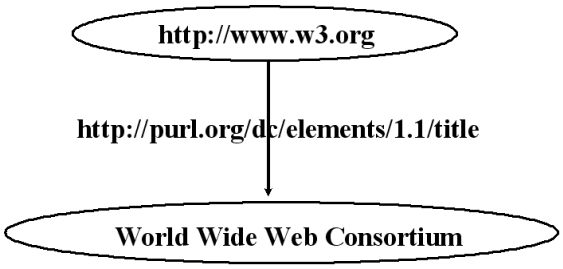



Fig. 2.1: **A Small Example of RDF Graph**

RDF Schema (RDFS) [10] is used to control the set of terms, properties, domains and ranges of properties, and the "rdfs:subClassOf" and "rdfs:subPropertyOf" relationships used to define resources. However, RDF does not specify a way for reasoning and RDFS is not expressive enough to catch all the relationships between classes and properties. Built on top of XML, RDF and RDFS, DAML+OIL [11] provides a richer set of vocabulary to describe the resources on the Web. The semantics behind DAML+OIL is a variation of description logics with datatypes which makes efficient ontology reasoning possible. DAML+OIL is the basis for the current W3C's Web Ontology Language (OWL) [12]. OWL provides a richer set of vocabulary by further restricting on the set of triples that can be represented. Details about ontology, existing ontology languages and their logics and inferences will be presented in the next subsection.

### 2.1.2 What is Ontology?

The metaphysical studies on ontologies starts since Aristotle [13] time. In philosophy, "Ontology" is the study of the nature of being and existence in the universe. The term "ontology" is derived from the Greek word "onto" (means "being") and "logia" (means "written or spoken discourse"). Smith [136] defines ontology as "the science

[10] `http://www.w3.org/TR/2004/REC-rdf-schema-20040210/`
[11] `http://www.daml.org/2001/03/daml+oil-index`
[12] `http://www.w3.org/2001/sw/WebOnt/`
[13] `http://www.answers.com/Aristotle`

of what is, of the kinds and structures of objects, properties, events, processes and relations in every area of reality" and points out the essence of ontology as "to provide a definitive and exhaustive classification of entities in all spheres of being". In contrast to these studies, Quine's *ontological commitment* [14] [131] drove ontology research towards formal theories in the conceptual world and fostered ontology development in natural science: people build ontologies with commonly agreed vocabularies for representing and sharing knowledge. In the context of semantic web, by further extending Quine's work, computer scientists interpret the term "ontology" with a new meaning as "an explicit specification of a conceptualization" [58], which is used to describe a particular domain by capturing the concepts and their relations in the domain for the purpose of information exchange and knowledge sharing, and provides a common understanding about this domain.

Although ontologies could be stored in one's mind, written in a document or embedded in software, such *implicit* ontologies do obstruct communication as well as interoperability [146]. In semantic web, ontologies are explicitly represented in a well defined knowledge representation language. Over the past few years, several ontology definition languages have emerged, including RDF(S), SHOE [15], OIL [16], DAML [17], DAML+OIL, and OWL. Among them, OWL is the standard recommendation by W3C, which has DAML+OIL as its basis but with simpler primitives. Fig. 2.2 shows the evolution of these languages [18]. Brief descriptions about OIL, DAML, DAML+OIL, and OWL, the four description logic [7] based languages, will be presented next.

OIL [49] stands for "Ontology Inference Layer", it is an extension of RDF(S),

[14] That is, one is committed as an existing thing when it is referenced or implied in some statements, and the statements are commitments to the thing.

[15] `http://www.cs.umd.edu/projects/plus/SHOE/`

[16] `http://www.ontoknowledge.org/oil/`

[17] `http://www.daml.org/`

[18] For a language feature comparison among XML, RDF(S), DAML+OIL and OWL, please refer to `http://www.daml.org/language/features.html`.

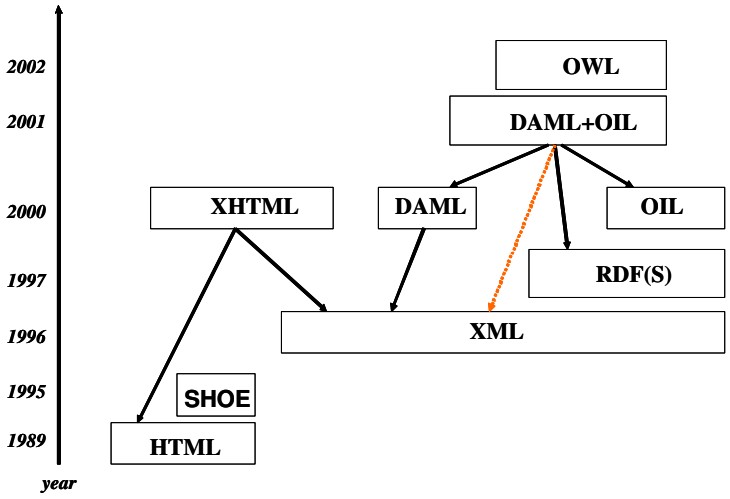



Fig. 2.2: **Development of Markup Languages**

its modeling primitives are originated from frame-based languages [100], its formal semantics and reasoning services are from description logics [7], while its language syntax is in well-defined XML [19]. OIL provides a layered approach for web-based representation and inference with ontologies: 1) Core OIL largely overlaps with RDFS, with the exception of the reification of RDFS, 2) Standard OIL tries to capture the modeling constructs (Tbox in DL), 3) Instance OIL deals with individual integration and database capability (Abox in DL), and 4) Heavy OIL is left for additional representational and reasoning capabilities in the future.

DAML is the abbreviation of "DARPA Agent Markup Language", it provides a basic infrastructure that allows machines to make some simple inferences, for example, if "fatherOf" is a "subProperty" of "parentOf", and "Tom" is the "fatherOf" "Lisa", then machine can infer that "Tom" is also the "parentOf" "Lisa". DAML is also built on XML. While XML does not provide semantics to its tags, DAML does.

Although DAML and OIL were resulted from different initiatives, the capabilities of these two languages are quite similar [20]. DAML+OIL is a semantic markup language for web resources built on DAML and OIL by a joint effort from both

[19] `http://www.w3.org/XML/`
[20] http://www.ontoknowledge.org/oil/oil-faq.html

the US and European society. The latest version was released in March 2001. A DAML+OIL ontology will have zero or more headers, followed by zero or more class elements, property elements and instances. A DAML+OIL knowledge base is a collection of restricted RDF triples: DAML+OIL assigns specific meaning to certain RDF triples using DAML+OIL vocabularies. DAML+OIL divides the instance universe into two disjoint parts: the *datatype* domain consists of the values that belong to XML Schema datatypes, while the *object* domain consists of individual objects that are instances of classes described within DAML+OIL or RDF(S). Correspondingly there are two kinds of restrictions in DAML+OIL: *ObjectRestriction* and *DatatypeRestriction*. In DAML+OIL, subclass relations between classes can be cyclic, in that case all classes involved in the cycle are treated as equivalent classes. DAML+OIL can introduce class definition at any time. DAML+OIL also provides decidable and tractable reasoning capability.

OWL, the standard web ontology language recently recommended by W3C, is intended to be used by applications to represent terms and their interrelationships. It is an extension of RDF(S) and goes beyond its semantics. OWL is largely based on DAML+OIL with removal of qualified restrictions, renaming of various properties and classes, and some other updates [21], and it includes three increasingly complex variations [22]: OWL Lite, OWL DL and OWL Full.

An OWL document can include an optional ontology header and any number of class, property, axiom, and individual descriptions. In an ontology defined by OWL, a named class is described by a class identifier via "rdf:ID". An anonymous class can be described by value (owl:hasValue, owl:allValuesFrom, owl:someValuesFrom) or cardinality (owl:maxCardinality, owl:minCardinality, owl:cardinality) restriction on property (owl:Restriction); by exhaustive enumeration of all individuals that are

[21] Refer to `http://www.daml.org/2002/06/webont/owl-ref-proposed\#appd` for all the changes.

[22] `http://www.w3.org/TR/owl-guide/`

the instances of this class (owl:oneOf); or by logical operations on two or more other classes (owl:intersectionOf, owl:unionOf, owl:complementOf). The three logical operators correspond to AND (conjunction), OR (disjunction) and NOT (negation) in logic, they define classes of all individuals by standard set-operations of intersection, union, and complement, respectively. Three class axioms (rdfs:subClassOf, owl:equivalentClass, owl:disjointWith) can be used for defining necessary and sufficient conditions of a class.

Two kinds of properties can be defined in an OWL ontology: object property (owl:ObjectProperty) which links individuals to individuals, and datatype property (owl:DatatypeProperty) which links individuals to data values. Similar to classes, "rdfs:subPropertyOf" is used to define that one property is a subproperty of another property. There are constructors to relate two properties (owl:equivalentProperty and owl:inverseOf), to impose cardinality restrictions on properties (owl:FunctionalProperty and owl:InverseFunctionalProperty), and to specify logical characteristics of properties (owl:TransitiveProperty and owl:SymmetricProperty). There are also constructors to relate individuals (owl:sameAs, owl:sameIndividualAs, owl:differentFrom and owl:AllDifferent).

The semantics of OWL is defined based on model theory [23] in the way analogous to the semantics of description logics (DLs). With the set of vocabularies (mostly as described above), one can define an ontology as a set of (restricted) RDF triples which can be represented as an RDF graph.

### 2.1.3 Brief Introduction to Description Logics

Description logics (DLs) [7] are a family of knowledge representation languages originated from semantic networks [137] and frame-based systems [99] in the 1980s. DLs deal with the representation and reasoning of structured concepts by providing an

[23] `http://www.w3.org/TR/owl-semantics/`

explicit model-theoretic semantics [46, 93]. DLs are suitable for capturing the knowledge about a domain in which instances can be grouped into classes and relationships among classes are binary. The family of DLs includes systems such as KL-ONE (1985) [20], LOOM (1987) [88], BACK (1987) [154], CLASSIC (1989) [19], KRIS (1991) [8], FaCT (1998) [24], RACER (2001) [25], Pellet (2003) [26] and KAON2 (2005) [27]. In recent years DLs also inspire the development of ontology languages such as OIL, DAML, DAML+OIL, and OWL, and act as their underlying logical basis and inference mechanism.

DLs describe a domain using concepts, individuals, and roles (which are binary relations among concepts to specify their properties or attributes). Concepts are used to describe classes of individuals and are denoted by conjoining superconcepts with any additional restrictions via a set of constructors. For example, the concept description "Professor $\sqcap$ Female $\sqcap \forall$ hasStudent.PhD" represents the classes of female professors all of whose students are PhD students. There are two kinds of concepts: primitive concepts and defined concepts. Primitive concepts are defined by giving only necessary conditions while defined concepts are specified by both necessary and sufficient conditions [93]. For example, "Human" can be a primitive concept and can be introduced as a subclass of another primitive concept "Animal" by description "Human $\sqsubset$ Animal", if an individual is a human then it must be an animal but not vice versa. On the other hand, "Man" can be thought as a defined concept by description "Man $\equiv$ Human $\sqcap$ Male", an individual is a man if and only if it is both a male and a human. The relationship between subconcepts and superconcepts is similar to an "**isa**" hierarchy, on the very top of the hierarchy is the concept **THING** (denoted as $\top$), which is a superconcept of all other concepts, and at the bottom is **NOTHING** (denoted as $\bot$), which is a subconcept of all other concepts. Roles are

[24] http://www.cs.man.ac.uk/~horrocks/FaCT/
[25] http://www.racer-systems.com/
[26] http://www.mindswap.org/2003/pellet/
[27] http://kaon2.semanticweb.org/

binary relationships between two concepts. If the number of fillers allowed for a role is larger than 1, one individual may relate by the same role to many individuals; otherwise, roles with exactly one filler are called "attributes". There are two kinds of restrictions that can be applied to a role. Value restrictions restrict the value of the filler of a role, while number restriction provides a lower or upper bound on the number of fillers of a role. Individuals are generally asserted to be instances of concepts and have roles filled with other individuals.

A DL-based knowledge base usually includes two components: Tbox (terminological KB, denoted as $\mathcal{T}$) and Abox (assertional KB, denoted as $\mathcal{A}$). Tbox consists of concepts and roles defined for a domain and a set of axioms used to assert relationship (subsumption, equivalence, disjointness etc) with respect to other classes or properties. Abox includes a set of assertions on individuals by using concepts and roles in Tbox. If $C$ is a concept, $R$ is a role, and $a$, $b$ are individuals, then $C(a)$ is a concept membership assertion and $R(a, b)$ is a role membership assertion [46].

The semantics of a description logic is given by an interpretation $\boldsymbol{I} = (\Delta^{\boldsymbol{I}}, \ .^{\boldsymbol{I}})$ which consists of a non-empty domain of objects $\Delta^{\boldsymbol{I}}$ and an interpretation function $.^{\boldsymbol{I}}$. This function maps every concept to a subset of $\Delta^{\boldsymbol{I}}$, every role and attribute to a subset of $\Delta^{\boldsymbol{I}} \times \Delta^{\boldsymbol{I}}$, and every individual to an element of $\Delta^{\boldsymbol{I}}$. An interpretation $\boldsymbol{I}$ is a model of a concept $C$ if $C^{\boldsymbol{I}}$ is non-empty (i.e., $C$ is said "satisfiable"). An interpretation $\boldsymbol{I}$ is a model of an inclusion axiom $C \sqsubseteq D$ if $C^{\boldsymbol{I}} \subseteq D^{\boldsymbol{I}}$. Moreover, an interpretation $\boldsymbol{I}$ is a model of $\mathcal{T}$ if $\boldsymbol{I}$ satisfies each element of $\mathcal{T}$, and an interpretation $\boldsymbol{I}$ is a model of $\mathcal{A}$ if $\boldsymbol{I}$ satisfies each assertation in $\mathcal{A}$.

Subsumption is the main reasoning service provided by DLs with regard to concepts. Suppose $A$ and $B$ are two concepts in $\mathcal{T}$, $A$ subsumes $B$, or $B$ is subsumed by $A$, if and only if $B^{\boldsymbol{I}} \subseteq A^{\boldsymbol{I}}$ for every model $\boldsymbol{I}$ of $\mathcal{T}$, $A$ is called a subsumer of $B$ while $B$ is a subsumee of $A$. Subsumption can be thought as a kind of "**isa**" relation, if $B$ is subsumed by $A$ then any instance of $B$ should also be an instance of $A$.

There are two major approaches used to perform concept subsumption.

- The first approach, "*structural subsumption*", is based on structural comparisons between concept descriptions which include all properties and all superconcepts of the concepts. The description is normalized into a canonical form first by making all implicit information explicit and then eliminating redundant information. Then a structural comparison between subexpressions of a concept with those of the other concept is performed. For this method, subsumption will easily be sound but hard to be complete due to high computational complexity. Subsumption is complete only if the comparison algorithm checks all parts of the structure and the normalization algorithm performs all the inferences that it should. In fact, most implemented normalize-and-compare subsumption algorithms are incomplete.

- The second approach, called "*tableau method*", aiming to make subsumption complete, is based on tableaux-like theorem proving techniques. Concept $C$ is subsumed by concept $D$ if and only if $C \sqcap \neg D$ is not satisfiable, or, $C$ is not subsumed by $D$ if and only if there exists a model for $C \sqcap \neg D$. This method tries to generate such a finite model by using an approach similar to first-order tableaux calculus with a guaranteed termination. If it succeeds then the subsumption relationship does not hold, if it fails to find a model then the subsumption relationship holds.

Some other reasoning tasks can be easily reduced to subsumption. For example, the problem of checking whether a concept $C$ is satisfiable or not can be reduced to the problem of checking if it is impossible to create an individual that is an instance of $C$, that is, whether $C$ is subsumed by **NOTHING** or not. Similarly, disjointness between two concepts $A$ and $B$ can be decided by checking whether $A \sqcap B$ is subsumed by **NOTHING** or not, and equivalence between two concepts $A$ and $B$ can be decided

by checking if both $A$ is subsumed by $B$ and $B$ is subsumed by $A$. Moreover, with subsumption, it is not hard to do concept classification: given a concept description $C$, identify its most specific subsumer and the most general subsumee in the hierarchy.

Recognition is the analog of subsumption with respect to individuals. An individual $a$ is recognized to be an instance of a concept $C$ if and only if $a^{\boldsymbol{I}} \in C^{\boldsymbol{I}}$ for every model $\boldsymbol{I}$ of $\mathcal{A}$. Besides recognition, other inferences regarding to individuals include propagation, inconsistency checking, rule firing, and test application etc.

An example description language, $ALC$, has the following syntax rules:

$$
\begin{array}{lcll}
C, D & \rightarrow & A \mid & (\textit{atomic concept}) \\
 & & \neg A \mid & (\textit{atomic negation}) \\
 & & C \sqcap D \mid & (\textit{intersection}) \\
 & & C \sqcup D \mid & (\textit{union}) \\
 & & \forall R.C \mid & (\textit{value restriction}) \\
 & & \exists R.C \mid & (\textit{full existential quantification}) \\
 & & \top \mid & (THING) \\
 & & \bot & (NOTHING)
\end{array}
$$

The description language $SHIQ$ augments $ALC$ with qualifying number restrictions, role hierarchies, inverse roles ($I$), and transitive roles. The semantics of OIL is captured by a description logic called $SHIQ$(d) which extends $SHIQ$ with concrete datatypes [69]. A translation function $\delta(.)$ is defined to map OIL ontologies into equivalent $SHIQ$(d) terminologies, and $SHIQ$(d) reasoner is implemented in the FaCT system [28]. $SHOQ$(D) [71] is an expressive description logic which extends $SHQ$ with named individuals ($O$) and concrete datatypes ($D$) but without inverse roles ($I$), it has almost the same expressive power as DAML+OIL (which has inverse roles). DAML+OIL can be viewed as the combination of $SHOQ$(D) with inverse

[28] `http://www.cs.man.ac.uk/~horrocks/FaCT/`

roles and RDF(S)-based syntax [70]. OWL-DL corresponds to the description language $SHOIN(\mathrm{D}_n)$, which extends $SHIQ$ with concrete XML Schema datatypes and nominals.

## 2.2 Bayesian Belief Networks

Uncertainty arises from the incomplete or incorrect understanding of the domain, it exists in many applications, including diagnosis in medicine, diagnosis for man-made systems, natural language disambiguity, and machine learning, to mention just a few. Probability theory has been proven to be one of the most powerful approaches to capturing the degree of belief about uncertain knowledge. A probability of **0** for a given sentence $L$ means a belief that $L$ is **false**, while a probability of **1** for $L$ means a belief that $L$ is **true**. A probability between **0** and **1** means an intermediate degree of belief in the truth of $L$. According to probability theory, the joint probability distribution of all variables involved can be used to compute the answer to any probabilistic queries about the domain through conditioning [133]. However, the joint probability distribution becomes intractably large as the number of variables increases. Bayesian networks (BNs), also called Bayesian belief networks, belief networks, or probabilistic causal networks, are widely used for knowledge representation under uncertainty [121] by graphically representing the dependence between variables and decomposing the joint probability distribution into a set of conditional probability tables associated with individual variables. In this section, a brief introduction to BNs and their semantics is presented first in Subsection 2.2.1, followed by a brief review of the inference mechanisms in Subsection 2.2.2 and learning methods related to BNs in Subsection 2.2.3.

### 2.2.1 Definition and Semantics

In its most general form, a Bayesian network (BN) of $n$ variables consists of a directed acyclic graph (DAG) of $n$ nodes and a number of arcs, with conditional probability tables (CPTs) attached to each cluster of parent-child nodes. Nodes $X_i$ ($i \in [1, n]$) in a DAG correspond to variables [29], and directed arcs between two nodes represent direct causal or influential relation from one node to the other. The uncertainty of the causal relationship is represented locally by CPT $\Pr(X_i|\pi_i)$ associated with each node $X_i$, where $\pi_i$ is the parent node set of $X_i$ [30]. A conditional independence assumption is made for BNs: $\Pr(X_i|\pi_i, S) = \Pr(X_i|\pi_i)$, where $S$ is any set of variables, excluding $X_i$, $\pi_i$, and all descendants of $X_i$. Under this conditional independence assumption, the graphical structures of BNs allow an unambiguous representation of interdependencies between variables, which leads to one of the most important feature of BNs: the joint probability distribution of $X = (X_1, \ldots, X_n)$ can be factored out as a product of the CPTs in the network (named "the chain rule of BN"):

$$\Pr(X = x) = \prod_{i=1}^{n} \Pr(x_i|\pi_i)$$

Here $x = \{x_1, ..., x_n\}$ represents a joint assignment or an instantiation to the set of all variables $X = \{X_1, ..., X_n\}$ and the lower case $x_i$ denotes an instantiation of $X_i$.

Evidence is a collection observation or findings on some of the variables. There are three types of evidences can be applied to a BN:

- Hard Evidence: A collection of hard findings. A hard finding instantiates a node $X_i$ to a particular state $x_i$, i.e., $\Pr(X_i = x_i) = 1$ and $\Pr(X_i = x_i' \neq x_i) = 0$.
- Soft Evidence: A collection of soft findings. Instead of giving the specific state a node $X_i$ is in, a soft finding gives a distribution $Q(X_i)$ of $X_i$ on its states.

[29] Variables may have a discrete or continuous state set, here we only consider variables with a finite set of mutual exclusive states.

[30] If $X_i$ is a root in the DAG which has no parent nodes, $\Pr(X_i|\pi_i)$ becomes $\Pr(X_i)$.

Hard evidence is thus a special case of soft evidence.

- Virtual Evidence: The likelihood of a variable's distributions, i.e., the probability of observing $X_i$ being in state $x_i$ if its true state is $x_i'$. It represents another type of uncertain findings: uncertain on a hard finding. Pearl [121, 122] has provided a method for reasoning with virtual evidence in BN by creating a virtual node $O_i$ for a virtual evidence $ve$ as a child of $X_i$ which has $X_i$ as its only parent and constructing its CPT by the likelihood ratio concerning $ve$. Virtual evidence is equivalent to soft evidence in expressiveness, so this method can also be used to soft evidence update by first converting soft evidence into equivalent virtual evidence [117, 147].

With the conditional independence assumption, interdependencies between variables in a BN can be determined by the network topology. This is illustrated next with the notion of "**d-separation**". There are three types of connections in the network: serial, diverging, and converging connections, as depicted in Fig. 2.3. In the situation of serial connection, hard evidence $e$ can transmit its influence between $A$ and $C$ in either direction unless $B$ is instantiated ($A$ and $C$ are said to be d-separated by $B$). In the diverging connection case, $e$ can transmit between $B$ and $C$ unless $A$ is instantiated ($B$ and $C$ are said to be d-separated by $A$). In converging connection, $e$ can only transmit between $B$ and $C$ if either $A$ or one of its descendants has received hard evidence, otherwise, $B$ and $C$ are said to be d-separated by $A$.

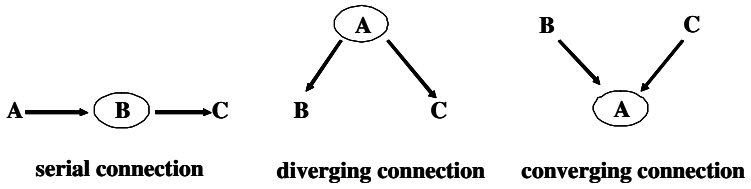



Fig. 2.3: **D-Separation in Three Types of BN Connections**

If nodes $A$ and $B$ are d-separated by a set of variables $V$, then changes in the certainty of $A$ will have no impact on the certainty of $B$, i.e., $A$ and $B$ are independent

of each other, given $V$, or, $\Pr(A|V,B) = \Pr(A|V)$. From the above three cases of connections, it can be shown that the probability distribution of a variable $X_i$ is only influenced by its parents, its children, and all the variables sharing a child with $X_i$, which form the Markov Blanket $M_i$ of $X_i$. If all variables in $M_i$ are instantiated, then $X_i$ is d-separated from the rest of the network by $M_i$, i.e., $\Pr(X_i|\overline{X_i}) = \Pr(X_i|M_i)$, where $\overline{X_i} = X - \{X_i\}$.

Noisy-or networks (Fig. 2.4) are special BNs of binary nodes (1 or 0), and it associates a single probability measure, called causal strength and denoted $p_i$, to each arc $A_i \rightarrow B$ to capture the degree of uncertainty of the causal relation from $A_i$ to $B$. If $B = 1$ then at least one of its parents is 1; when more than one parents are 1, then their effects on causing $B = 1$ are independent. $p_i$ indicates how likely $A_i = 1$ alone causes $B = 1$, i.e. $p_i = \Pr(B = 1|A_i = 1, A_k = 0, \forall k \neq i)$. The posterior probability of $B$ given an instantiation of its parents is:

$$\Pr(B = 1|A_1, ..., A_n) = 1 - \prod_{i=1}^{n} (1 - p_i a_i)$$

where $a_i$ denotes an instantiation of $A_i$.

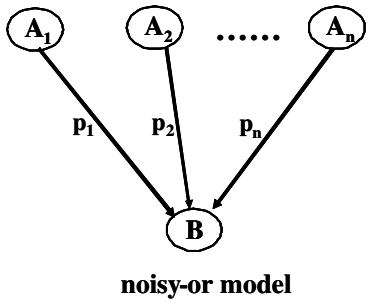



Fig. 2.4: **A Special Type of BNs**

This noisy-or model tremendously reduces the number of conditional probabilities needed to specify a BN, saves some table look up time, and makes it easy for domain experts to provide and assess conditional probabilities.

To understand the semantics of a BN, one way is to treat the network as a rep-

resentation of the joint probability distribution (see "chain rule" above), the second way is to view it as an encoding of a set of conditional independence statements. The two views are equivalent. The first is helpful in understanding how to construct networks, whereas the second is helpful in designing inference algorithms.

### 2.2.2 Inference

With the joint probability distribution, BNs support, at least in theory, any inference in the joint space, given some evidence $e$. Three related yet distinct types of probabilistic inference tasks have received wide attention in BN community. They all start with evidence $e$ but differ on what are to be inferred.

- Belief Update: Given $e$, compute the posterior probability $\Pr(X_i|e)$ for any or all uninstantiated variable $X_i$.
- Maximum *a posteriori* probability (MAP): Given $e$, find the most probable joint value assignment to all uninstantiated variables. MAP is also known as "belief revision".
- Most probable explanation (MPE): Given $e$, find the most probable joint assignment for all "hypothesis" or "explanation" variables. Such a joint assignment forms an explanation for $e$.

It has been well established that general probabilistic inference, including those mentioned above, in BNs, is NP-hard [29]. Approximate solutions of MAPs with a given error rate is also in NP-hard [1].

A number of algorithms have been developed for both exact and proximate solutions to these and other probabilistic inference tasks. In our context we are particularly interested in belief updating methods. There are three main approaches developed for belief updating: belief propagation [119], junction tree [83], and stochastic simulation [120]. The first two are for exact solutions by exploring the causal

structures in BNs for efficient computation, while the last one is for an approximate solution. Belief propagation based on local message passing [119] works for polytrees (singly connected BNs) only, it can be extended to work for general belief networks (multiply connected BNs) with some additional processing such as clustering (node collapsing), conditioning, etc. Junction tree approach [83] works for all belief networks, but the construction of junction tree from belief network is non-trivial. Stochastic simulation [120] aims to reduce the time and space complexity of exact solutions via a two-phase cycle: local numerical computation followed by logical sampling, sampling method includes forward sampling, Gibbs sampling etc.

Interested readers may refer to [60] for a survey of various exact and approximate Bayesian network inference algorithms, including those for MAPs (e.g. [124]) and MPEs.

### 2.2.3 Learning

In some cases, both the network structure and the associated CPT of a belief network are constructed by human experts based on their knowledge and experience. However, experts' opinions are often biased, inaccurate, incomplete, and sometimes contradicting to each other, so it is desirable to validate and improve the model using data. In many other cases, prior knowledge does not exist or is only partially available or is too expensive to obtain; network structure and corresponding CPT need to be learned from case data.

Depends on whether the network structure is known or unknown and the variables in the network is observable or hidden, there are 4 kinds of learning varieties [133]. The first is "Known structure, fully observable", in which the only task is to learn the CPTs by using statistical information from the case data. The second is "Unknown structure, fully observable", in which the main task is to reconstruct the topology of the network through a search in the space of structures. The third is "Known

structure, hidden variables", which is similar to neural network learning. The last is "Unknown structure, hidden variables", no good algorithms are developed for this problem at present. In general, structure learning (learning the DAG) is harder, parameter learning (learning CPT) is easier if the DAG is known.

An early effort in learning is the CI-algorithm [121], which is based on variable interdependencies. It applies standard statistical method on the database to find all pairs of variables that are dependent of each other, eliminate indirect dependencies as much as possible, and then determine directions of dependencies. This method often only produces incomplete results (learned structure contains indirect dependencies and undirected links).

A second approach is Bayesian approach [30]. The goal is to find the most probable DAG $B_S$ , given database $D$, i.e. $max(\Pr(B_S|D))$ or $max(\Pr(B_S, D))$. The approach develops a formula to compute $\Pr(B_S, D)$ for a given pair of $B_S$ and $D$, based on some assumptions and Bayes' theorem. A hill-climbing algorithm named K2 is developed to search for the best $B_S$ depending on a pre-determined variable ordering. This approach has solid theoretical foundation and great generality, but the computational cost is high and the heuristic search may lead to sub-optimal results.

A third method is Minimum Description Length (MDL) approach [81] which tries to achieve a balance between accuracy (how well a learned BN fits case data) and complexity (size of CPT) of the learned BN. A MDL $L$ is defined as: $L = a*L_1+b*L_2$, where $L_1$ is the length of encoding of the BN (more complex BNs have large $L_1$), $L_2$ is the length of encoding of the data, given the BN model (a BN that better fits the DB has smaller $L_2$). The algorithm then tries to find a BN by best-first search that minimizes $L$. This approach also has high time and space complexity.

For noisy-or BNs of binary variable, neural networks can be used to maximize the similarity between the probability distribution of the learned BN and the probability distribution of the case data. Existing works include Boltzmann Machine Model

[105], and Extended Hebbian Learning Model [125] etc. These approaches can learn structure while learning the causal strengths.

All the aforementioned approaches belong to the second, "Unknown structure, fully observable" learning task. "Fully observable" means a training sample is a complete instantiation of all variables involved. No one has investigated the learning of BN (either structure or parameter learning) with low-dimensional data (i.e., the samples are instantiations of subset of $X$).

## 2.3 Uncertainty for the Semantic Web

There are two different directions of researches related to handling uncertainty in semantic web. The first is trying to extend the current ontology representation formalism with uncertainty reasoning, the second is to represent probabilistic information using an OWL or RDF(S) ontology.

Earliest works have tried to add probabilities into full first-order logic [9, 64], in which syntax are defined and semantics of the result formalisms are clarified, but the logic was highly undecidable just as pure first-order logic. An alternative direction is to integrate probabilities into less expressive subsets of first-order logic such as rule-based (for example, probabilistic horn abduction [129]) or object-centered (for example, probabilistic description logics [66, 73, 76, 159, 56, 61, 87, 106, 40, 34, 68, 128]) systems. Works in the latter category are particularly relevant to our research because 1) description logics (DLs), as a subset of first-order logic, provide decidable and sound inference mechanism; and 2) OWL and several other ontology languages are based on description logics. An overview of approaches in this category is provided in Subsection 2.3.1.

While it is hard to define an "ontology of probability" in a general setting, it is possible to represent selected forms of probabilistic information using pre-defined

OWL or RDF(S) ontologies which are tailored to the application domains. Several existing works (e.g., [128, 51, 40]) in this topic will be presented in Subsection 2.3.2.

### 2.3.1 Uncertainty Modeling and Reasoning

Many of the suggested approaches to quantifying the degree of overlap or inclusion between two concepts are based on ad hoc heuristics, others combine heuristics with different formalisms such as fuzzy logic, rough set theory, and Bayesian probability (see [141] for a brief survey). Among them, works that integrate probabilities with DL-based systems are most relevant to ***BayesOWL***. These include:

- Probabilistic extensions to $ALC$ based on probabilistic logics [66, 73];
- Probabilistic generalizations to DLs using non-graphical models (e.g., 1) Lukasiewicz's works [87, 86] on combining description logic programs with probabilistic uncertainty; 2) Haarsler's generic framework [61] for DLs with uncertainty which unifies a number of existing works; 3) P-$SHOQ$(D) [56], a probabilistic extension of $SHOQ$(D) based on the notion of probabilistic lexicographic entailment; and 4) pDAML+OIL [106], an extension of DAML+OIL by mapping its models onto probabilistic Datalog while preserving as much of the original semantics as possible; etc.);
- Works on extending DLs with Bayesian networks (BNs) (e.g., 1) P-CLASSIC [76] that extends CLASSIC; 2) PTDL [159] that extends TDL (Tiny Description Logic with only "Conjunction" and "Role Quantification" operators); 3) PR-OWL [34] that extends OWL with full first-order expressiveness by using Multi-Entity Bayesian Networks (MEBNs) [82] as the underlying logical basis; 4) OWL_QM [128] that extends OWL to support the representation of probabilistic relational models (PRMs) [31] [55]; and 5) the work of Holi and Hyvönen [67, 68]

[31] A PRM specifies a probability distribution over the attributes of the objects in a relational database, which includes a relational component that describes schemas and a probabilistic component that describes the probabilistic independencies held among ground objects.

which uses BNs to model the degree of subsumption for ontologies encoded in RDF(S); etc.).

Next we introduce P-$SHOQ$(D) and P-CLASSIC, the two most important extensions, in more details, followed by a discussion of the works in the last category.

**Introduction to P-$SHOQ$(D)**

P-$SHOQ$(D) [56] is a probabilistic extension of $SHOQ$(D) [71], which is the semantics behind DAML+OIL (without inverse roles). In P-$SHOQ$(D), the set of individuals $I$ is partitioned into $I_C$ (the set of classical individuals) and $I_P$ (the set of probabilistic individuals). A concept is generic iff no $o \in I_P$ occurs in it. A probabilistic terminology $P = (P_g, (P_o)_{o \in I_p})$, which is based on the language of conditional constraints. $P_g = (T, D)$ is the generic probabilistic terminology where $T$ is a generic classical terminology and $D$ is a finite set of generic conditional constraints, $P_o$ is the assertional probabilistic terminology for every $o \in I_P$. A conditional constraint has the form $(D|C)[l, u]$, where $C$ and $D$ are concepts and real numbers $l, u \in [0, 1]$, $l < u$, it can be used to represent different kinds of probabilistic knowledge. For examples, $(D|C)[l, u]$ means "an instance of the concept $C$ is also an instance of the concept $D$ with a probability in $[l, u]$"; $(D|\{o\})[l, u]$ means "the individual $o \in I_P$ is an instance of the concept $D$ with a probability in $[l, u]$"; $(\exists R.\{o\}|C)[l, u]$ means "an arbitrary instance of $C$ is related to a given individual $o \in I_C$ by a given abstract role $R$ with a probability in $[l, u]$"; $(\exists R.\{o'\}|\{o\})[l, u]$ means "the individual $o \in I_P$ is related to the individual $o' \in I_C$ by the abstract role $R$ with a probability in $[l, u]$". The semantics of P-$SHOQ$(D) is based on the notion of probabilistic lexicographic entailment from probabilistic default reasoning. Sound, complete and decidable probabilistic reasoning techniques based on reductions to classical reasoning in $SHOQ$(D) and to linear programming are presented in [56].

**Introduction to P-CLASSIC**

P-CLASSIC [76] aims to answer any probabilistic subsumption queries as $\Pr(D|C)$: what is the probability that an object belongs to concept $D$ given that it belongs to concept $C$? It includes two components: a standard terminological component which is based on a variant of the CLASSIC description logic, and a probabilistic component which is based on Bayesian networks.

The non-probabilistic DL component does not contain "same-as" constructor but supports negation on primitive concepts which are different from CLASSIC. A terminology in P-CLASSIC only includes the concept definition part (for defined concepts), while concept introductions (for primitive concepts) are given as part of the probabilistic component. Also, the number of fillers for each role $R$ is bounded.

The probabilistic component of P-CLASSIC consists of a set $\boldsymbol{P}$ of p-classes, each p-class $P \in \boldsymbol{P}$ is represented using a Bayesian network $\mathbf{N}_P$, and one of the p-classes is the root p-class $P^*$, denoting the distribution over all objects. $P^*$ describes the properties of concepts, all other p-classes describe the properties of role fillers. In general, $\mathbf{N}_P$ contains 1) a node for each primitive concept $A$, which is either **true** or **false**, 2) a node FILLS(Q) for each attribute filler $Q$, which consists of a finite set of abstract individuals, 3) a node NUMBER(R) for each role $R$ (non-functional binary relation here), which specifies the number of R-fillers and takes on values between 0 and some upper bound $b_R$, and 4) a node PC(R) for each role R, whose values range over the set of p-classes for the properties of role fillers. Arcs in $\mathbf{N}_P$ may point from superconcepts to subconcepts, from concepts to those FILLS(Q), NUMBER(R), and PC(R) nodes, NUMBER(R) nodes may only be parents of corresponding PC(R) nodes, and PC(R) nodes can only be a leaf node. However, no formal methods about how to construct $\mathbf{N}_P$ and its topology are discussed.

The semantics of P-CLASSIC is an extension of the semantics of CLASSIC by interpreting a p-class as an objective (statistical) probability: each p-class is associated with a distribution over the interpretation domain. For any P-CLASSIC

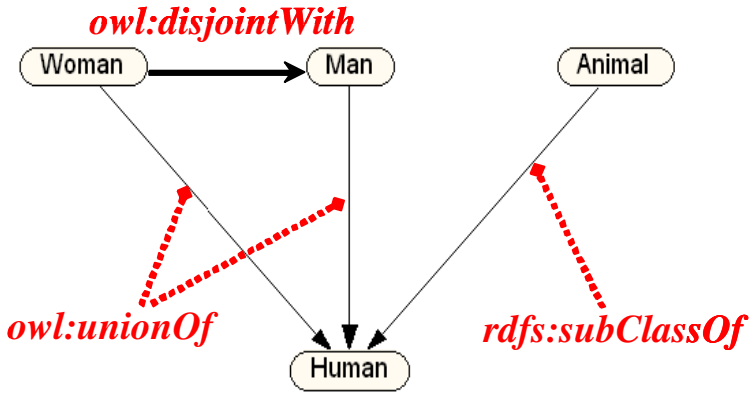
knowledge base $\triangle$ and any description $C$, there is a unique number $\rho \in [0, 1]$ such that $\Delta \models (\Pr(C) = \rho)$. A sound and complete inference algorithm "ComputeProbability" is provided to compute $\rho$. However, the complexity of the inference algorithm is no longer polynomial if P-CLASSIC is extended to handle $\bigvee$ (disjunction), $\exists$ (existential quantification), negation on arbitrary concepts (not only primitive ones), and qualified number restrictions.

P-CLASSIC has been used in [90] to provide a probabilistic extension of the *LCS* (least common subsumer) operator for description logic *ALN*. The framework of P-CLASSIC has also been extended, in somewhat different settings, to probabilistic frame-based systems [78] which annotates a frame with a local probabilistic model (a BN representing a distribution over the possible values of the slots in the frame) and object-oriented Bayesian networks (OOBN) [77, 127] which describes complex domains in terms of inter-related objects by combining clear declarative probabilistic semantics with many of the organizational benefits of an object-oriented framework.

**Discussion about Existing BN-Based Approaches**

PTDL [159] uses a simple description logic to extend the capabilities of BNs, it is most closely allied to P-CLASSIC [76], but different in the way of handling role quantifications. Neither of the two works has provided any mechanism to construct CPTs. They assume that CPTs will be assigned by domain experts. However, it is often difficult and sometimes even impossible for human experts to assign a CPT to a node if this node has large number of parents or its parents come from different sources. For example, as in Fig. 2.5, if "Human" is the union of two disjoint concepts "Woman" and "Man", as well as a subclass of "Animal", by using P-CLASSIC, the translated network will have arcs going into "Human" from all the other three, and there is no way to specify some entries in "Human"'s CPT (e.g., $\Pr(Human = True | Woman = False, Man = True, Animal = False)$ can not be specified since a

man must be an animal according to the defined relations.).




| Woman | Man | Animal | True | False | |
|---|---|---|---|---|---|
| True | True | True | | | contradictory |
| True | True | False | | | contradictory |
| True | False | True | 1.000 | 0.000 | |
| True | False | False | | | contradictory |
| False | True | True | 1.000 | 0.000 | |
| False | True | False | | | contradictory |
| False | False | True | 0.000 | 1.000 | |
| False | False | False | 0.000 | 1.000 | |

Fig. 2.5: **CPT Construction Problem of P-CLASSIC**

PR-OWL and OWL_QM are similar in spirit, but OWL_QM is specialized to the Quiddity*Modeler [32] toolset developed by IET [33] and thus provides a smaller extension with less parsing and reasoning support. While PR-OWL extends OWL with full MEBN-logic [82], P-CLASSIC and PTDL use the standard BN model.

The work of Holi and Hyvönen [67, 68] models an RDF(S) concept subsumption with arcs from child subconcept nodes to parent superconcept nodes, and places one node for each possible concept overlap. The translated BN will be extremely large and complicated when there are many relations and overlaps among concepts. And same as P-CLASSIC and PTDL, it would be extremely painful for a domain expert to assign CPTs for each of the nodes.

[32] `http://www.iet.com/quiddity.html`
[33] Information Extraction and Transport, Inc.

On the other side, to deal with vague and imprecise knowledge, research in extending description logics with fuzzy reasoning has gained some attention recently. Interested readers may refer to [139, 140, 116, 2, 91, 138] for a rough picture about this topic.

### 2.3.2 Representation of Probabilistic Information

Not many works exist in this field, according to googling [34] or swoogling [35] on the web, it is not surprising that one can not even find a simplest ontology of probability or for annotating probabilistic information.

The work of Fukushige [50, 51] proposes a vocabulary for representing probabilistic relationships in an RDF graph which is to be mapped to a Bayesian network (BN) to perform inference on it. Three kinds of probabilistic information can be encoded in his framework: probabilistic relations (prior), probabilistic observation (data), and probabilistic belief (posterior). And any of them can be represented using probabilistic statements which are either conditional or unconditional. Compared to the "XML Belief Network File Format" (XBN) [36], his work is more on getting an extended vocabulary which can describe probabilistic relations in a way that is both semantic web compatible and easy to map to a BN, instead of just representing BNs by inventing a new format [37].

Unlike Fukushige's work, in this research we do not treat "prior" (probabilistic relation), "data" (probabilistic observation), "posterior" (probabilistic belief) differently, instead, we focus on the mathematical foundations of the discrete probability theory, where a piece of probabilistic information is either "prior" or "conditional".

The OWL_QM [128] system also includes an OWL implementation of PRM con-

[34] `http://www.google.com`

[35] `http://swoogle.umbc.edu`

[36] `http://research.microsoft.com/dtas/bnformat/default.htm`

[37] Which is, not that meaningful, since there are a bunch of well- and widely-used BN file formats already.

structs about facets, slot chains, an owl class named "ProbabilisticRelationship" for casual relations, and a set of vocabularies to define the probability distributions or tables in a probabilistic relationship. The "ProbabilisticRelationship" class is defined with three object properties: "parent_PR", "child_PR", and "slotList_PR". A user can also specify variable discretizations for a continuous variable. A "Conditional-ProbabilityTable" has values stored in instances of "CPTCell", and each "CPTCell" associates an attribute-value-pair list with a decimal probability value.

However, this representation is specific to the OWL_QM system, so that it can not be used to other places without modification. In this research we intend to define an ontology for annotating probabilistic information in more general forms, thus can be grabbed and used by anybody.

## 2.4 IPFP: Iterative Proportional Fitting Procedure

The well-known **iterative proportional fitting procedure** (***IPFP***) can be used to find a distribution which satisfies a set of consistent low-dimensional probabilistic constraints and is as close as to the original distribution. It was first published by Kruithof in [79] in 1937, and in [36] it was proposed as a procedure to estimate cell frequencies in contingency tables under some marginal constraints. In 1975, Csiszar [33] provided an ***IPFP*** convergence proof based on I-divergence geometry. Vomlel rewrote a discrete version of this proof in his PhD thesis [152] in 1999. ***IPFP*** was extended in [18, 31] as conditional iterative proportional fitting procedure (***C-IPFP***) to also take conditional distributions as constraints, and the convergence was established for the discrete case. In this section we will present the ***IPFP*** and ***C-IPFP*** in a way that is easier to be understood by non-math major readers. Subsection 2.4.1 gives some definitions in probability theory, which will be used in the definitions of ***IPFP*** and ***C-IPFP*** in Subsection 2.4.2 and throughout the rest

of the thesis.

### 2.4.1 The ABCs of Probability

We start this subsection with the notations and definitions used for discrete probability distributions in this text.

**Definition 2.1 (Random Experiment)** In probability theory, a random experiment is one whose outcome can not be predicted with certainty and can be repeated indefinitely under essentially the same conditions.

**Definition 2.2 (Sample Space)** The sample space (denoted as $\Omega = \{\omega\}$) of a random experiment is a set of all possible outcomes. For example, for tossing a single die, $\Omega$ is $\{1, 2, 3, 4, 5, 6\}$; for tossing a single coin, $\Omega$ is $\{head, tail\}$.

**Definition 2.3 (Random Event)** A random event E is a subset of $\Omega$ (or set of outcomes) to which a probability is assigned. An elementary random event is a single-element subset of $\Omega$ which contains only one of the outcomes. A given random event occurs in a random experiment only if the outcome of this random experiment is an element of this random event, and probability is defined to be a measure of how likely this random event is to occur.

**Definition 2.4 (Probability Measure)** Mathematically, a probability measure "Pr" of a random experiment is a real-valued function from the collections of random events to real numbers among [0..1]. The empty set (denoted as $\emptyset$) is an event which never occurs and defined to have the probability of **0**, the sample space $\Omega$ itself is an event which always occurs and defined to have the probability of **1**. Also, the probability of a union of a finite or countably infinite collection of disjoint random

events is the sum of the corresponding probabilities, i.e., $\Pr(\cup \mathrm{E_j}) = \sum_j \Pr(\mathrm{E_j})$ if $\{\mathrm{E_j}\}$ is a countable, pairwise disjoint collection of random events.

**Definition 2.5 (Probability Space)** A probability space is defined as a triple of $(\Omega, \Lambda, \Pr)$, and $\Lambda = \{\mathrm{E}\}$ is a set of random events and a $\sigma$-algebra on $\Omega$.

**Definition 2.6 (Discrete Random Variable)** A random variable $X_i$ is a function from $\Omega$ to another set T. Usually $\mathrm{T} \subseteq \Re$, a set of all real values. A random variable $X_i$ is discrete if T has a finite [38] set of possible values. For example, for tossing a single die, both $\Omega$ and T are $\{1, 2, 3, 4, 5, 6\}$, and a random variable $X_i$ can be defined as $X_i(\omega) = \omega$.

**Definition 2.7 (Probability Distribution of Discrete Random Variable)** The probability distribution of a random variable $X_i$ must be defined such that:

1. $\Pr(X_i = x_i) \geq 0$,
2. $\sum_{x_i} \Pr(X_i = x_i) = 1$ as $x_i$ runs through the set of all possible values of $X_i$, and
3. $\Pr(\mathrm{E}) = \sum_{\omega_i \in \mathrm{E}, X_i(\omega_i) = x_i} \Pr(X_i = x_i)$, and $E$ is a random event.

**Definition 2.8 JPD (Discrete Joint Probability Distribution)** Let $X = \{X_1, ..., X_n\}$ be a set of random variables, $\Pr(X) = \Pr(X_1, ..., X_n)$ denotes a $n$-dimensional joint probability distribution if for every $x = (x_1, ..., x_n) \in X$ [39], $0 \leq \Pr(x) = \Pr(X_1 = x_1, ..., X_n = x_n) \leq 1$ and $\sum_{x \in X} \Pr(X = x) = 1$ as $x$ runs through all possible assignments of $X$.

[38] In this text we do not consider the case of "countable infinite".

[39] We use a "$\in$" here only for convenience, or, $X$ is used for both "set of variables" and "set of different instantiations of all variables"

**Definition 2.9 MPD (Marginal Probability Distribution)** Let $X_K \subseteq X$, $\Pr(X_K)$ is defined as a marginal probability distribution of $\Pr(X)$ if

$$\Pr(x_K) = \sum_{y \in X, y^{X_K} = x_K} \Pr(y)$$

as $x_K$ runs through all possible assignments of $X_K$, and $y^{X_K}$ denotes a vector of variables' values with size $|X_K|$ from an assignment $y$ of $X$ (and these variables has one-to-one correspondences with variables in $X_K$). If $X_K = \emptyset$ then $\Pr(X_K) = 1$.

**Definition 2.10 CPD (Conditional Probability Distribution)** Let $X_A, X_B \subseteq X$ be disjoint, $X_A$ is nonempty, $\Pr(X_A|X_B)$ is defined as a conditional probability distribution of $\Pr(X)$ if $\Pr(x_A|x_B) \cdot \Pr(x_B) = \Pr(x^{X_A \cup X_B})$ for all assignments of $X_A$ and $X_B$. If $\Pr(X_B) = 0$ then $\Pr(X_A|X_B)$ is undefinite.

**Definition 2.11 (Probabilistic Conditional Independence)** Let $X_A, X_B, X_C \subseteq X$ be pair-wise disjoint and $X_A$ and $X_B$ are nonempty, $X_A$ is conditionally independent of $X_B$ given $X_C$ iff $\Pr(X_A, X_B|X_C) = \Pr(X_A|X_C) \cdot \Pr(X_B|X_C)$, i.e., $\Pr(X_A, X_B, X_C) \cdot \Pr(X_C) = \Pr(X_A, X_C) \cdot \Pr(X_B, X_C)$.

In this text, the distance between two JPDs is measured by *I-divergence* and *total variance*, which are defined as below.

**Definition 2.12 (I-divergence)** Let $\mathfrak{P}$ be the set of JPDs over $X = \{X_1, ..., X_n\}$, and $P$, $Q \in \mathfrak{P}$, *I-divergence* (also known as *Kullback-Leibler divergence* or *Cross-entropy*, which is often used as a distance measure between two JPDs) is defined as:

$$I(P\|Q) = \begin{cases} \sum\limits_{x \in X, P(x) > 0} P(x) \log \frac{P(x)}{Q(x)} & if\ P \ll Q \\ +\infty & if\ P \not\ll Q \end{cases} \tag{2.1}$$

here $P \ll Q$ means $P$ is **dominated** by $Q$, i.e.

$$\{x \in X | P(x) > 0\} \subseteq \{y \in X | Q(y) > 0\}$$

where $x$ (or $y$) is an assignment of $X$, or equivalently:

$$\{y \in X | Q(y) = 0\} \supseteq \{x \in X | P(x) = 0\}$$

since a probability value is always non-negative. The dominance condition in Eq. 2.1 guarantees division by zero will not occur because whenever the denominator $Q(x)$ is zero, the numerator $P(x)$ will be zero. Note that *I-divergence* is zero if and only if $P$ and $Q$ are identical and *I-divergence* is non-symmetric.

**Definition 2.13 (Total Variance)** Let $\mathfrak{P}$ be the set of JPDs over $X = \{X_1, ..., X_n\}$, and $P$, $Q \in \mathfrak{P}$, the *total variance* between $P$, $Q$ is defined as:

$$|P - Q| = \sum_{x \in X} |P(x) - Q(x)| \tag{2.2}$$

where $x$ is an assignment of $X$, and *total variance* is symmetric and be zero only if $P$ and $Q$ are identical.

**Theorem 2.1 (Lower Bound on I-divergence by Total Variance)** If $P, Q \in \mathfrak{P}$ are two JPDs over $X = \{X_1, ..., X_n\}$, then the following inequality holds [152]:

$$|P - Q| \leq 2\sqrt{I(P\|Q)} \tag{2.3}$$

Next, definitions of *I-projection*s are provided before introducing the details of ***IPFP*** in the next subsection.

**Definition 2.14 (I-projection)** Probability distributions from a given set minimizing *I-divergence* with respect to a given distribution are called *I-projection*s. Let $\mathfrak{P}$ be the set of JPDs over $X = \{X_1, ..., X_n\}$. The $I_1$-*projection* of a JPD $Q \in \mathfrak{P}$ on a given set of JPDs $\boldsymbol{\varepsilon} \subseteq \mathfrak{P}$ is a JPD $P \in \boldsymbol{\varepsilon}$ such that the *I-divergence* "$I(P\|Q)$" is minimal among all JPDs in $\boldsymbol{\varepsilon}$. Similarly, the $I_2$-*projection*s of $Q$ on $\boldsymbol{\varepsilon}$ are JPDs in $\boldsymbol{\varepsilon}$ that minimize the *I-divergence* "$I(Q\|P)$". We denote the $I_1$-*projection* as $\pi_{\boldsymbol{\varepsilon}}Q$ and the $I_2$-*projection* as $\pi'_{\boldsymbol{\varepsilon}}Q$. In this text, the convergence proof and geometry of *I-divergence* are using $I_1$-*projection*, and two theorems about $I_1$-*projection* are presented below.

**Theorem 2.2 (Three Points Property)** A JPD $R \in \boldsymbol{\varepsilon}$ is an $I_1$-*projection* of $Q \in \mathfrak{P}$ iff for every other $P \in \boldsymbol{\varepsilon}$, the "Three Points Property" holds [152]:

$$I(P\|Q) = I(P\|R) + I(R\|Q) \tag{2.4}$$

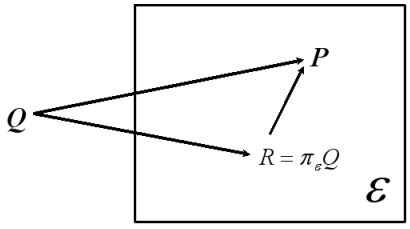



Fig. 2.6: **Three Points Property**

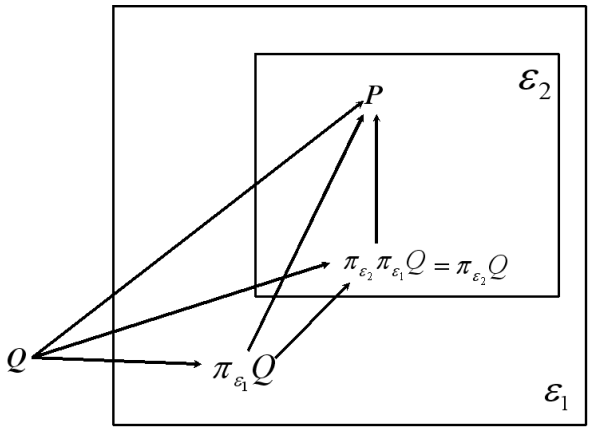



Fig. 2.7: **$\mathbf{I_1}$-projection on a Subset**

**Theorem 2.3 ($I_1$-projection on a Subset)** Let $\boldsymbol{\varepsilon_2} \subseteq \boldsymbol{\varepsilon_1}$ be two sets of JPDs over $X = \{X_1, ..., X_n\}$ and $Q \in \mathfrak{P}$ be a given JPD such that there exists a JPD $P \in \boldsymbol{\varepsilon_2}$ and $P \ll Q$, then the following equations holds [152]:

$$\pi_{\boldsymbol{\varepsilon_2}} \pi_{\boldsymbol{\varepsilon_1}} Q = \pi_{\boldsymbol{\varepsilon_2}} Q \tag{2.5}$$

Note that $I_1$-*projection* is unique but $I_2$-*projection* in general is not. If $\boldsymbol{\varepsilon}$ is the set of all JPDs that satisfies a set of given constraints, the $I_1$-*projection* $P \in \boldsymbol{\varepsilon}$ of $Q$ is a distribution that has the minimum distance from $Q$ while satisfying all constraints [152]. In this text, we will focus our attention on $I_1$-*projection* only.

### 2.4.2 IPFP and C-IPFP

In this subsection we presents the well-known **iterative proportional fitting procedure** (***IPFP***) for finding the $I_1$-*projection* of an initial distribution to a consistent set of probabilistic constraints, and its extension ***C-IPFP*** for handling conditional probabilistic constraints.

**Definition 2.15 (IPFP)** Let $X = \{X_1, X_2, ..., X_n\}$ be a space of $n$ discrete random variables and $\mathfrak{P}$ be the set of JPDs over $X$, given a consistent set of $m$ MPDs $\{R_i(Y^i)\}$ where $X \supseteq Y^i \neq \emptyset$ and an initial JPD $Q_{(0)} \in \mathfrak{P}$, **iterative proportional fitting procedure** (***IPFP***) is a procedure for determining a JPD $P(X) = P(X_1, X_2, ..., X_n) \in \mathfrak{P} \ll Q_{(0)}$ satisfying all constraints in $\{R_i(Y^i)\}$ by repeating the following computational process over $k$ and $i = ((k-1) \bmod m) + 1$:

$$Q_{(k)}(X) = \begin{cases} 0 & if\ Q_{(k-1)}(Y^i) = 0 \\ Q_{(k-1)}(X) \cdot \frac{R_i(Y^i)}{Q_{(k-1)}(Y^i)} & if\ Q_{(k-1)}(Y^i) > 0 \end{cases} \tag{2.6}$$

This process iterates over distributions in $\{R_i(Y^i)\}$ in cycle. It can be shown [152] that

in each step $k$, $Q_{(k)}(X)$ is an $I_1$-*projection* of $Q_{(k-1)}(X)$ that satisfies the constraint $R_i(Y^i)$ [40] and $Q^*(X) = \lim_{k\to\infty} Q_{(k)}(X)$ is an $I_1$-*projection* of $Q_{(0)}$ that satisfies all constraints, i.e., $Q_k(X)$ converges to $Q^*(X) = P(X) = P(X_1, X_2, ..., X_n)$.

**Definition 2.16 (C-IPFP)** ***C-IPFP*** from [18, 31] is an extension of ***IPFP*** to allow constraints in the form of CPDs, i.e. $R_i(Y^i|Z^i)$ where $Y^i$, $Z^i \subseteq X$. The procedure can be written as:

$$Q_{(k)}(X) = \begin{cases} 0 & if\ Q_{(k-1)}(Y^i|Z^i) = 0 \\ Q_{(k-1)}(X) \cdot \frac{R_i(Y^i|Z^i)}{Q_{(k-1)}(Y^i|Z^i)} & if\ Q_{(k-1)}(Y^i|Z^i) > 0 \end{cases} \tag{2.7}$$

***C-IPFP*** has similar convergence result [31] [41] as ***IPFP*** and Eq. 2.6 is in fact a special case of Eq. 2.7 with $Z^i = \emptyset$.

## 2.5 Other Related Works

Today data or information can be retrieved from many different sources, such as databases, web, knowledge bases, and other specific information systems. In order to answer user queries, the interoperability between different computer systems or agents can be solved by integration of the heterogeneous information sources. Heterogeneity problem can be classified into 4 levels [135]: the **system** level heterogeneity is about the physical layer of the systems such as incompatible hardware, network communication etc, the **syntactical** level heterogeneity refers to the different data representations or languages used, the **structural** level heterogeneity refers to the different data models used, and the **semantic** level heterogeneity refers to the meaning of the concepts defined. There are many technologies (for example, CORBA, DCOM,

[40] But $Q_{(k)}(X)$ may violate other constraints, so we need to have many iterations over each of the constraints.

[41] Pages 14 to 16 in this paper. Interested readers may also refer to [33] for a more mathematical explanation.

XML technologies, or other middleware software products) developed to solve the first three levels of heterogeneity, while semantic heterogeneity requires more complicated methods and satisfactory solutions have yet to emerge.

A standard way to achieve information integration is to build a global schema over all the related heterogeneous information sources, then user or agent queries will point to this global schema. This global integrated schema approach is often used in federated databases and data warehousing, and is sometimes called "data warehousing approach" [150]. In general, is very difficult to construct a global schema from individual database schemas, and even harder for other kind of information sources. Also, if any of the existing information sources is changed, the global schema need to be constructed all over again, this is inefficient and a waste of the computational resource.

An alternative "on-demand driven" [150] approach is to answer user queries and other requests on-demand by combining or joining information obtained from different sources at runtime based on the mediator architecture [4, 95, 155]. A common data model about the application domain and a common query language based on the model is required. This approach is more scalable, flexible and dynamic. A number of systems have been built using this approach, including SIMS from USC [3], TSIMMIS from Stanford [52], Information Manifold from AT&T [111], Garlic from IBM [118], DISCO from Bull-INRIA [145], HERMES from Army Research [144], Infomaster from Stanford [54], InfoSleuth from MCC [13] (based on the Carnot [157] technology), COIN from MIT [21, 22, 57], MOMIS from Italy [15, 14], the OBSERVER system [97] (based on inter-ontology relationships such as synonyms, hyponyms, hypernyms for semantic information brokering), OntoBroker from Germany [35], the DWQ project [24, 25, 23], the BUSTER [42] project and KRAFT from UK [151], etc.

Two methods are commonly adopted in implementing "on-demand driven" ap-

[42] http://www.semantic-translation.de/

proach. The first one is an "eager" paradigm, which collects all the data before answering any queries, while the second is a "lazy" approach, which postpones information collection to query evaluation stage. Most systems in existence today prefer the "lazy" approach, since it is more scalable, and easier to maintain consistency. However, in the core of both methods are algorithms for information combination or translation.

To solve the problem of information integration, how to deal with semantic heterogeneity is the key part. In next subsection I will focus on the approaches that have been developed for semantic integration, especially ontology merging, matching, or translation.

### 2.5.1 Ontology-Based Semantic Integration

The Semantic Web puts the onus of ontology creation on the user by providing common ontology languages such as RDF(S) and OWL. However, ontologies defined by different applications or agents usually describe their domains in different terminologies, even when covering the same domain. The semantic-level heterogeneity between two information sources refers to the use of conflicted or mismatched terms about concepts in their corresponding ontologies, which can be classified into the following categories:

- *ambiguous reference* – the same term (i.e., the symbolic identifier of a concept in an ontology) means differently in different ontologies;
- *synonymical reference* – two terms of different ontologies have the same meaning;
- *one-to-many matching* – one term of one of the ontologies matches [43] to several terms of the other ontology;

[43] 'match' means that the subject and the object refer to exactly the same concept.

- *uncertain matching* – one term of one of the ontologies has similar but not exactly the same meaning to any terms of the other ontology; and

- *structural difference* – two terms with the same or similar meaning are structured differently in different ontologies (e.g., different paths from their respective root concepts).

In order to support ontology-based information integration, tools and effective mechanisms are needed to resolve the semantic heterogeneity problem and align the terms in different ontologies. This subsection briefly reviews the existing works in this topic, which is grouped into five different research directions in tackling the problem.

- **One Centralized Global Ontology.** Enforcing one centralized global ontology prevents semantic heterogeneity since no more ontology exists and everyone is using the same ontology. However, this approach is obviously impractical since 1) the creation and maintenance of such an ontology is usually prohibitively expensive and 2) it is usually impractical to develop an ontology with consent from the user community at large. A user may wish to express his or her own point of view about the domain for his or her own purpose.

- **Merging Ontologies.** Merging different ontologies into a unified one is another natural approach to semantic integration when those ontologies overlap significantly over a common domain. There are many heuristics to merge two terms, such as 1) linguistic heuristics which uses term spelling or additional natural language processing (NLP) techniques with manual validation, e.g., *FCA-MERGE* [143, 142], 2) syntactic and semantic heuristics, e.g., *PROMPT* [108] [44] and *Chimaera* [94], and 3) hybrid approaches [72]. However, this approach is usually costly and not scalable. The merging procedure has to restart from

[44] It initializes term-matching suggestions using linguistic similarity among class names, and then updates suggestions automatically by resolving newly detected syntactic and semantic conflicts.

scratch when any of the input ontologies has been modified. When merging a large number of ontologies, the merging result may not always meet the need of the application.

- **Mapping Ontologies.** Building a set of mappings (or matches) between two ontologies is an alternative way to merging ontologies. A mapping between two terms from two different ontologies conveys the fact that the terms have similar or the same meaning. Besides manually specifying mappings, there are some semi-automated methods such as: 1) lexical similarity analysis on linguistic or lexical ontologies [59, 75, 148] such as WordNet, Cyc, and SENSUS; 2) textual description analysis, which assigns a set of relevant documents to each term so as to capture the meaning of the term, measures similarity between terms using machine learning based text classification techniques, and searches for mappings based on the similarity matrix obtained, e.g., *CAIMAN* [80], *OntoMapper* [130], and *GLUE* [42, 44, 43, 45]; 3) ontology algebra and articulation, e.g., *SKAT* [103], *ONION* [104], which are semi-automatic, with good scalability, easy to maintenance, but slow; 4) information flow and channel theory based approach [74]; 5) structural analysis, i.e., 'similarity flooding' – a graph matching algorithm based on fixpoint computation [96]; and 6) hybrid heuristics, sometimes combined with the structural information of the ontology taxonomy, e.g., *Anchor-PROMPT* [109] and *PROMPTDIFF* [110]. Ehrig and Sure [48] presents an approach to integrate various similarity measures in ontology mapping. A brief survey of existing approaches is provided by [107], however, most of these approaches only study exact mappings, without taking the degree of uncertainty [45] into consideration [46]. Since semantic similarities

[45]It is often the case that a concept defined in one ontology can only find partial matches to one or more concepts in another ontology

[46]Note that the methods in (ii) fail to completely address uncertainty in mapping since the degree of similarity found between concepts will not be considered in further reasoning

between concepts can be easily represented probabilistically (but not logically), Bayesian Networks (BNs) [121] stand out as a natural choice in tackling this problem: 1) Mitra et al. [101, 102] improve existing mapping results by applying a set of meta-rules to capture the structural influence and the semantics of ontology relations; and 2) Ding et al. [41] and Pan et al. [117] proposed a principled methodology by first translating the source and target ontologies into BNs, and then mapping the concepts from the two ontologies based on evidential reasoning between the two translated BNs. Note that [6] reports some methods on mapping evaluation.

- **Ontology Translation.** Given two ontologies, ontology translation is to translate one of the ontologies into a target ontology which uses the representation and semantics of the other ontology, sometimes with the help of an intermediate shared ontology. Based on a set of defined rules and transformation operators, *Ontomorph* [27] offers syntactic rewriting and semantic rewriting to support the translation between two different knowledge representation languages. *OntoMerge* [47], an online ontology translation system [47] based on ontology merging (which requires a set of ontology bridging axioms produced manually by domain experts) and automated reasoning, achieves term translations using a first order theorem prover built on top of PDDAML (PDDL-DAML Translator) [48] (based on Jena) and OntoEngine [49] (an inference engine based on JTP), in either forward or backward chaining way. Ontology translation takes a further step after mapping or merging, and is one of the most difficult tasks towarding information integration.

- **Runtime Ontology Resolution.** Semantic differences can arise during runtime interaction in a multi-agent environment since it is impractical to restrict

[47] http://cs-www.cs.yale.edu/homes/dvm/daml/ontology-translation.html
[48] http://www.cs.yale.edu/homes/dvm/daml/pddl_daml_translator1.html
[49] http://projects.semwebcentral.org/projects/ontoengine/

all agents to use the same ontology. None of merging, mapping, or translating ontologies is practical since they are usually offline approaches which need to be done before the deployment of a multi-agent system. One family of approaches [156, 11, 10, 126] is inspired by language games, where agents identify and resolve ontology conflicts through incremental interpretation, clarification, and explanation by negotiating with one another when semantic differences have been detected. An alternative approach utilizes approximate classification methods for semantic-preserving context transformations, such as rough set theory, fuzzy set, or probabilistic Bayes' Theorem [28, 141].

Since the interoperability between different knowledge systems or agents relies on their full understanding of the terminologies used by peers, the resolution of semantic heterogeneity between different information sources is necessary and important. Hence, this aspect currently attracts significant attention from the Semantic Web research community.

### 2.5.2 Database Schema Integration

Ontologies and database schemas are very closely related, they serve different purposes but have very similar functionalities. Ontology can be considered as a kind of conceptual schema, and the ontology language can be treated as the corresponding conceptual data model. Although ontology is syntactically and semantically richer than common database schema, methodologies or ideas emerged from schema integration are worth to investigate and some can be adopted to solve the semantic integration problem. This section gives a brief overview of existing works in schema integration field. Schema integration, especially database schema integration, is a well-developed area for which many mature approaches have been developed (e.g., [5, 12, 15, 16, 53, 62, 84, 89, 98, 115, 134, 63]). Database schema integration tries to construct a global view from a set of given schemas with different structures and

terminologies.

An operation that plays an important role in schema integration is "match", which finds mappings between elements of two source schemas, since a first step in integrating schemas is to identify those inter-schema relationships between their elements. A classification of schema matching approaches is given in [132]:

- Instance-level vs. Schema-level: Instance-level matching also takes consideration of data contents while schema-level matching only cares about schema information.
- Element-level vs. Structure-level: Element-level matching performs 'match' for individual schema elements, while the latter can perform 'match' for complex schema structures.
- Linguistics-based vs. Constraint-based: The former approach is based on linguistic knowledge of the names and descriptions about elements, while the latter is based on keys and relationships among elements.
- Matching cardinality (1:1, 1:n, n:1, n:m)
- The use of auxiliary information.

SemInt [84, 85] is an instance-based element-level matching prototype with 1:1 match cardinality. It uses a neural network to determine matching candidates, this method takes no consideration of structures. TransScm [98] transforms input schemas into labelled graphs, applies multiple handcrafted matching rules at each node, and performs top-down match node by node, it is a schema-based element-level matching prototype with 1:1 match cardinality. This method performs well when two schemas are very similar.

DIKE [113, 114, 112, 115] is based on the principle that nearby elements will influence a match more than the ones farther away. It uses a linguistic matching

algorithm to automatically determine synonym and inclusion (is-a, hypernyms) relationships between elements by performing a pairwise comparison based on a set of manually-specified synonym, homonym and inclusion properties with a "plausibility factor" between **0** and **1**. ARTEMIS [16, 26] matches elements based on their name affinity and structure affinity, it serves as the schema integration component of the MOMIS [15, 14] mediator system. Cupid [89] models the interconnected elements of a schema as a schema tree, computes the similarity coefficients (which is in [0, 1]) between the elements of the source schemas in three phases and then derived mappings from these coefficients. The first is the linguistic matching phase, which, with the help of a thesaurus, produces a linguistic similarity coefficient ($lsim$); the second is the structural matching phase, which, based on the similarity of the elements' contexts or vicinities, produces a structural similarity coefficient ($ssim$); in the final phase, the weighted similarity ($wsim$) is computed according to: $wsim = wstruct * ssim + (1 - wstruct) * lsim$ ($wstruct$ is in [0, 1]). The pair of schema elements with maximal weighted similarity will be identified as a mapping. All of DIKE, ARTEMIS and Cupid are hybrid schema-based matching prototypes with both element- and structure-level matching.

Unlike above methods, Automatch [17] uses machine learning techniques to automate schema matching. Examples are attached to schema nodes by domain experts, statistical feature selection techniques are used to learn an efficient representation of the examples, the learned probabilistic knowledge is stored in a KB called "attribute dictionary" and used to find an optimal matching based on Bayesian learning.

There are many other works in this area such as the ones described in [5, 53, 62, 63]. Same as semantic integration, most works here are semi-automatic, either need user to specify some initial information, or to validate results. [132] provides a survey of approaches to automatic schema matching.

## 2.6 Summary

This chapter provides an overview on five research areas that are closely related to our work presented in this dissertation: 1) an introduction to semantic web, ontology, and description logics (DLs); 2) an introduction to Bayesian belief networks (BNs) and their inference and learning methods; 3) a survey of existing works on uncertainty reasoning for knowledge representation, especially for the semantic web; 4) a simple introduction to the "**iterative proportional fitting procedure**" (***IPFP***) and its extension ***C-IPFP***; and 5) a survey of existing works on information integration, especially on ontology-based semantic integration and database schema integration.

Uncertainty modeling and reasoning for the semantic web was rarely addressed, until the first publication of our initial results on ***BayesOWL*** in January 2004 [38]. Moreover, at that time, no proposal has been made to represent probabilistic information using RDF(S) or OWL. To realize the true Semantic Web vision and its full potential, effective and theoretically well-founded mechanism for uncertainty reasoning arise as an inevitable demand among semantic web researcher and developers. Our work, ***BayesOWL***, is one of the pioneers in this field.

In parallel, existing ***IPFP*** and ***C-IPFP*** work only on full joint probability tables, which is extremely time- and space-consuming. In case that JPDs are given as BNs, how can one modify the BNs to satisfy a given set of probabilistic constraints by only changing their CPTs and make the resulting BNs have JPDs as close as to the original JPDs? We extend ***IPFP*** and ***C-IPFP*** to ***E-IPFP***, ***D-IPFP***, and ***SD-IPFP*** to reduce the computational cost, as well as to handle JPDs represented by BNs. Since ***BayesOWL*** uses ***SD-IPFP*** for its CPT construction, in next chapter, we will present our work in extending ***IPFP*** and ***C-IPFP*** first.

# Chapter 3

# Modifying Bayesian Networks by Probabilistic Constraints

Consider a Bayesian network (BN) [121] $\mathcal{N}$ on a set of $n$ variables $X = \{X_1, ..., X_n\}$ that models a particular domain. $\mathcal{N}$ defines a JPD $P(X)$. Suppose you are given a probability distribution $R(Y)$ on a non-empty subset of the variables $Y \subseteq X$ and $R(Y)$ does not agree with $P(X)$ (i.e., $P(Y) \neq R(Y)$, $P(Y)$ denotes the MPD of $P(X)$ on $Y$). Is it possible to change $\mathcal{N}$ to $\mathcal{N}'$ so that its distribution $P'(X)$ satisfies $R(Y)$? Can you do so with more than one such probabilistic constraints $R_1(Y^1), R_2(Y^2),\ ...,\ R_m(Y^m)$? Can you do so if the constraints given are in the form of CPDs (i.e., $R(Y|Z)$ *and* $Y, Z \subseteq X, Y \cap Z = \emptyset, Y \neq \emptyset, Z \neq \emptyset$)? Moreover, can you do so by only modifying CPTs of $\mathcal{N}$ (i.e., $\mathcal{N}$ and $\mathcal{N}'$ have the same structure)?

Problems of this kind can be found in designing new BNs, merging small BNs into a large one, or refining an existing one with new or more reliable probabilistic information. For example, when designing a BN for heart disease diagnosis, it is relatively easy to obtain a consensus among domain experts on what factors affect heart diseases and how they are causally related to one another. This knowledge of qualitative associations can then be used to define the networks structure, i.e., the DAG of the BN.

However, it is not that easy to obtain the CPTs for each of the variables. Experts' opinions are often coarse (e.g., in Fig. 3.1, the likelihood of $A$ causes $B$ is "high" but that of $C$ causes $B$ is "low"), not in a uniform scale (e.g., "high" given for one association may not mean exactly the same for another association), not in the form of CPTs (e.g., in Fig. 3.1, not the likelihood of causing $B$ by the combination of

all possible states of $A$ and $C$). Learning CPTs from statistical data is also often problematic. Most learning methods require samples of complete instantiations of all variables (i.e., fully observable), but in many real word applications, especially those involving a large number of variables, statistical data are fragmented, represented by, say, a number of low-dimensional distributions over subsets of the variables. In the heart disease example (see Fig. 3.1), one may obtain a distribution of *drinking* and *heart diseases* from a survey concerning effects of drinking on people's health, and a distribution of *smoking* and *heart diseases* from a survey concerning effects of smoking on people's health. But none of the surveys includes both *drinking* and *smoking*, two of the important causal factors to *heart diseases*. Moreover, a new survey on drinking with larger samples and improved survey methods may give a more accurate distribution of *drinking* and *heart diseases*, the BN needs to adapt itself to the new data. This kind of needs to modifying BNs to satisfy certain probabilistic constraints by only changing its CPTs arises very often in many domains, especially in diagnosis and sociology research.

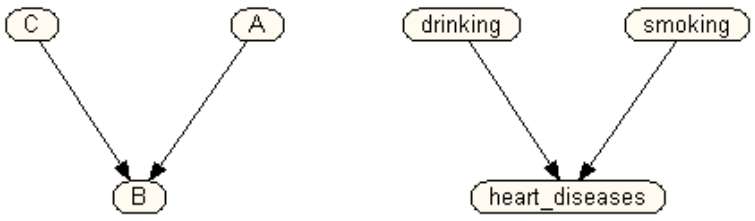



Fig. 3.1: **Two Simple BNs**

One would think this kind of BN modification tasks can be accomplished by applying ***IPFP*** [1] on the JPD of the given BN. This approach will not work well for at least two reasons. First, theoretically the joint distribution resulted from the ***IPFP*** process, although satisfying all the constraints, may not always be consistent with

[1] In this chapter, unless a distinction is explicitly made, the term "***IPFP***" is used to mean that ***IPFP*** in Eq. 2.6 of Definition 2.15 is applied for marginal constraints, while ***C-IPFP*** in Eq. 2.7 of Definition 2.16 is applied for conditional constraints.

the interdependencies imposed by the network structure, and thus cannot be used to generate new CPTs properly. Secondly, since ***IPFP*** works on the JPD of all variables of the BN, it becomes computational intractable with large BNs. For example, a middle-sized BN with only 32 binary variables has $2^{32}$ float (or double) entries in its JPD, which requires a super large memory (usually it will be out of memory if using only one single computer) and the ***IPFP*** process itself will be extremely slow because for each constraint every entry of the JPD needs to be examined and modified.

In this chapter, we describe our approach to address both of these problems. The first problem is resolved by algorithm ***E-IPFP***, which extends ***IPFP*** by converting the structural invariance to a new probabilistic constraint. The second problem is resolved by algorithm ***D-IPFP***. This algorithm decomposes a global ***E-IPFP*** into a set of smaller, local ***E-IPFP*** problems, each of which corresponds to one constraint and only involves variables that are relevant to those in that constraint. ***SD-IPFP***, the algorithm adopted by ***BayesOWL*** to construct CPTs for the translated BN, is in fact a simplified version of ***D-IPFP*** when some special forms of constraints are given.

The rest of this chapter is organized as follows. Section 3.1 defines the notations used in this chapter and reproduces the convergence proof of ***IPFP*** (i.e., Eq. 2.6 in Definition 2.15). Section 3.2 states precisely the BN modification problems we intend to solve. Section 3.3 gives ***E-IPFP*** and its convergence proof. Section 3.4 describes ***D-IPFP*** and shows that a significant saving is achieved with reasonable relaxation of the minimum distance requirement. Convergence proof of the algorithm is also given. Section 3.5 presents ***SD-IPFP***, by rewriting ***D-IPFP*** for a special type of constraints whose variables are confined locally to within individual CPTs. Section 3.6 describes the implementation of various ***IPFP*** algorithms. Computer experiments of limited scope were conducted to validate the algorithms and to give us a sense of how expensive this approach may be. Experiment results are given in

Section 3.7. Section 3.8 concludes this chapter with comments on related works and suggestions for future research.

## 3.1 Preliminaries

First we define the notations used in this chapter.

- $X = \{X_1, X_2, ..., X_n\}$ is a space of $n$ discrete random variables. In general, upper case $S$, $X$, $Y$, $Z$, ..., etc. are used for the sets of variables. Different sets of variables can be differentiated by superscripts, for example, $Y^1$ and $Y^2$ are two different sets of variables.

- Low case $x = \{x_1, x_2, ..., x_n\}$ is an assignment or instantiation of $X$, for convenience, we denote it as $x \in X$, and $X$ in this case is interpreted as a space of instantiations over all $n$ variables. Same for $s$, $y$, $z$, ..., etc.

- Individual variables are indicated by subscripts, for example, $X_i$ is a variable in $X$ and $x_i$ its instantiation.

- Capital letters $P$, $Q$, $R$, ..., are for probability distributions. It can be differentiated by subscripts.

- A marginal probabilistic constraint $R_i(Y^i)$ to distribution $P(X)$ is a distribution on $Y^i \subseteq X, Y^i \neq \emptyset$. $P(X)$ is said to satisfy $R_i(Y^i)$ if $P(Y^i) = R_i(Y^i)$.

- A conditional probabilistic constraint $R_i(Y^i|Z^i)$ to distribution $P(X)$ is a distribution on $Y^i, Z^i \subseteq X, Y^i \cap Z^i = \emptyset, Y^i \neq \emptyset, Z^i \neq \emptyset$. $P(X)$ is said to satisfy $R_i(Y^i|Z^i)$ if $P(Y^i|Z^i) = R_i(Y^i|Z^i)$.

- $\mathcal{R}_m$ denotes a set of marginal constraints $\{R_i(Y^i)\}$. $\mathcal{R}_c$ denotes a set of conditional constraints $\{R_i(Y^i|Z^i)\}$. $\mathcal{R} = \mathcal{R}_m \cup \mathcal{R}_c$ denotes a set of constraints, either marginal, or conditional.

- $\boldsymbol{\mathcal{P}}$ denotes the set of JPDs over $X$.

- $\boldsymbol{\varepsilon_{R_i(Y^i)}} \subseteq \boldsymbol{\mathcal{P}}$ denotes the set of JPDs over $X$ such that for each JPD $Q \in \boldsymbol{\varepsilon_{R_i(Y^i)}}$, its MPD over $Y^i$ is equal to $R_i(Y^i)$, i.e., $Q(Y^i) = R_i(Y^i)$.

- $\boldsymbol{\varepsilon_{\{R_i(Y^i)\}}} \subseteq \boldsymbol{\mathcal{P}}$ denotes the set of JPDs over $X$ such that for each JPD $Q \in \boldsymbol{\varepsilon_{\{R_i(Y^i)\}}}$, its MPDs over $\{Y^i\}$ are equal to all the corresponding probabilistic constraints, i.e., $Q(Y^i) = R_i(Y^i)$ for all the $m$ ones. Note that $\boldsymbol{\varepsilon_{\{R_i(Y^i)\}}} = \bigcap_{i=1}^{m} \boldsymbol{\varepsilon_{R_i(Y^i)}}$.

- $Q_{(0)}, Q_{(1)}, ..., Q_{(k-1)}, Q_{(k)}, ...$ denotes the sequence of JPDs resulted from each iteration of the various ***IPFP*** algorithms.

- A BN is denoted as $\boldsymbol{\mathcal{N}}$, $\boldsymbol{\mathcal{G}}$ denotes the structure (i.e., the DAG) of $\boldsymbol{\mathcal{N}}$, $\boldsymbol{\mathcal{C}}$ denotes the set of CPTs of $\boldsymbol{\mathcal{N}}$. Different BNs can be differentiated by subscripts or superscripts.

- $\pi_i$ denotes the set of parents of $X_i$ specified in $\boldsymbol{\mathcal{G}}$.

Next we rewrite the convergence proof for ***IPFP*** in Eq. 2.6 of Definition 2.15 [2]. The convergence proof includes three parts. The inheritance of dominance was shown first, followed by the $I_1$-*projection* on one probabilistic constraint, and finally the convergence of the process on all the given probabilistic constraints. Again the assumption here is that the given probabilistic constraints are consistent, which makes $\boldsymbol{\varepsilon_{\{R_i(Y^i)\}}} \neq \emptyset$ and there exists at least one JPD $P$ over $X$ such that $P \in \boldsymbol{\varepsilon_{\{R_i(Y^i)\}}}$ and $P \ll Q_{(0)}$.

**Part 1: Inheritance of Dominance**

**Goal:** To show that for each $Q_{(k)}$ $(k = 1, 2, 3, ...)$ and $i = ((k-1) \bmod m) + 1$, $P(Y^i) \ll Q_{(k-1)}(Y^i)$ if $P \in \boldsymbol{\varepsilon_{\{R_i(Y^i)\}}}$ and $P \ll Q_{(0)}$.

[2] ***C-IPFP*** in Eq. 2.7 of Definition 2.16 has similar convergence result in the discrete finite case.

**Proof.** If $P \ll Q_{(k-1)}$ then $P(Y^i) \ll Q_{(k-1)}(Y^i)$. So we can prove the goal by proving $P \ll Q_{(k-1)}$. Since $P \ll Q_{(0)}$, we only need to show that:

$$P \ll Q_{(k-1)} \Rightarrow P \ll Q_{(k)}, \quad for \ \ each \ \ k = 1, 2, 3, ...$$

by induction over $k$. From Eq. 2.6 it follows that for all $x \in X$ it holds:

$$Q_{(k)}(x) = 0 \quad iff \quad either \ \ Q_{(k-1)}(x) = 0 \ \ or \ \ R_i(x^{Y^i}) = 0 \ (i.e., P(x^{Y^i}) = 0)$$

When $P(x^{Y^i}) = 0$, for all $y \in X$ that is used to compute this marginal probability value (i.e. $y^{Y^i} = x^{Y^i}$), we have: $P(y) = 0$. On the other hand, since $P \ll Q_{(k-1)}$, for all $x \in X$, we know that: $Q_{(k-1)}(x) = 0 \Rightarrow P(x) = 0$. So, in either case, whenever $Q_{(k)}(x) = 0$, we have $P(x) = 0$, which means $P \ll Q_{(k)}$. □

**Part 2: $I_1$-projection on $\boldsymbol{\varepsilon_{R_i(Y^i)}}$**

**Goal:** In each step $k$, $Q_{(k)}$ is an $I_1$-*projection* of $Q_{(k-1)}$ that satisfies the constraint $R_i(Y^i)$, i.e., $Q_{(k)} = \pi_{\boldsymbol{\varepsilon_{R_i(Y^i)}}} Q_{(k-1)}$.

**Proof.** From Eq. 2.6 we know that $Q_{(k)} \ll Q_{(k-1)}$, so the *I-divergence* $I(Q_{(k)} \| Q_{(k-1)})$ is always non-negative, according to Eq. 2.4 of Theorem 2.2, we only need to show that the following assertion is true:

$$For \ \ every \ \ Q \in \boldsymbol{\varepsilon_{R_i(Y^i)}}, I(Q \| Q_{(k-1)}) = I(Q \| Q_{(k)}) + I(Q_{(k)} \| Q_{(k-1)}) \tag{3.1}$$

**Case A. When $\boldsymbol{Q \not\ll Q_{(k-1)}}$**, $I(Q \| Q_{(k-1)}) = \infty$. Since $Q \not\ll Q_{(k-1)}$ and $Q_{(k)} \ll Q_{(k-1)}$, then $Q \not\ll Q_{(k)}$, and consequently, $I(Q \| Q_{(k)}) = \infty$ and $I(Q_{(k)} \| Q_{(k-1)}) < \infty$, which proves Eq. 3.1 in this case.

**Case B. When $\boldsymbol{Q \ll Q_{(k-1)}}$**. Consider the case $x \in X$: $Q_{(k)}(x) > 0$, since $Q_{(k)} \ll Q_{(k-1)}$, $I(Q_{(k)} \| Q_{(k-1)})$ is always finite and can be written as (based on Eq. 2.6 and Eq. 2.1):

$$I(Q_{(k)} \| Q_{(k-1)})$$

$$= \sum_{x \in X, Q_{(k)}(x)>0} Q_{(k)}(x) \log \frac{Q_{(k)}(x)}{Q_{(k-1)}(x)}$$

$$= \sum_{x \in X, Q_{(k-1)}(x)>0, R_i(x^{Y^i})>0} Q_{(k-1)}(x) \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})} \log \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})}$$

$$= \sum_{x^{Y^i} \in Y^i, R_i(x^{Y^i})>0} \sum_{x^{\overline{Y^i}} \in \overline{Y^i}, Q_{(k-1)}(x)>0} Q_{(k-1)}(x^{Y^i}, x^{\overline{Y^i}}) \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})} \log \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})}$$

$$= \sum_{x^{Y^i} \in Y^i, R_i(x^{Y^i})>0} \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})} \left( \log \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})} \right) \sum_{x^{\overline{Y^i}} \in \overline{Y^i}, Q_{(k-1)}(x)>0} Q_{(k-1)}(x^{Y^i}, x^{\overline{Y^i}})$$

$$= \sum_{x^{Y^i} \in Y^i, R_i(x^{Y^i})>0} \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})} \left( \log \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})} \right) Q_{(k-1)}(x^{Y^i})$$

$$= \sum_{x^{Y^i} \in Y^i, R_i(x^{Y^i})>0} R_i(x^{Y^i}) \log \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})} \tag{3.2}$$

Here $\overline{Y^i}$ denotes $X \backslash Y^i$. Since $Q \in \boldsymbol{\varepsilon_{R_i(Y^i)}}$, it follows that $Q(Y^i) = R_i(Y^i)$, also, since $Q \ll Q_{(k-1)} \Rightarrow Q(Y^i) \ll Q_{(k-1)}(Y^i) \Rightarrow R_i(Y^i) \ll Q_{(k-1)}(Y^i)$, Eq. 3.2 can be further written as:

$$I(Q_{(k)} || Q_{(k-1)})$$

$$= \sum_{x^{Y^i} \in Y^i, Q(x^{Y^i})>0} Q(x^{Y^i}) \log \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})}$$

$$= \sum_{x \in X, Q(x)>0} Q(x) \log \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})}$$

$$= \sum_{x \in X, Q(x)>0} Q(x) \log \frac{Q_{(k-1)}(x) \frac{R_i(x^{Y^i})}{Q_{(k-1)}(x^{Y^i})}}{Q_{(k-1)}(x)}$$

$$= \sum_{x \in X, Q(x)>0} Q(x) \log \frac{Q_{(k)}(x)}{Q_{(k-1)}(x)} \tag{3.3}$$

Since $Q_{(k)} \ll Q_{(k-1)}$, for every $x \in X$, it holds that $Q_{(k)}(x) = 0$ iff $Q_{(k-1)}(x) = 0$ or $R_i(x^{Y^i}) = Q(x^{Y^i}) = 0$. Since $Q \ll Q_{(k-1)}$, $Q_{(k-1)}(x) = 0 \Rightarrow Q(x) = 0$. It is obvious that $Q(x^{Y^i}) = 0 \Rightarrow Q(x) = 0$. Thus it holds that $Q \ll Q_{(k)}$. Then, using Eq. 2.1 and

Eq. 3.3, we have:

$$
\begin{aligned}
& I(Q\|Q_{(k-1)}) \\
&= \sum_{x\in X, Q(x)>0} Q(x)\log\frac{Q(x)}{Q_{(k-1)}(x)} \\
&= \sum_{x\in X, Q(x)>0} Q(x)\log\frac{Q(x)\cdot Q_{(k)}(x)}{Q_{(k)}(x)\cdot Q_{(k-1)}(x)} \\
&= I(Q\|Q_{(k)}) + \sum_{x\in X, Q(x)>0} Q(x)\log\frac{Q_{(k)}(x)}{Q_{(k-1)}(x)} \\
&= I(Q\|Q_{(k)}) + I(Q_{(k)}\|Q_{(k-1)}) \qquad (3.4)
\end{aligned}
$$

That completes the proof. □

**Part 3: Convergence of *IPFP***

**Goal:** If there exists at least one $P \in \boldsymbol{\varepsilon_{\{R_i(Y^i)\}}}$ and $P \ll Q_{(0)}$, then $Q^*(X) = \lim_{k\to\infty} Q_{(k)}$ is an $I_1$-*projection* of $Q_{(0)}$ that satisfies all probabilistic constraints, i.e., $Q^*(X) = \pi_{\boldsymbol{\varepsilon_{\{R_i(Y^i)\}}}} Q_{(0)}$.

**Proof.** From "**Part 2**" we have:

$$Q_{(k)} = \pi_{\boldsymbol{\varepsilon_{R_i(Y^i)}}} Q_{(k-1)}, for\ \ all\ \ k = 1, 2, 3, ..., i = ((k-1) \bmod m) + 1$$

Take an arbitrary $P \in \boldsymbol{\varepsilon_{\{R_i(Y^i)\}}}$, using Eq. 2.4 of Theorem 2.2, we have:

$$
\begin{aligned}
& I(P\|Q_{(0)}) = I(P\|Q_{(1)}) + I(Q_{(1)}\|Q_{(0)}) \\
& I(P\|Q_{(1)}) = I(P\|Q_{(2)}) + I(Q_{(2)}\|Q_{(1)}) \\
& ... \\
& I(P\|Q_{(k-1)}) = I(P\|Q_{(k)}) + I(Q_{(k)}\|Q_{(k-1)})
\end{aligned}
$$

Adding them together, we have:

$$I(P\|Q_{(0)}) = I(P\|Q_{(k)}) + I(Q_{(k)}\|Q_{(k-1)}) + ... + I(Q_{(1)}\|Q_{(0)})$$

$$\Rightarrow I(P\|Q_{(0)}) = \lim_{k\to\infty} I(P\|Q_{(k)}) + \sum_{k=1}^{\infty} I(Q_{(k)}\|Q_{(k-1)}) \tag{3.5}$$
$$\Rightarrow I(P\|Q_{(0)}) \geq \sum_{k=1}^{\infty} I(Q_{(k)}\|Q_{(k-1)})$$

From "**Part 1**", we have $P \ll Q_{(k)}$ for all $k = 1, 2, 3, ...$, so $\lim_{k\to\infty} I(P\|Q_{(k)})$ is always non-negative. Also, since $Q_{(k)} \ll Q_{(k-1)}$, all $I(Q_{(k)}\|Q_{(k-1)})$ are non-negative. Further, since $P \ll Q_{(0)}$, $I(P\|Q_{(0)})$ is finite. Thus $I(Q_{(k)}\|Q_{(k-1)}) \to 0$. Using Theorem 2.1, we have the *total variance* $\left|Q_{(k)} - Q_{(k-1)}\right| \to 0$, so there exists a limit probability distribution of the sequence $Q_{(k)}, k = 1, 2, 3, ...$, and we denote it as $Q^*(X)$.

Given an arbitrary index $1 \leq i \leq m$, from "**Part 2**" we know that all distributions in the subsequence $Q_{(i+j*m)}, j = 1, 2, 3, ...$ are $I_1$-*projection*s of some distributions on $\boldsymbol{\varepsilon_{R_i(Y^i)}}$. But all these subsequences will converge to the same limit, i.e., $Q^*(X)$, so we will get: $Q^*(X) \in \boldsymbol{\varepsilon_{\{R_i(Y^i)\}}} = \bigcap_{i=1}^{m} \boldsymbol{\varepsilon_{R_i(Y^i)}}$. Now Eq. 3.4 also holds for $Q^*(X)$, we can rewrite Eq. 3.4 as:

$$\begin{aligned} & I(Q^*(X)\|Q_{(0)}) \\ &= \lim_{k\to\infty} I(Q^*(X)\|Q_{(k)}) + \sum_{k=1}^{\infty} I(Q_{(k)}\|Q_{(k-1)}) \\ &= \sum_{k=1}^{\infty} I(Q_{(k)}\|Q_{(k-1)}) \end{aligned} \tag{3.6}$$

Then for $P \in \boldsymbol{\varepsilon_{\{R_i(Y^i)\}}}$, using Eq. 3.4 and Eq. 3.5 we get:

$$\begin{aligned} & I(P\|Q_{(0)}) \\ &= \lim_{k\to\infty} I(P\|Q_{(k)}) + \sum_{k=1}^{\infty} I(Q_{(k)}\|Q_{(k-1)}) \\ &= I(P\|Q^*(X)) + \sum_{k=1}^{\infty} I(Q_{(k)}\|Q_{(k-1)}) \\ &= I(P\|Q^*(X)) + I(Q^*(X)\|Q_{(0)}) \end{aligned} \tag{3.7}$$

Again, based on Eq. 2.4 of Theorem 2.2, Eq. 3.7 means $Q^*(X) = \pi_{\boldsymbol{\varepsilon}_{\{\boldsymbol{R_i(Y^i)}\}}} Q_{(0)}$, that finishes the whole convergence proof. □

## 3.2 The Problem of Modifying BNs with Probabilistic Constraints

Based on the notations, a network $\mathbf{\mathcal{N}}_0$ on $X = \{X_1, ..., X_n\}$ has DAG $\mathbf{\mathcal{G}}_0$ and CPT set $\mathbf{\mathcal{C}}_0$ where each CPT in $\mathbf{\mathcal{C}}_0$ is in the form of $P_0(X_i|\pi_i)$, and the JPD of $\mathbf{\mathcal{N}}_0$ is $P_0(X) = \prod_{i=1}^n P_0(X_i|\pi_i)$.

Given a JPD $P(X)$ and a BN structure $\mathbf{\mathcal{G}}$ of $X$, a CPT $P(X_i|\pi_i)$ can be *extracted* from $P(X)$ by computing $P(\pi_i)$ and $P(X_i, \pi_i)$ from $P(X)$ through marginalization or any other methods. When $P(X)$ and $\mathbf{\mathcal{G}}$ are given, CPT extraction is unique. When all CPTs of $\mathbf{\mathcal{N}}$ are replaced by those extracted from an arbitrary $P(X)$ according to $\mathbf{\mathcal{G}}$, its distribution $P'(X) = \prod_{i=1}^n P(X_i|\pi_i)$ may not be equal to $P(X)$ even though the conditional distribution of $X_i$, given $\pi_i$, are the same in both $P(X)$ and $P'(X)$. This is because certain conditional independences of $P'(X)$, dictated by the network structure, do not hold for $P(X)$.

A distribution $P(X)$ is said to be (structurally) *consistent* with $\mathbf{\mathcal{G}}$ of $\mathbf{\mathcal{N}}$ if and only if there exists a set of CPTs $\mathbf{\mathcal{C}} = \{Q(X_i|\pi_i)\}$ such that $P(X) = \prod_{i=1}^n Q(X_i|\pi_i)$. Since when $\mathbf{\mathcal{G}}$ is given, $P(X)$ uniquely determines $P(X_i|\pi_i)$ for all $X_i$, so if $P(X)$ is consistent with $\mathbf{\mathcal{G}}$ then $P(X) = \prod_{i=1}^n P(X_i|\pi_i)$. Consequently, if both $P(X)$ and $P'(X)$ are consistent with $\mathbf{\mathcal{G}}$, then $P(X) = P'(X)$ if and only if $\mathbf{\mathcal{C}} = \mathbf{\mathcal{C}'}$.

With the above notations, we can state precisely the problem we are trying to solve as follows: for a given $\mathbf{\mathcal{N}}$ over variables $X$ with distribution $Q(X)$ and a set of consistent constraints $\mathcal{R}$, find $\mathbf{\mathcal{N}}^*$ that meets the following three requirements:

1. $\mathbf{\mathcal{G}} = \mathbf{\mathcal{G}}^*$ (both networks have the same structure);

2. $Q^*(X)$, the distribution of $\mathfrak{N}^*$, satisfies all constraints in $\mathcal{R}$; and

3. *I-divergence* $I(Q^*(X)\|Q(X))$ is minimum among all distributions that meet requirements 1 and 2.

For a given $\mathfrak{N}_0$ and its distribution $Q_0(X) = \prod_{i=1}^{n} Q_0(X_i|\pi_i)$ and constraint set $\mathcal{R}$, one can always obtain an $I_1$-*projection* $Q^*(X)$ of $Q_0(X)$ on $\mathcal{R}$ by ***IPFP*** (i.e., requirement 1 and 3). However, $Q^*(X)$ is not guaranteed to be consistent with $\mathcal{G}_0$ (i.e., requirement 2). This is especially true if some constraints involve more than one variables and they span over more than one CPT. This problem is illustrated in the following examples with a small network $\mathfrak{N}_4$ of four binary variables $\{A, B, C, D\}$, as depicted in Fig. 3.2. In our context, "**1**" is used for a "True" state and "**0**" is used for a "False" state.

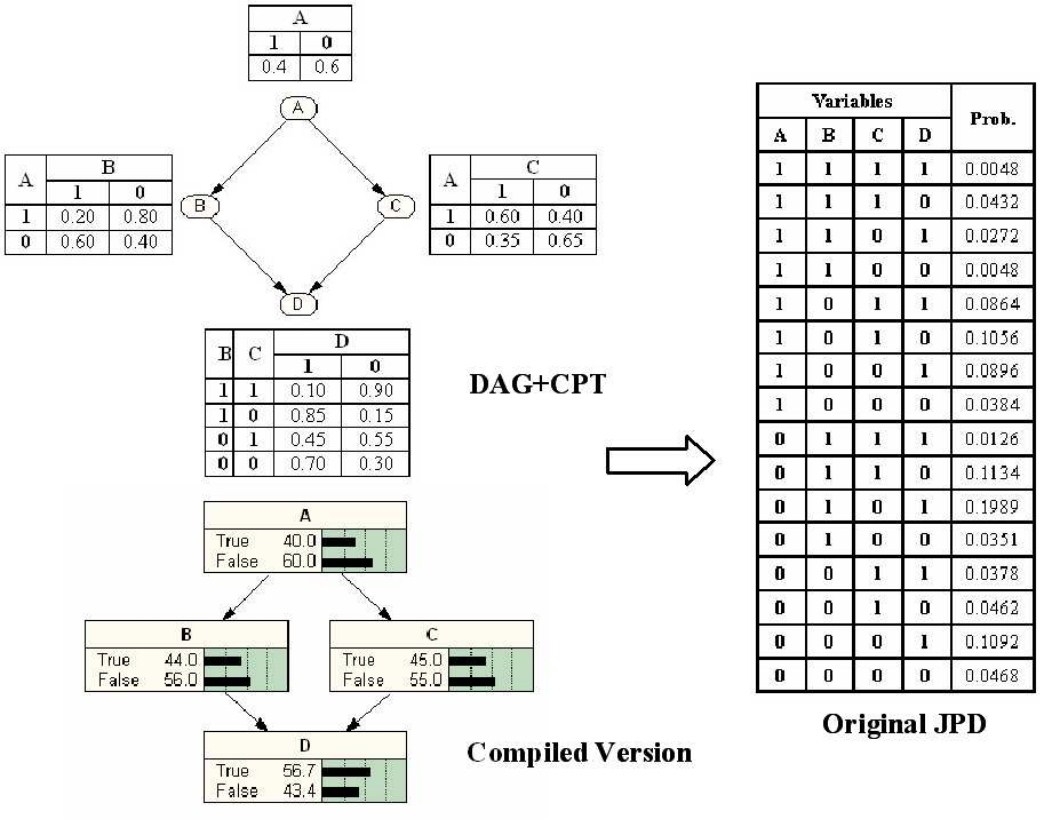



Fig. 3.2: **Network $\mathfrak{N}_4$ of $X = \{A, B, C, D\}$ and its CPTs**

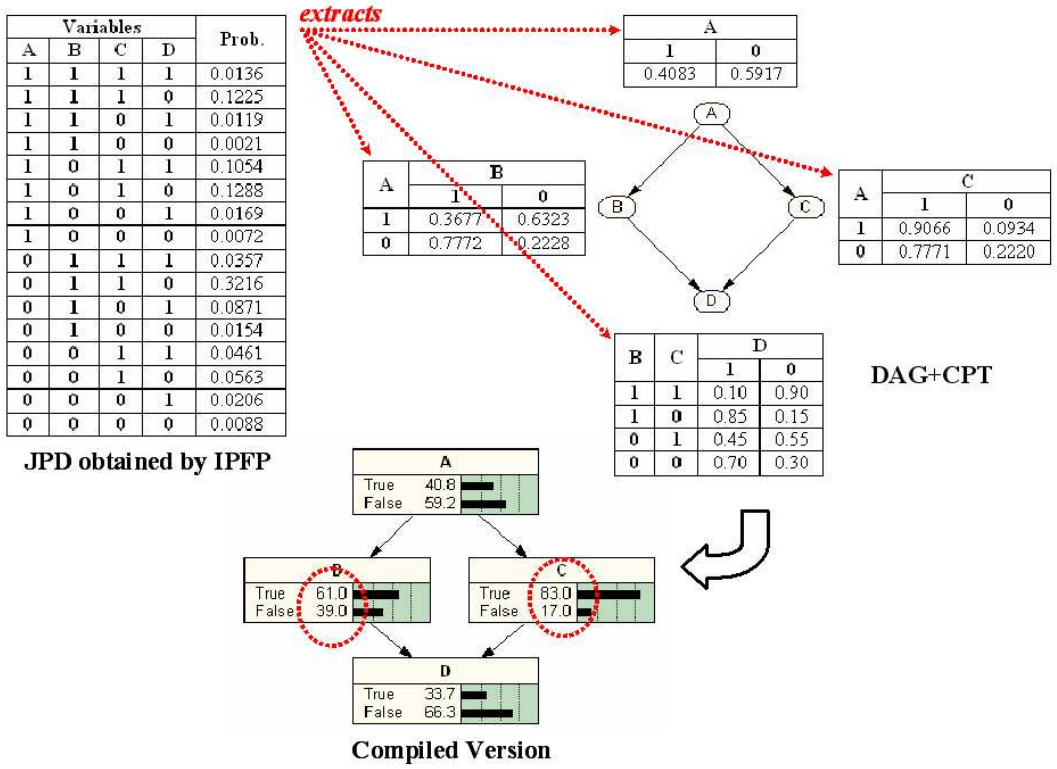



Fig. 3.3: **Running *IPFP* with** $R_1(B)$ **and** $R_2(C)$

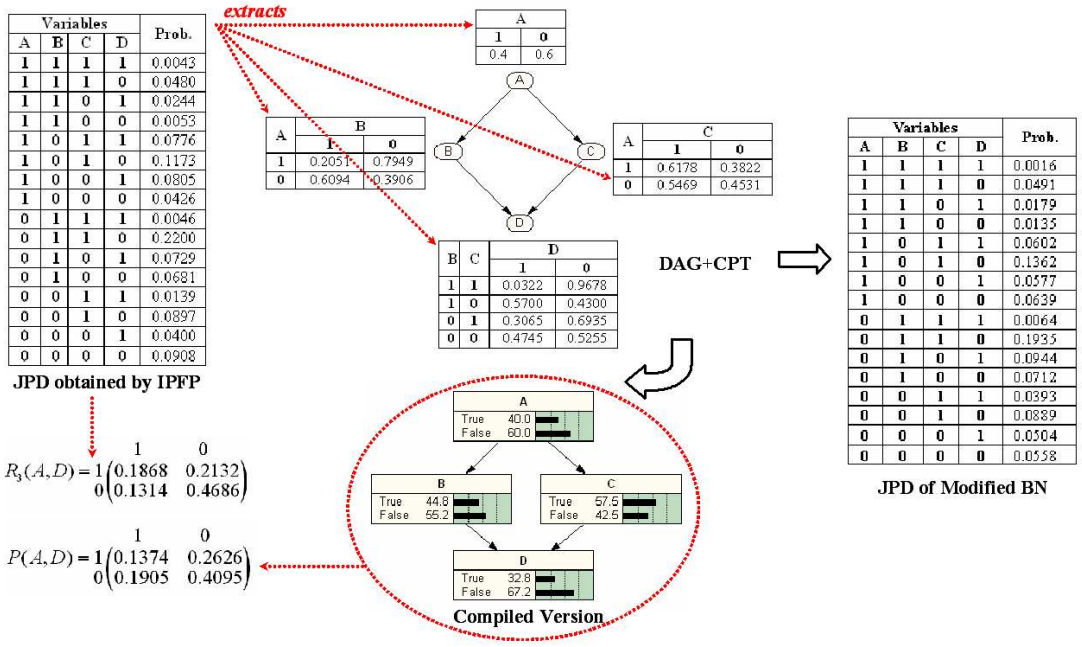



Fig. 3.4: **Running *IPFP* with** $R_3(A, D)$

Fig. 3.3 gives $Q^*(A, B, C, D)$, the JPD resulted from ***IPFP*** on $\mathfrak{N}_4$ with two constraints $\{R_1(B) = (0.61, 0.39), R_2(C) = (0.83, 0.17)\}$. *I-divergence* of $Q^*$ to the original distribution is **0.5708**. Also given are the CPTs of the four variables extracted from $Q^*$ according to the network structure. We can verify that 1) $Q^*(B) = R_1(B)$ and $Q^*(C) = R_2(C)$ (i.e., $Q^*$ satisfies both constraints), and 2) $Q^*(A, B, C, D) = Q^*(A) \cdot Q^*(B|A) \cdot Q^*(C|A) \cdot Q^*(D|B, C)$ (i.e., $Q^*$ is consistent with the network structure). Note here that CPTs of three nodes ($A$, $B$, $C$) have been changed.

However, it is different when a single constraint $\{R_3(A, D) = (0.1868,\ 0.2132,\ 0.1314,\ 0.4686)\}$ is applied. As can be seen from the left upper corner of Fig. 3.4, the resulting distribution, although satisfying $R_3(A, D)$, is not consistent with the structure of $\mathfrak{N}_4$, i.e., $Q^*(A, B, C, D) \neq Q^*(A) \cdot Q^*(B|A) \cdot Q^*(C|A) \cdot Q^*(D|B, C)$. We can modify the BN by extracting CPTs from $Q^*(A, B, C, D)$ while keeping the structure unchanged. The new CPTs and the JPD of the modified BN are given in the right part of Fig. 3.4. It can be seen that, $P(A, D)$, the joint distribution computed from the modified BN with probabilities (0.1374, 0.2626, 0.1905, 0.4095), is not equal to $R_3(A, D)$. This is because $A$ and $D$ are not within a single CPT and the interdependency among variables has been altered by ***IPFP*** while attempting to satisfy the constraint $R_3(A, D)$ and minimize *I-divergence*. *I-divergence* of the JPD of the modified BN to the original distribution is **0.2611**.

## 3.3 E-IPFP

To solve the BN modification problem defined in Section 3.2, we first extend ***IPFP*** to handle the requirement that the solution distribution should be consistent with $\mathfrak{G}_0$, the structure of the given BN. Recall that whether a distribution $Q(X)$ is consistent with $\mathfrak{G}_0$ can be determined by whether $Q(X) = \prod_{i=1}^{n} Q(X_i|\pi_i)$, where the parent-child relation in the right hand of the equation is determined by $\mathfrak{G}_0$. We can thus treat

this requirement as a probabilistic constraint $R_r(X) = \prod_{i=1}^{n} Q_{(k-1)}(X_i|\pi_i)$ in ***IPFP***. Here $Q_{(k-1)}(X_i|\pi_i)$ are extracted from $Q_{(k-1)}(X)$ according to $\mathfrak{S}_0$. We call $R_r(X)$ a structural constraint.

Like any other constraint $R_i(Y^i)$, this constraint, when applied at step $k$ of ***IPFP***, changes $Q_{(k-1)}(X)$ to $Q_{(k)}(X)$. By Eq. 2.6, $Q_{(k)}(X) = R_r(X) = \prod_{i=1}^{n} Q_{(k-1)}(X_i|\pi_i)$, thus meeting the structural consistency requirement.

Let $Q_0(X) = \prod_{i=1}^{n} Q_0(X_i|\pi_i)$ be the distribution of a given network $\mathfrak{N}_0$, and $\mathcal{R}$ be the set of $m$ given constraints. ***E-IPFP*** is a simple extension of ***IPFP*** by including the structural constraint as the $(m+1)^{th}$ constraint $R_{m+1}(X)$. The algorithm ***E-IPFP*** is stated in Table 3.1. Note that for convenience Step 2.2 skips the "zero" case of Eq. 2.6 and Eq. 2.7. As a practical matter, convergence of ***E-IPFP*** can be determined by testing if the difference between $Q_{(k)}(X)$ and $Q_{(k-1)}(X)$ (by any of a number of metrics) is below a given threshold.

All constraints remain constant during the iteration process except $R_{m+1}(X)$, which changes its value every time it is applied. Nonetheless, as a distribution, when $R_{m+1}(X)$ is applied to $Q_{(k-1)}(X)$, the resulting $Q_{(k)}(X) = R_{m+1}(X)$ is an $I_1$-*projection* of $Q_{(k-1)}(X)$ on $R_{m+1}(X)$. This is because $Q_{(k)}(X)$ is the only distribution that satisfies $R_{m+1}(X)$ since $R_{m+1}(X)$ is a distribution of $X$, not of a subset of $X$. As can be seen from [33, 152, 31] and Section 3.1, convergence of the original ***IPFP*** is a consequence of the property that each iteration of ***IPFP*** produces an $I_1$-*projection* of the previous distribution on a constraint. Since this condition holds for our ***E-IPFP***, the process converges to a distribution $Q^*(X)$, and $Q^*(X)$ is an $I_1$-*projection* of $Q_0(X)$ on $\{R_1, R_2, \ ..., \ R_m, R_{m+1}(X)\}$. Since $Q^*(X)$ satisfies $R_{m+1}(X)$, we have $Q^*(X) = \prod_{i=1}^{n} Q^*(X_i|\pi_i)$, so it also satisfies the structural consistency requirement. Therefore, among those distributions that satisfy given constraints in $\mathcal{R}$ and are consistent with $\mathfrak{S}_0$, $Q^*(X)$ has the minimum *I-divergence* to $Q_0(X)$.

Application of ***E-IPFP*** to the network $\mathfrak{N}_4$ of Fig. 3.2 with a single constraint

***E-IPFP***$(\mathfrak{N}_0(X),\ R = \{R_1, R_2,\ ...,\ R_m\})$ {

1. Computing $Q_0(X) = \prod_{i=1}^{n} Q_0(X_i|\pi_i)$ where $Q_0(X_i|\pi_i) \in \mathfrak{C}_0$;
2. Starting with $k = 1$, repeat the following procedure until convergence {
   - 2.1. $i = ((k-1) \bmod (m+1)) + 1$;
   - 2.2. if $i < m+1$ {
     - if $(R_i \in \mathcal{R}_m)$ { /* for marginal constraints */
       - $Q_{(k)}(X) = Q_{(k-1)}(X) \cdot \frac{R_i(Y^i)}{Q_{(k-1)}(Y^i)}$ ; (from Eq. 2.6)
     - } else if $(R_i \in \mathcal{R}_c)$ { /* for conditional constraints */
       - $Q_{(k)}(X) = Q_{(k-1)}(X) \cdot \frac{R_i(Y^i|Z^i)}{Q_{(k-1)}(Y^i|Z^i)}$ ; (from Eq. 2.7)
     - }
   - }
   - 2.3. else {
     - extract $Q_{(k-1)}(X_i|\pi_i)$ from $Q_{(k-1)}(X)$ according to $\mathfrak{S}_0$;
     - $Q_{(k)}(X) = \prod_{i=1}^{n} Q_{(k-1)}(X_i|\pi_i)$;
   - }
   - 2.4. $k = k + 1$;
   }
3. return $\mathfrak{N}^*(X)$ with $\mathfrak{S}^* = \mathfrak{S}_0$ and $\mathfrak{C}^* = \{Q_{(k)}(X_i|\pi_i)\}$;

}

Table 3.1: **The *E-IPFP* Algorithm**

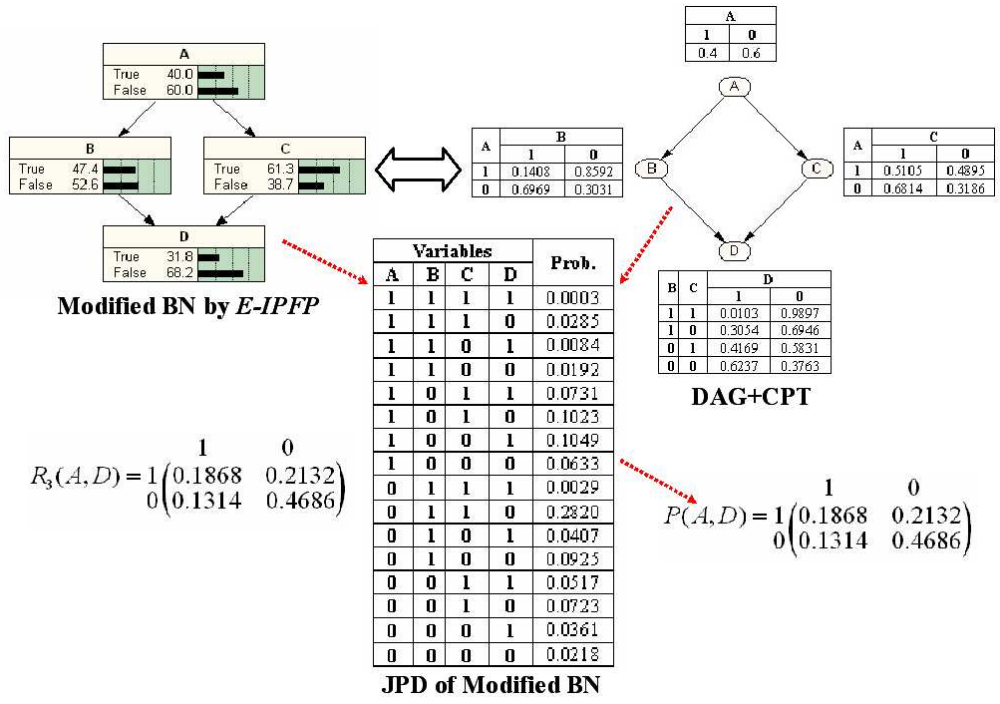



Fig. 3.5: **Running *E-IPFP* with** $R_3(A, D)$

$\{R_3(A, D) = (0.1868, 0.2132, 0.1314, 0.4686)\}$ converges to a distribution (Fig. 3.5). Comparing with the result in Fig. 3.4 (using ***IPFP***), this distribution not only satisfies $R_3(A, D)$, but is also structurally consistent with $\mathfrak{N}_4$. However, its *I-divergence* to the original distribution increases slightly in absolute value (from **0.2611** in Fig. 3.4 to **0.4419**).

## 3.4 D-IPFP

As can be seen in Eq. 2.6 and Eq. 2.7, the computation of both ***IPFP*** and ***E-IPFP*** is on the entire joint distribution of $X$ at every iteration. This distribution becomes prohibitively large with large $n$, making the process computationally intractable for BNs of large size. Roughly speaking, when $Q_{(k-1)}(X)$ is modified by constraint $R_i(Y^i)$ (or $R_i(Y^i|Z^i)$), Eq. 2.6 (or Eq. 2.7) requires to check each entry in $Q_{(k-1)}(X)$ against every entry of $R_i(Y^i)$ (or $R_i(Y^i|Z^i)$) and makes the update if $x$ is consistent with $y^i$

(or $x$ is consistent with $y^i$ and $z^i$). The cost can be roughly estimated as $O(2^n * 2^{|Y^i|})$ (or $O(2^n * 2^{|Y^i|+|Z^i|})$), which grows exponentially with $n$.

Since the joint distribution of a BN is a product of distributions of much smaller size (i.e., its CPTs), the cost of ***E-IPFP*** may be reduced if we can utilize the interdependencies imposed on the distribution by the network structure and only update some selected CPTs. This has motivated the development of algorithm ***D-IPFP*** which decomposes the *global* ***E-IPFP*** (the one involving all $n$ variables) into a set of *local* ***E-IPFP***, each for one constraint $R_i(Y^i)$ (or $R_i(Y^i|Z^i)$), on a small subnet of $\mathbf{N}_0$ that contains $Y^i$ (or $Y^i \cup Z^i$).

Without loss of generality, now we assume all the constraints are from $\mathcal{R}_m$. Consider one such constraint $R_i(Y^i)$ at step $k$ where $Y^i$ is a non-empty subset of $X$. Let $Y$ be some non-empty subset of $X$ (i.e., $Y \subseteq X$ *and* $Y \neq \emptyset$) such that $Y^i \subseteq Y$, and let $S = (\bigcup_{X_j \in Y} \pi_j) \backslash Y$, i.e., $S$ contains parent nodes of all variables in $Y$ except those that are also in $Y$. Multiplying all CPTs for variables in $Y$, one can construct a conditional distribution $Q'_{(k-1)}(Y|S)$:

$$Q'_{(k-1)}(Y|S) = Q_{(k-1)}(Y|S) = \prod_{X_j \in Y} Q_{(k-1)}(X_j|\pi_j) \tag{3.8}$$

With Eq. 3.8, we can define $Q'_{(k-1)}(X)$ as follows:

$$Q'_{(k-1)}(X) = Q_{(k-1)}(X) = Q'_{(k-1)}(Y|S) \cdot \prod_{X_j \notin Y} Q_{(k-1)}(X_j|\pi_j) \tag{3.9}$$

Now $R_i(Y^i)$ becomes local to the table $Q'_{(k-1)}(Y|S)$, and we can obtain:

$$Q'_{(k)}(X) = Q'_{(k)}(Y|S) \cdot \prod_{X_j \notin Y} Q_{(k)}(X_j|\pi_j)$$

by obtaining $Q'_{(k)}(Y|S)$ using Eq. 2.6 in the subspace of $Y \cup S$ while keeping CPTs

for variables outside $Y$ unchanged:

$$\begin{cases} Q'_{(k)}(Y|S) = Q'_{(k-1)}(Y|S) \cdot \frac{R_i(Y^i)}{Q'_{(k-1)}(Y^i)} \cdot \alpha_k \\ Q'_{(k)}(X_j|\pi_j) = Q'_{(k-1)}(X_j|\pi_j) = Q_{(k-1)}(X_j|\pi_j) \quad for\ \forall X_j \notin Y \end{cases} \tag{3.10}$$

$\alpha_k$ is a normalization vector. Next, we could extract $Q'_{(k)}(X_j|\pi_j)$ for all $X_j \in Y$ from $Q'_{(k)}(Y|S)$, and let $Q_{(k)}(X_j|\pi_j) = Q'_{(k)}(X_j|\pi_j)$, then we can get $Q_{(k)}(X)$ by:

$$Q_{(k)}(X) = \prod_{X_j \in Y} Q'_{(k)}(X_j|\pi_j) \cdot \prod_{X_j \notin Y} Q_{(k-1)}(X_j|\pi_j) \tag{3.11}$$

Though $Q'_{(k)}(Y|S)$ satisfies $R_i(Y^i)$, $Q_{(k)}(X)$ might not, so the process from Eq. 3.8 to Eq. 3.11 need to be repeated until converge. In summary, update of $Q_{(k-1)}(X)$ to $Q_{(k)}(X)$ by $R_i(Y^i)$ can be seen to consist of iterations over three steps: 1) form $Q'_{(k-1)}(Y|S)$ from CPTs for $X_j \in Y$ by Eq. 3.8; 2) update $Q'_{(k-1)}(Y|S)$ to $Q'_{(k)}(Y|S)$ by $R_i(Y^i)$ using Eq. 3.10; and 3) extract $Q'_{(k)}(X_j|\pi_j)$ from $Q'_{(k)}(Y|S)$ and compute the new distribution $Q_{(k)}(X)$ by Eq. 3.11. Comparing Eq. 3.8, Eq. 3.10 and Eq. 3.11 with Step 1, Step 2.2 and Step 2.3 in algorithm ***E-IPFP***, this procedure of ***D-IPFP*** for one constraint amounts to one application of the ***E-IPFP*** algorithm with two constraints (i.e., $R_i(Y^i)$ and local structural constraint $R_r(Y) = \prod_{X_j \in Y} Q'_{(k)}(X_j|\pi_j)$) on local distribution $Q'_{(k-1)}(Y|S)$ and it can be easily extended to handle constraints from $\mathcal{R}_c$. Then given a set of constraints $\mathcal{R}$, the ***D-IPFP*** algorithm can be presented as Table 3.2. For efficiency consideration, in implementing ***D-IPFP***, the "while" loop of Step 2.3 can be replaced by a single iteration.

Next we analyze the convergence of ***D-IPFP*** by first examining the behavior involving a single constraint that iterates over Eq. 3.8 to Eq. 3.11 (i.e., Step 2.3 in Table 3.2). This is given in Theorem 3.1 below.

**Theorem 3.1 (Convergence of *D-IPFP* for One Constraint)**

***D-IPFP***$(\mathfrak{N}_0(X), \mathcal{R} = \{R_1, R_2, \ ..., \ R_m\})$ {

1. Computing $Q_0(X) = \prod_{i=1}^{n} Q_0(X_i|\pi_i)$ where $Q_0(X_i|\pi_i) \in \mathfrak{C}_0$;

2. Starting with $k = 1$, repeat the following procedure until convergence {

   2.1 $i = ((k-1) \bmod m) + 1$;

   2.2 getting the $Y$ and $S$ of this constraint, let counter $kk = 0$;

   2.3 while not converge {

      2.3.1 $Q'_{(k-1)}(Y|S) = \prod\limits_{X_j \in Y} Q_{(k-1)}(X_j|\pi_j)$ ;

      2.3.2 if $(R_i \in \mathcal{R}_m)$ { /* for marginal constraints */

         $Q'_{(k)}(Y|S) = Q'_{(k-1)}(Y|S) \cdot \frac{R_i(Y^i)}{Q'_{(k-1)}(Y^i)} \cdot \alpha_k$;

      } else if $(R_i \in \mathcal{R}_c)$ { /* for conditional constraints */

         $Q'_{(k)}(Y|S) = Q'_{(k-1)}(Y|S) \cdot \frac{R_i(Y^i|Z^i)}{Q'_{(k-1)}(Y^i|Z^i)} \cdot \alpha_k$;

      }

      2.3.3 Updating CPTs for all $X_j \in Y$ and compiling the network; {

         $Q_{(k)}(X_j|\pi_j) = Q'_{(k)}(X_j|\pi_j) \quad \forall X_j \in Y$

         $Q_{(k)}(X_j|\pi_j) = Q_{(k-1)}(X_j|\pi_j) \quad \forall X_j \notin Y$

      }

      2.3.4 $Q_{(k-1)}(X_j|\pi_j) = Q_{(k)}(X_j|\pi_j)$, for all $X_j \in X$ ; $kk = kk + 1$ ;

   }

   2.4 $k = k + 1$;

}

3. return $\mathfrak{N}^*(X)$ with $\mathfrak{G}^* = \mathfrak{G}_0$ and $\mathfrak{C}^* = \{Q_{(k)}(X_i|\pi_i)\}$;

}

Table 3.2: **The *D-IPFP* Algorithm**

Let $Q_{(k-1)}(X) = \prod_{j=1}^{n} Q_{(k-1)}(X_j|\pi_j)$ be a probability distribution over variables $X$ where each $Q_{(k-1)}(X_j|\pi_j)$ is the CPT for variable $X_j$ in a Bayesian network $\mathbf{\mathcal{N}}$ of $n$ variables. Let $R_i(Y^i)$ be a probability distribution over variables $Y^i \subseteq X$ that is consistent with the structure of $\mathbf{\mathcal{N}}$. Then:

1. The iterations of Eq. 3.8 - Eq. 3.11 (i.e., Step 2.3 in Table 3.2), starting with $Q_{(k-1)}(X)$, will converge to a distribution $Q^*_{(k)}(X)$;
2. $Q^*_{(k)}(X)$ satisfies $R_i(Y^i)$, i.e., $Q^*_{(k)}(Y^i) = R_i(Y^i)$;
3. $Q^*_{(k)}(X)$ is consistent with the structure of $\mathbf{\mathcal{N}}$;
4. $Q^*_{(k)}(X)$ is not always the $I_1$-*projection* of $Q_{(k-1)}(X)$ on $R_i(Y^i)$, but on constraint set $\{R_i(Y^i), R_r(Y)\}$.

**Proof.**

*Part 1.* Note that Eq. 3.8 and Eq. 3.9 do not change the distribution, they only change its representation. Eq. 3.11 imposes a local structural constraint on $Q'_{(k-1)}(Y|S)$, as argued in Section 3.3 for ***E-IPFP***, $Q_{(k)}(Y|S)$ is thus an $I_1$-*projection* of $Q'_{(k)}(Y|S)$ on $R_r(Y)$, i.e., $Q_{(k)}(X)$ is thus an $I_1$-*projection* of $Q'_{(k)}(X)$ on $R_r(Y)$ since all other CPTs are unchanged. Now we show that, with Eq. 3.10, $Q'_{(k)}(X)$ is an $I_1$-*projection* of $Q'_{(k-1)}(X)$. Combining Eq. 3.8, Eq. 3.9, and Eq. 3.10, we have

$$
\begin{aligned}
Q'_{(k)}(X) &= Q'_{(k)}(Y|S) \cdot \prod_{X_j \notin Y} Q'_{(k-1)}(X_j|\pi_j) \\
&= [Q'_{(k-1)}(Y|S) \cdot \prod_{X_j \notin Y} Q'_{(k-1)}(X_j|\pi_j)] \cdot \frac{Q'_{(k)}(Y|S)}{Q'_{(k-1)}(Y|S)} \\
&= Q'_{(k-1)}(X) \cdot \frac{Q'_{(k)}(Y|S)}{Q'_{(k-1)}(Y|S)}
\end{aligned}
$$

Therefore, $Q'_{(k)}(X)$ is an $I_1$-*projection* of $Q'_{(k-1)}(X)$ on constraint $Q'_{(k)}(Y|S)$. Since each update generates a distribution that is an $I_1$-*projection* of the previous distri-

bution, again, according to [33, 152, 31] and Section 3.1, the process converges with $\lim_{kk\to\infty} Q_{(k)}(x) = Q^*_{(k)}(X)$. Note that $kk$ is the counter for Step 2.3 which accumulates the number of iterations for the internal "while" loop in Table 3.2.

*Part 2.* We prove this part by showing that when $kk \to \infty$, $\frac{R_i(Y^i)}{Q'_{(k-1)}(Y^i)} \to 1$. Note,

$$\begin{aligned}
&Q'_{(k-1)}(Y|S) \cdot \frac{R_i(Y^i)}{Q'_{(k-1)}(Y^i)} \\
&= Q'_{(k-1)}(Y|S) \cdot \frac{Q'_{(k-1)}(S)}{Q'_{(k-1)}(S)} \cdot \frac{R_i(Y^i)}{Q'_{(k-1)}(Y^i)} \\
&= \frac{Q'_{(k-1)}(Y,S)}{Q'_{(k-1)}(S)} \cdot \frac{R_i(Y^i)}{Q'_{(k-1)}(Y^i)} \\
&= \frac{Q'_{(k)}(Y,S)}{Q'_{(k-1)}(S)} \\
&= Q'_{(k)}(Y|S) \cdot \frac{Q'_{(k)}(S)}{Q'_{(k-1)}(S)} \qquad (3.12)
\end{aligned}$$

By Part 1, when $kk \to \infty$, $Q'_{(k)}(X) - Q'_{(k-1)}(X) \to 0$. Then we have $\frac{Q'_{(k)}(S)}{Q'_{(k-1)}(S)} \to 1$ and $\frac{Q'_{(k)}(Y|S)}{Q'_{(k-1)}(Y|S)} \to 1$. Substituting these limits into Eq. 3.12, we have $\frac{R_i(Y^i)}{Q'_{(k-1)}(Y^i)} \to 1$.

*Part 3.* This is to show $Q_{(k)}(X) = \prod_{X_i \in X} Q_{(k)}(X_i|\pi_i)$. Similarly, by Part 1, when $kk \to \infty$, $Q_{(k)}(X) - Q'_{(k)}(X) \to 0$. Since $\prod_{X_j \notin Y} Q_{(k-1)}(X_j|\pi_j)$ has never changed, it can be factored out. Then according to Eq. 3.10 and Eq. 3.11, we have:

$$Q_{(k)}(Y|S) - Q'_{(k)}(Y|S) = \prod_{X_j \in Y} Q'_{(k)}(X_j|\pi_j) - Q'_{(k)}(Y|S) \to 0$$

Thus $Q'_{(k)}(Y|S)$ is consistent with the network structure with variables in $Y$. Since other CPT's have not been changed, $Q^*_{(k)}(X)$ is still consistent with the network structure of $\mathfrak{N}$.

*Part 4.* We prove it by a counter example. In the example in Fig. 3.4 at the end of Section 1, an $I_1$-*projection* on $R_3(A, D)$ is not consistent with the network structure.

On the other hand, $Q^*_{(k)}(X)$ from ***D-IPFP*** must be consistent with the network structure. Since $I_1$-*projection* is unique, $Q^*_{(k)}(X)$ therefore cannot be an $I_1$-*projection* of $Q_{(k-1)}(X)$ on $R_i(Y^i)$ only. Actually, as proved earlier [3], $Q^*_{(k)}(X)$ is an $I_1$-*projection* of $Q_{(k-1)}(X)$ on constraint set $\{R_i(Y^i), R_r(Y)\}$. □

Theorem 3.1 can be easily extended to the case of conditional constraints. When ***D-IPFP*** is applied to a set of constraints, according to Theorem 3.1, each iteration of ***D-IPFP*** for one constraint produces an $I_1$-*projection* of the previous distribution on a constraint set $\{R_i(Y^i), R_r(Y)\}$, so, similar to "Part 3" of the ***IPFP*** convergence proof in Section 3.1, the complete ***D-IPFP*** process converges to a distribution $Q^*(X)$ which is an $I_1$-*projection* of $Q_0(X)$ on $\Re \cup \{\forall R_r(Y)\} \cup \{R_r(X)\}$. $R_r(X)$ is also satisfied since in each iteration all other CPTs not related to $Y$ will be unchanged. Compare this result to that of ***E-IPFP***, the *I-divergence* $I(Q^*(X)\|Q_0(X))$ of ***D-IPFP*** will be slightly larger than that of ***E-IPFP***, since ***D-IPFP*** satisfies on more constraints. There is a trade off between accuracy and efficiency when choosing which algorithm to use.

Now the remaining problem is how to get a good $Y$ from $Y^i$?

**(Y1)** The extreme case is to let $Y = X$, and thus $S = \emptyset$, which reduces the ***D-IPFP*** process to ***E-IPFP***, or we could say that ***E-IPFP*** is a special case of ***D-IPFP*** with $Y = X$.

**(Y2)** A simplest case is to let $Y = Y^i$ (or $Y = Y^i \cup Z^i$ for conditional constraint). In this case, it is possible that some $X_i \in S$, which is the parent of $X_t \in Y^i$, is also a child of some $X_j \in Y^i$. Based on the BN independence assumption, if the CPT of $X_i$ is also allowed to be changed, the resulting distribution will have smaller *I-divergence* to the original distribution than that of **(Y2)** and this *I-divergence* will be very close to that of ***E-IPFP***, thus brings out the third method to get $Y$.

[3] As stated earlier, this ***D-IPFP*** for one constraint $R_i(Y^i)$ amounts to one application of a local ***E-IPFP***, so the convergence result of ***E-IPFP*** in Section 3.3 can be applied to here directly.

**(Y3)** Originally, $Y = Y^i$ (or $Y = Y^i \cup Z^i$ for conditional constraint) and $S = (\bigcup_{X_j \in Y^i} \pi_j) \backslash Y^i$, then repeat the following process until nothing more could be added to $Y$: if $X_i \in S$ and $X_j \in Y^i$ and $X_j \in \pi_i$, then $Y = Y \cup \{X_i\}$, $S = (S - \{X_i\}) \cup (\pi_i \backslash Y)$.

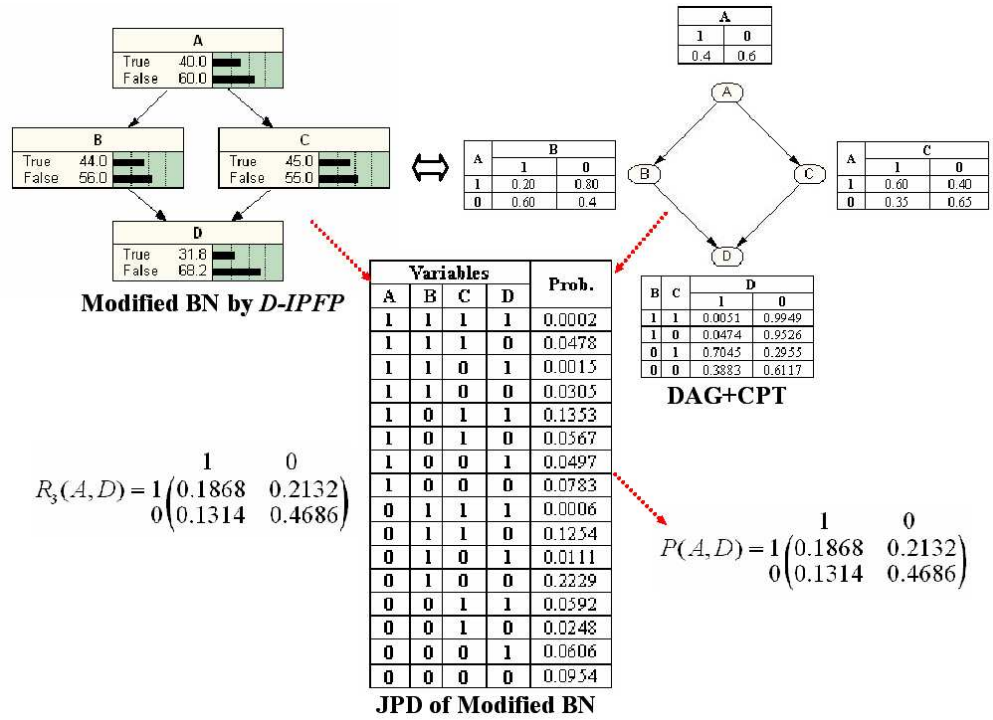



Fig. 3.6: **Running *D-IPFP*(Y2) with** $R_3(A, D)$

Consider again the network $\mathfrak{N}_4$ in Fig. 3.2 with a single non-local constraint $\{R_3(A, D)\}$, if we have $Y = \{A, D\}$ and $S = \{B, C\}$ by **(Y2)**, the new table $Q'(A, D|B, C)$ can be computed as the product of $Q(A)$ and $Q(D|B, C)$ of the original BN. For example, one entry of this table $Q'(A = 1, D = 0|B = 1, C = 1)$ is $0.4 * 0.9 = 0.36$. Then we applied ***D-IPFP*** to the BN in Fig. 3.2 with the non-local constraint $R_3(A, D)$. The process converged. The resulting BN satisfies the constraint $R_3(A, D)$, and only CPT for $D$ has been changed (See Fig. 3.6, note that the CPT for $A$ is not changed in this case but it is possible to be changed in other cases, but the CPTs for $B$ and $C$ will never be changed.). As expected, the *I-divergence* with ***D-IPFP*** was worse than that with ***E-IPFP*** (increased from **0.4419** to **0.7815**).

The moderate sacrifice in *I-divergence* with ***D-IPFP*** is rewarded by a signifi-

cant saving in computation. Since $R_i(Y^i)$ is now used to modify $Q'_{(k-1)}(Y|S)$, not $Q_{k-1}(X)$, the cost for each step is reduced from $O(2^n * 2^{|Y^i|})$ to $O(2^{|S|+|Y|} * 2^{|Y^i|})$, where $O(2^{|S|+|Y|})$ is the size of CPT $Q'_{(k-1)}(Y|S)$. The saving is thus in the order of $O(2^{n-|S|-|Y|})$.

## 3.5 SD-IPFP

A probabilistic constraint is *local* if it contains only one variable and some of its parents, i.e., $R_i(Y^i) = R_i(X_j, Z^j \subseteq \pi_j)$ for marginal constraint or $R_i(Y^i|Z^i) = R_i(X_j|Z^j \subseteq \pi_j)$ for conditional constraint. In either case, when applying ***D-IPFP*** to the constraint, $Y = \{X_j\}$, $S = \pi_j$, and Step 2.3 in Table 3.2 can be replaced by one step:

$$\begin{cases} Q_{(k)}(X_j|\pi_j) = Q_{(k-1)}(X_j|\pi_j) \cdot \frac{R_i(Y^i)}{Q_{(k-1)}(Y^i)} \cdot \alpha_k \\ Q_{(k)}(X_l|\pi_l) = Q_{(k-1)}(X_l|\pi_l) \quad for\ l \neq j \end{cases} \tag{3.13}$$

for marginal constraint $R_i(Y^i)$, where

$$\alpha_k = \sum_{x_j} Q_{(k-1)}(x_j|\pi_j) \frac{R_i(y^i)}{Q_{(k-1)}(y^i)}$$

$\alpha_k$ is the normalization factor. Similar equations can be obtained in case of conditional constraint. Since only the table for $X_j$ is changed, Eq. 3.11 is rewritten to:

$$Q_{(k)}(X) = Q_{(k)}(X_j|\pi_j) \cdot \prod_{l \neq j} Q_{(k-1)}(X_l|\pi_l) \tag{3.14}$$

Therefore $Q_{(k)}(X)$ is consistent with $G_0$, i.e., it satisfies the structural constraint. Eq. 3.14 can also be written as:

$$\begin{aligned} & Q_{(k)}(X) \\ & = Q_{(k-1)}(X_j|\pi_j) \cdot \frac{R_i(Y^i)}{Q_{(k-1)}(Y^i)} \cdot \alpha_k \cdot \prod_{l \neq j} Q_{(k-1)}(X_l|\pi_l) \end{aligned}$$

$$= Q_{(k-1)}(X) \cdot \frac{R_i(Y^i)}{Q_{(k-1)}(Y^i)} \cdot \alpha_k$$

Therefore, according to Eq. 2.6, $Q_{(k)}(X)$ is not an $I_1$-*projection* of $Q_{(k-1)}(X)$ on $R_i(Y^i)$ unless $\alpha_k = 1$.

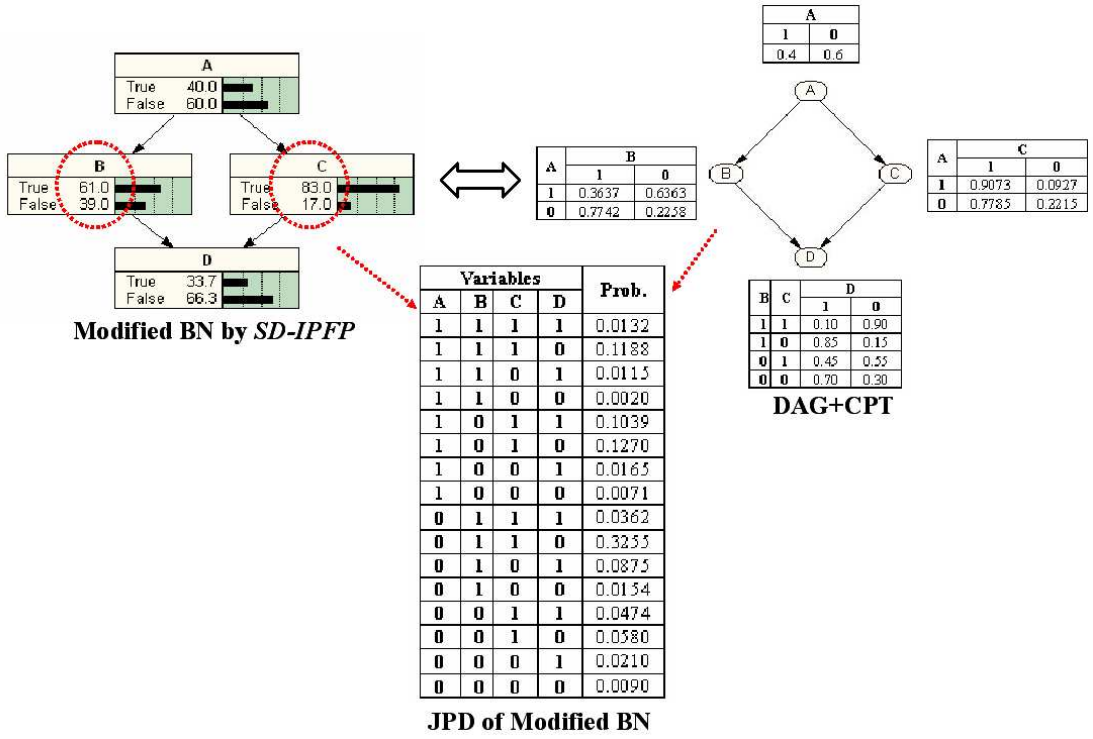



Fig. 3.7: **Running *SD-IPFP* with** $R_1(B)$ **and** $R_2(C)$

Recall the example in Fig. 3.3 where the standard ***IPFP*** of Eq. 2.6 is used to process two local constraints $R_1(B)$ and $R_2(C)$, three variables ($B$, $C$, and $A$) have their CPTs changed in the final BN. When Eq. 3.13 is applied, only tables for $B$ and $C$ have been changed in the final BN (Fig. 3.7). Its *I-divergence* to the original distribution is slightly larger than the one obtained by ***IPFP*** of Eq. 2.6 (increased from **0.5708** to **0.5711**).

## 3.6 The *IPFP* API

Surprisingly, one can not find any available code about ***IPFP***, which motivated me to implement an API for all the variants of ***IPFP*** algorithms, as discussed in previous sections. It is organized into three packages: "DiscreteProb" which includes classes and methods for storing and updating probability distributions, "GenericIPFP" which includes the implementations of the existing ***IPFP*** and ***C-IPFP*** algorithms, and "ExtendedIPFP" which includes the implementations of the extended ***E-IPFP***, ***D-IPFP***, ***SD-IPFP*** algorithms, as well as methods (included in the "Transform" module) used for extracting CPTs for a BN DAG from given JPD and methods used for obtaining MPDs for a set of variables from a given BN. The class diagram is shown in Fig. 3.8, the dashed arrow indicates the dependency between packages.

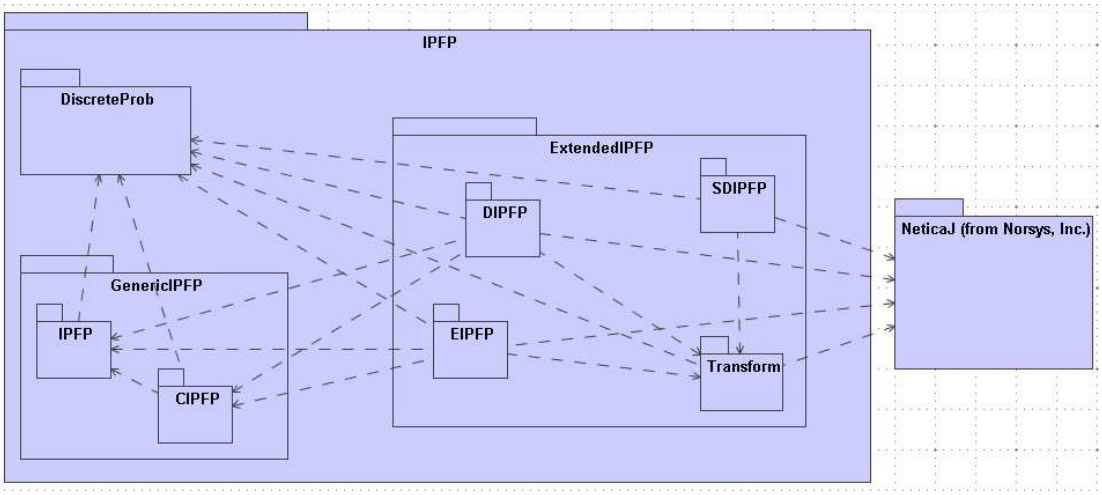



Fig. 3.8: **Class Diagram of the *IPFP* API**

There are many existing software packages for Bayesian networks that are written in various languages and provide different features in reasoning and learning. Interested readers may refer to `http://www.cs.ubc.ca/~murphyk/Bayes/bnsoft.html` for a complete list of packages and a tabular comparison among them, which is maintained by Kevin Murphy [4] in University of British Columbia, Canada. In my imple-

[4] `http://www.cs.ubc.ca/~murphyk/`

mentation, I used the NeticaJ API purchased from Norsys [5]. NeticaJ is implemented in Java and provided with complete Javadocs. It is powerful and easy to use. It can do belief updating using junction trees, parameter learning from case files, specifies findings to variables, and provides a graphic representation of the network. The classes and methods implemented in the "Transform" module are based on this API.

The realization of the different variants of ***IPFP*** algorithms depends on the successful implementation of the "DiscreteProb" module and the "Transform" module. While the latter can be easily implemented using the NeticaJ API, the former need to be dealt with great care. The core component of the "DiscreteProb" module is the simulation of a dynamic multi-dimensional array which is used to hold probability values. Classes for random variables and probability distributions are built upon this multi-dimensional array. A random variable has a name and a set of states. A JPD has a set of random variables, and an corresponding multi-dimensional array for probability values. A CPD has a set of prior random variables, a set of condition random variables, and an corresponding multi-dimensional array for probability values. Methods for JPD marginalization and for computation of distance measures between two JPDs such as *I-divergence* and *total variance* are also provided. The various ***IPFP*** algorithms are then implemented based on these methods. The experimental results shown in next section are obtained using this API.

## 3.7 Experiments

First, as shown in Fig. 3.9, a comparison is made among ***E-IPFP***, ***D-IPFP***($\mathbf{Y2}$), and ***D-IPFP***($\mathbf{Y3}$) for modifying $\mathbf{\mathcal{N}}_4$ in Fig. 3.2 with the constraint sets $\{R_3(A, D)\}$ and $\{R(B), R(C)\}$, respectively, when using the same stop criteria (i.e., when the *total variance* between JPDs obtained from two consecutive iterations is smaller than 0.0001). ***E-IPFP*** always has the minimal *total variance* and *I-divergence*, as proved

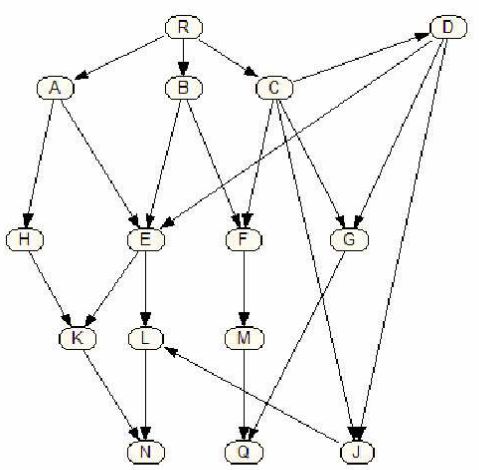
[5] `http://www.norsys.com/`

in Section 3.3. For constraint set $\{R_3(A, D)\}$, ***D-IPFP*(Y3)** is actually reduced to ***E-IPFP*** since $Y = \{A, B, C, D\}$ and $S = \emptyset$ in this particular case, so they have the same convergence results, as can be seen from the distance measures. Similarly, for constraint set $\{R(B), R(C)\}$, ***D-IPFP*(Y2)** and ***D-IPFP*(Y3)** are also reduced to same running steps in this particular case since they have obtained the same $Y$ and $S$ for both constraints, and their distance measures, are the same for sure. One thing to note is that for a BN with very small size, the actual running time of ***E-IPFP*** is not much worse than that of ***D-IPFP***, which we believe, is due to the overhead of ***D-IPFP*** caused by Step 2.2 and Step 2.3.1 in Table 3.2. So, in practice, for a network with small size, ***E-IPFP*** might be a better choice.

| Constraints | Num. of Iterations | | | Time Used (ms) | | | Total Variance $\lvert Q^* - Q_0 \rvert$ | | | I-divergence $I(Q^* \parallel Q_0)$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | E-IPFP | D-IPFP (Y2) | D-IPFP (Y3) | E-IPFP | D-IPFP (Y2) | D-IPFP (Y3) | E-IPFP | D-IPFP (Y2) | D-IPFP (Y3) | E-IPFP | D-IPFP (Y2) | D-IPFP (Y3) |
| $R_3$(A,D) | 21 | 29 | 10 | 218 | 378 | 217 | 0.6410 | 0.7772 | 0.6410 | 0.4419 | 0.7815 | 0.4419 |
| $R_1$(B), $R_2$(C) | 4 | 4 | 4 | 62 | 46 | 16 | 0.7600 | 0.7600 | 0.7600 | 0.5708 | 0.5711 | 0.5711 |

Fig. 3.9: **Experiment Results - 1**

To empirically validate the algorithms and to get a sense of how expensive this approach may be, we have conducted experiments within limited scope with an artificially made network of 15 discrete variables. The network structure is given in the top part of Fig. 3.10. Three sets of 4, 8, and 16 constraints, respectively, are selected for the experiments (as in the bottom part of Fig. 3.10). Each set contains a mix of local and non-local constraints. Number of variables in a constraint ranges from 1 to




**4 constraints: (2 local ones + 2 non-local ones)**
Local Marginal (1): {P(B)}
Local Conditional (1): {P(G|C)}
Non-local Marginal (1): {P(R,D)}
Non-local Conditional (1): {P(J|R)}

**8 constraints: (5 local ones + 3 non-local ones)**
Local Marginal (3): {P(B), P(C), P(H)}
Local Conditional (2): {P(F|C), P(N|K)}
Non-local Marginal (1): {P(R,D)}
Non-local Conditional (2): {P(N|R,D), P(Q|R,D)}

**16 constraints: (10 local ones + 6 non-local ones)**
Local Marginal (5): {P(A), P(B), P(C), P(H), P(M)}
Local Conditional (5): {P(E|B,D), P(F|B), P(F|C), P(G|C), P(N|K)}
Non-local Marginal (3): {P(R,D), P(K,L), P(N,Q)}
Non-local Conditional (3): {P(J|R), P(N|R,D), P(Q|R,D)}

Fig. 3.10: **A Network of 15 Variables**

3, the size of the subnet associated with a constraint ($|Y| + |S|$) ranges from 2 to 6. Therefore a saving in computational time would be in the order of $O(2^{15-6}) = O(2^9)$ if not including the overhead caused by Step 2.2 and Step 2.3.1 in Table 3.2. Both ***E-IPFP***, ***D-IPFP*(Y2)**, and ***D-IPFP*(Y3)** were run for each of the three sets using the same stop criteria (i.e., when the *total variance* between JPDs obtained from two consecutive iterations is smaller than 0.005). The program is a brute force implementation of the two algorithms without any optimization. The experiments were run on a DELL OPTIPLEX GX270 Intel Pentium 4 Desktop of 2.4GHz CPU, 1GB RAM, and 784M maximum memory for the JVM (Java Virtual Machine). The

results are reported in Fig. 3.11.

| Num. of Constraints | Num. of Iterations | | | Time Used (seconds) | | | Total Variance $\|Q^* - Q_0\|$ | | | I-divergence $I(Q^* \| Q_0)$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | E-IPFP | D-IPFP (Y2) | D-IPFP (Y3) | E-IPFP | D-IPFP (Y2) | D-IPFP (Y3) | E-IPFP | D-IPFP (Y2) | D-IPFP (Y3) | E-IPFP | D-IPFP (Y2) | D-IPFP (Y3) |
| 4 | 8 | 3 | 7 | 533 | 0.75 | 0.406 | 0.2757 | 0.4113 | 0.2785 | 0.0811 | 0.3401 | 0.0826 |
| 8 | 8 | 9 | 4 | 581 | 107 | 15 | 0.6192 | 0.6694 | 0.6226 | 0.5618 | 0.6292 | 0.5665 |
| 16 | 9 | 7 | 5 | 769 | 45 | 189 | 1.2579 | 1.2595 | 1.2593 | 2.5284 | 2.6146 | 2.5321 |

Fig. 3.11: **Experiment Results - 2**

Each of the 9 experimental runs converged to a distribution that satisfies all given constraints and is consistent with the network structure. As expected, ***D-IPFP*** is significantly faster than ***E-IPFP*** but with moderately larger *I-divergence*s when using (**Y2**) to get the $Y$ and $S$ in the algorithm. Also, from both Fig. 3.9 and Fig. 3.11 we can see that in general ***E-IPFP*** has smaller I-divergences, then ***D-IPFP***(**Y3**), and finally ***D-IPFP***(**Y2**). This is consistent with our theoretical analysis. The rate of speed up of ***D-IPFP*** is roughly in the theoretically estimated range ($O(2^9)$) for the case of 4 constraints, when the overhead is small. For the case of 8 and 16 constraints, the overhead used to find $Y$ and $S$ and extract local distributions $Q'_{(k-1)}(Y|S)$ from BN for each of the constraints in each iteration become significant with a network of size 15. However, ***D-IPFP*** is still much faster than ***E-IPFP***.

## 3.8 Summary

In this chapter, we developed algorithm ***E-IPFP*** that extends ***IPFP*** to modify probability distributions represented as Bayesian networks. The modification is done by only changing the conditional probability tables of the network while leaving the network structure intact. We also show a significant saving in computational cost can be achieved by decomposing the global ***E-IPFP*** into local ones with a much smaller scale, as described in algorithm ***D-IPFP***. Computer experiments within limited scope seem to validate the analysis results. These algorithms can be valuable tools in Bayesian network construction, merging and refinement when low-dimensional distributions need to be incorporated into the network. ***D-IPFP*** can be simplified and rewritten to ***SD-IPFP*** when only dealing with local constraints (priors or pair-wise marginals), which will be further extended in ***BayesOWL*** for CPT construction under the condition of a given set of hard evidences.

Several pieces of existing work are particularly relevant to this work, besides those related to the development of the original ***IPFP*** and proofs of its convergence. Diaconis and Zabell (1982) [37], in studying the role of Jeffrey's rule in updating subjective probability, consider ***IPFP*** as one of methods for mechanical updating of probability distribution. In contrast to other methods that are based on different assumptions on the subjectivity of the probabilities, the mechanical updating methods are based on some distance metrics, rather than "attempt to quantify one's new degree of belief via introspection".

Vomlel (1999) [152] studied in detail how ***IPFP*** can be used for probabilistic knowledge integration in which a joint probability distribution (the knowledge base) is built from a set of low dimensional distributions, each of which models a subdomain of the problem. Besides providing a cleaner, more readable convergence proof for ***IPFP***, he also studied the behavior of ***IPFP*** with input set generated by decomposable generating class. If such input distributions can be properly ordered,

***IPFP*** may converge in one or two cycles. This kind of input set roughly corresponds to ordering constraints for a Bayesian network in such a way that the constraint involving ancestors are applied before those involving descendants, if such order can be determined. For example, if all three constraints $\{R_1(B), R_2(C), R_3(A, D)\}$ must be met, we may be better off by applying $R_3(A, D)$ before the other two.

In all of these works, ***IPFP*** is applied to update joint distributions, none has discussed its application in modifying distributions represented by a BN.

To the best of our knowledge, the only work that applies ***IPFP*** to BN is the one by Valtorta et al (2000) [147]. In this work, ***IPFP*** is used to support belief update in BN by a set of soft evidences that are observed simultaneously. However, this work does not concern itself with updating the BN itself.

Algorithms developed in this chapter only work with consistent constraints. What will happen when the given probabilistic constraints are not consistent with each other? A number of computational experiments [152, 153] show that ***IPFP*** will either fail to find a distribution because of the violation of "dominance" or the $Q_{(k)}, k = 1, 2, 3, ...$ sequence will oscillate in cycles and never converge. How to handle inconsistent constraint is one of the important directions for future research. In Vomlel's thesis [152], he presents two basic approaches in solving this problem. The first is to define some "distance measure" from the marginals of a distribution in the oscillating sequence to the given constraints, and choose the one that minimizes the distance measure as the best solution of running ***IPFP***, however, this approach does not work in the case of "fails". The second approach, referred as "missing data methods", aims to modify the given inconsistent probabilistic constraints to make it workable for ***IPFP***, and is based on the assumption that the given probabilistic constraints are estimated as relative frequencies from data and the inconsistency comes from incomplete, incorrect, or missing data. In this case, methods from Statistics can be borrowed to analysis and process the inconsistent data.

Another direction is to investigate in what situations modification of only conditional probability tables is no longer sufficient or desirable, the network structure need also be changed in order to better satisfy given constraints.

Efficiency of this approach also needs serious investigation. As our experiments show, ***EIPFP*** in general is very expensive. The convergence time in our experiments with a small BN (15 nodes) and moderate number of constraints is in the order of tens of minutes when the stop criteria is low or hours when the stop criteria is high. The performance of even ***D-IPFP*** can be worse if some input distributions involve larger number of variables. Complexity can be reduced if we can divide a large constraint into smaller ones by exploring independence between the variables (possibly based on the network structure). Properly ordering the constraints may also help. Ultimately, this problem can only be solved by parallelizing the algorithms or by approximation when the network is really large.

# Chapter 4

# BayesOWL - A Probabilistic Extension to OWL

This chapter presents ***BayesOWL*** in detail. As mentioned earlier, ***BayesOWL*** is a framework which augments and supplements the semantic web ontology language OWL [1] for representing and reasoning with uncertainty based on Bayesian networks (BN) [121]. ***BayesOWL*** provides a set of rules and procedures for direct translation of an OWL taxonomy ontology into a BN directed acyclic graph (DAG), it also provides a method based on **iterative proportional fitting procedure** (***IPFP***) [79, 36, 33, 152, 18, 31] that incorporates available probabilistic constraints when constructing the conditional probability tables (CPTs) of the translated BN. The translated BN, which preserves the semantics of the original taxonomy ontology and is consistent with all the given probabilistic constraints, can support ontology reasoning, both within and across ontologies as Bayesian inferences. If two taxonomy ontologies are translated to two BNs, then concept mapping between these taxonomy ontologies can be accomplished by evidential reasoning across the translated BNs. Discussion and some preliminary works on this issue will be presented at the end of Chapter 5.

This chapter is organized as follows: Section 4.1 proposes a representation in OWL of probabilistic information concerning the entities and relations in ontologies which will be used as constraints to construct CPTs of the translated BN; Section 4.2 presents the structural translation rules; Section 4.3 presents the method used for CPT construction; Section 4.4 presents the semantics of ***BayesOWL***; Section 4.5 talks about the possible reasoning tasks. Section 4.6 describes the ***OWL2BN*** API

[1] http://www.w3.org/2001/sw/WebOnt/

for structural translation, which, together with the ***IPFP*** API described in Section 3.6, builds up an initial version of the ***BayesOWL*** framework. An example that translates an OWL taxonomy ontology of over 70 defined concepts into a BN DAG is presented. Section 4.7 compares ***BayesOWL*** to other related works. The chapter ends with discussion and suggestions for future research in Section 4.8.

## 4.1 Representing Probabilistic Information

Information about the uncertainty of the classes and relations in an ontology can often be represented as probability distributions (e.g., $P(C)$ and $P(C|D)$), which we refer to as probabilistic constraints on the ontology. These probabilities can be either provided by domain experts or learned from data.

The model-theoretic semantics [2] of OWL treats the domain as a non-empty collection of individuals. If class $A$ represents a concept, we treat it as a random binary variable of two states $a$ and $\bar{a}$, and interpret $P(A = a)$ as the prior probability or one's belief that an arbitrary individual belongs to class $A$, and $P(a|b)$ as the conditional probability that an individual of class $B$ also belongs to class $A$. Similarly, we can interpret $P(\bar{a})$, $P(\bar{a}|b)$, $P(a|\bar{b})$, $P(\bar{a}|\bar{b})$ and with the negation interpreted as "not belonging to".

Although not necessary, it is beneficial to represent the probabilistic constraints as OWL statements. We have developed such a representation. Currently, our translation framework only allows to encode two types of probabilities into the original ontology:

1. prior or marginal probability $P(C)$;
2. conditional probability $P(C|O_C)$ where $O_C \subseteq \pi_C$, $\pi_C \neq \emptyset$, $O_C \neq \emptyset$.

for a concept class $C$ and its parent superconcept class set $\pi_C$. This is because they correspond naturally to classes and relations (RDF triples) in an ontology, and are

[2] http://www.w3.org/TR/owl-semantics/direct.html

most likely to be available to ontology designers. The representation can be easily extended to constraints of other more general forms if needed.

We treat a probability as a kind of resource, and define two OWL classes: "PriorProb", "CondProb". A prior probability $P(C)$ of a variable $C$ is defined as an instance of class "PriorProb", which has two mandatory properties: "hasVarible" (only one) and "hasProbValue" (only one). A conditional probability $P(C|O_C)$ of a variable $C$ is defined as an instance of class "CondProb" with three mandatory properties: "hasCondition" (at least has one), "hasVariable" (only one), and "hasProbValue" (only one). The range of properties "hasCondition" and "hasVariable" is a defined class named "Variable", which has two mandatory properties: "hasClass" and "hasState". "hasClass" points to the concept class this probability is about and "hasState" gives the "True" (belong to) or "False" (not belong to) state of this probability. The defined ontology "prob.owl" is attached in "Appendix".

```
<Variable rdf:ID="c">
   <hasClass>C</hasClass>
   <hasState>True</hasState>
</Variable>
<PriorProb rdf:ID="P(c)">
   <hasVariable>c</hasVariable>
   <hasProbValue>0.8</hasProbValue>
</PriorProb>
```

Table 4.1: **Representing $P(c) = 0.8$ in OWL**

For example, $P(c) = 0.8$, the prior probability that an arbitrary individual belongs to class $C$, can be expressed as Table 4.1 and $P(c|p1, p2, p3) = 0.8$, the conditional probability that an individual of the intersection class of $P1$, $P2$, and $P3$ also belongs to class $C$, can be expressed as Table 4.2. For simplicity we did not consider the

namespaces in these examples.

| | |
|---|---|
| <Variable rdf:ID="c"> | <Variable rdf:ID="p3"> |
| <hasClass>C</hasClass> | <hasClass>P3</hasClass> |
| <hasState>True</hasState> | <hasState>True</hasState> |
| </Variable> | </Variable> |
| <Variable rdf:ID="p1"> | <CondProb rdf:ID="P(c\|p1, p2, p3)"> |
| <hasClass>P1</hasClass> | <hasCondition>p1</hasCondition> |
| <hasState>True</hasState> | <hasCondition>p2</hasCondition> |
| </Variable> | <hasCondition>p3</hasCondition> |
| <Variable rdf:ID="p2"> | <hasVariable>c</hasVariable> |
| <hasClass>P2</hasClass> | <hasProbValue>0.8</hasProbValue> |
| <hasState>True</hasState> | </CondProb> |
| </Variable> | |

Table 4.2: **Representing** $P(c|p1, p2, p3) = 0.8$ **in OWL**

## 4.2 Structural Translation

At the present time, ***BayesOWL*** is restricted to translating only OWL-DL concept taxonomies into BNs. This section focuses on the translation of an OWL taxonomy ontology into the network structure, i.e., the DAG of a BN. The task of constructing CPTs will be considered in the next section. For simplicity, constructors for header components in the ontology, such as "owl:imports" (for convenience, assume an ontology involves only one single OWL file), "owl:versionInfo", "owl:priorVersion", "owl:backwardCompatibleWith", and "owl:incompatibleWith" are ignored since they are irrelevant to the concept definition. Since the domain of discourse is treated as a non-empty collection of individuals ("owl:Thing"), then every concept class (either primitive or defined) can be thought as a countable subset (or subclass) of

"owl:Thing".

In the semantic web, an important component of an ontology defined in OWL or RDF(S) is the taxonomical concept subsumption hierarchy based on class axioms and logical relations among the concept classes. At the present time, we focus our attention to OWL ontologies defined using only constructors in these two categories (as in Table. 4.3). Constructors related to properties, individuals, and datatypes will be considered in the future.

| **Constructor** | **DL Syntax** | **Class Axiom** | **Logical Operator** |
|---|---|---|---|
| rdfs:subClassOf | $C_1 \sqsubseteq C_2$ | * | |
| owl:equivalentClass | $C_1 \equiv C_2$ | * | |
| owl:disjointWith | $C_1 \sqsubseteq \neg C_2$ and $C_2 \sqsubseteq \neg C_1$ | * | |
| owl:unionOf | $C \equiv C_1 \sqcup ... \sqcup C_n$ | | * |
| owl:intersectionOf | $C \equiv C_1 \sqcap ... \sqcap C_n$ | | * |
| owl:complementOf | $\neg C$ | | * |

Table 4.3: **Supported Constructors**

Conversion of an OWL concept taxonomy into a BN DAG is done by a set of structural translation rules. The general principle underlying these rules is that all classes (specified as "subjects" and "objects" in RDF triples of the OWL file) are translated into nodes (named **concept node**s) in BN, and an arc is drawn between two concept nodes in BN only if the corresponding two classes are related by a "predicate" in the OWL file, with the direction from the superclass to the subclass. A special kind of nodes (named **L-Node**s) are created during the translation to facilitate modeling relations among concept nodes that are specified by OWL logical operators. These structural translation rules are summarized as follows:

1. Every primitive or defined concept class $C$ is mapped into a binary variable node in the translated BN. Node $C$ in the BN can be either "True" or "False",

represented as $c$ or $\bar{c}$, indicating whether a given instance $o$ belongs to concept $C$ or not.

2. Constructor "**rdfs:subClassOf**" is modeled by a directed arc from the parent superclass node to the child subclass node. For example, a concept class $C$ defined with superconcept classes $C_i(i = 1, ..., n)$ by "rdfs:subClassOf" is mapped into a subnet in the translated BN with one converging connection from each $C_i$ to $C$, as illustrated in (Fig. 4.1).

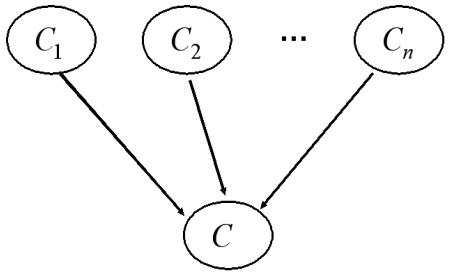



Fig. 4.1: **"rdfs:subClassOf"**

3. A concept class $C$ defined as the intersection of concept classes $C_i(i = 1, ..., n)$, using constructor "**owl:intersectionOf**" is mapped into a subnet (Fig. 4.2) in the translated BN with one converging connection from each $C_i$ to $C$, and one converging connection from $C$ and each $C_i$ to an L-Node called "LNodeIntersection".

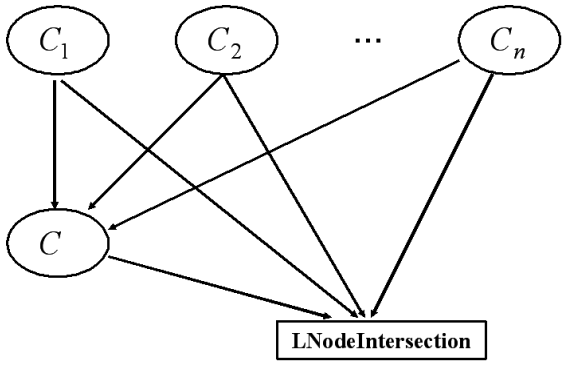



Fig. 4.2: **"owl:intersectionOf"**

4. A concept class $C$ defined as the union of concept classes $C_i (i = 1, ..., n)$, using constructor "**owl:unionOf**" is mapped into a subnet (Fig. 4.3) in the translated BN with one converging connection from $C$ to each $C_i$ , and one converging connection from $C$ and each $C_i$ to an L-Node called "LNodeUnion".

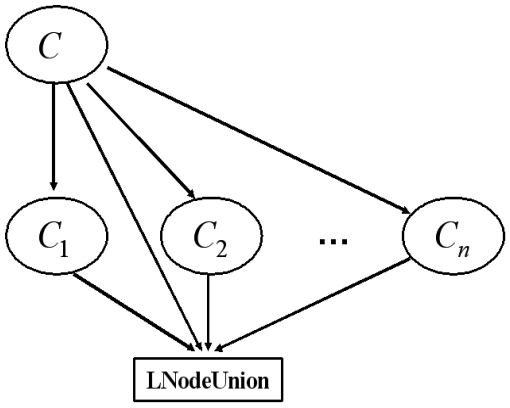



Fig. 4.3: **"owl:unionOf"**

5. If two concept classes $C_1$ and $C_2$ are related by constructors "**owl:complementOf**", "**owl:equivalentClass**", or "**owl:disjointWith**", then an L-Node (named "LNodeComplement", "LNodeEquivalent", "LNodeDisjoint" respectively, as in Fig. 4.4) is added to the translated BN, and there are directed links from $C_1$ and $C_2$ to the corresponding L-Node.

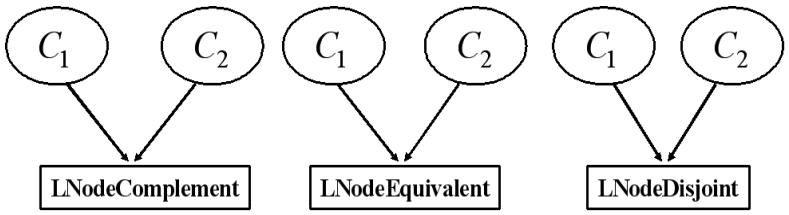



Fig. 4.4: **"owl:complementOf, owl:equivalentClass, owl:disjointWith"**

Based on rules 1 to 5, the translated BN contains two kinds of nodes: concept nodes for regular concept classes and L-Nodes which bridge concept nodes that are associated by logical relations. L-nodes are leaf nodes, with only in-arcs. With all logical relations, except "rdfs:subClassOf", handled by L-nodes, the in-arcs to a

concept node can only come from its parent superclass nodes. This makes $C$'s CPT smaller and easier to construct. L-nodes also help avoid forming cycles in translated BN. Since L-nodes are leaves, no cycles can be formed with L-nodes. The only place where cycles can be defined for OWL taxonomies is by "rdf:subClassOf" (e.g., $A$ is a subclass of $B$ and $B$ is a subclass of $A$). However, according to OWL semantics, all concepts involved in such a 'subclass' cycle are equivalent to each other. We can always detect this type of cycles in the pre-processing step and use rule 5, instead of rule 2, to handle the translation.

In the translated BN, all arcs are directed based on OWL statements, two concept nodes without any defined or derived relations are d-separated with each other, and two implicitly dependent concept nodes are d-connected with each other but there is no arc between them. Note that, this translation process may impose additional conditional independence to the nodes by the d-separation in the BN structure [121]. For example, consider nodes $B$ and $C$, which are otherwise not related except that they both are subclasses of $A$. Then in the translated BN, $B$ is conditionally independent of $C$, given $A$. Such independence can be viewed as a default relationship, which holds unless information to the contrary is provided. If dependency exists, it can be modeled by using additional nodes similar to the L-Nodes.

## 4.3 CPT Construction

To complete the translation the remaining issue is to assign a conditional probability table (CPT) $P(C|\pi_C)$ to each variable node $C$ in the DAG, where $\pi_C$ is the set of all parent nodes of $C$. As described earlier, the set of all nodes $X$ in the translated BN can be partitioned into two disjoint subsets: concept nodes $X_C$ which denote concept classes, and L-Nodes $X_L$ for bridging concept nodes that are associated by logical relations. In theory, the uncertainty information about concept nodes and

their relations may be available in probability distributions of any arbitrary forms, our observation, however, is that it is most likely to be available from the domain experts or statistics in the forms of prior probabilities of concepts and pair-wise conditional probabilities of concepts, given a defined superclass. Therefore, the method developed in this section accommodates two types of probabilities with respect to a concept node $C \in X_C$: prior probability $P(C)$, and conditional probability $P(C|O_C \subseteq \pi_C)$ where $O_C \neq \emptyset$, as mentioned earlier in Section 4.1. Methods for utilizing probabilities in arbitrary forms and dimensions [123] is reported in Chapter 3. Before going into the details of constructing CPTs for concept nodes in $X_C$ based on available probabilistic information, CPTs for the L-Nodes in $X_L$ are discussed first.

### CPTs for L-Nodes

CPT for an L-Node can be determined by the logical relation it represents so that when its state is "**True**", the corresponding logical relation holds among its parents. Based on the structural translation rules, there are five types of L-Nodes corresponding to the five logic operators in OWL: "LNodeComplement", "LNodeDisjoint", "LNodeEquivalent", "LNodeIntersection", and "LNodeUnion", their CPTs can be specified as follows:

1. **LNodeComplement**: The complement relation between $C_1$ and $C_2$ can be realized by "LNodeComplement = True iff $c_1\bar{c_2} \vee \bar{c_1}c_2$", which leads to the CPT in Table 4.4;

| C1 | C2 | True | False |
|---|---|---|---|
| True | True | 0.000 | 1.000 |
| True | False | 1.000 | 0.000 |
| False | True | 1.000 | 0.000 |
| False | False | 0.000 | 1.000 |

Table 4.4: **CPT of LNodeComplement**

2. **LNodeDisjoint**: The disjoint relation between $C_1$ and $C_2$ can be realized by "LNodeDisjoint = True iff $c_1\bar{c_2} \vee \bar{c_1}c_2 \vee \bar{c_1}\bar{c_2}$", which leads to the CPT in Table 4.5;

| C1 | C2 | True | False |
|---|---|---|---|
| True | True | 0.000 | 1.000 |
| True | False | 1.000 | 0.000 |
| False | True | 1.000 | 0.000 |
| False | False | 1.000 | 0.000 |

Table 4.5: **CPT of LNodeDisjoint**

3. **LNodeEquivalent**: The equivalence relation between $C_1$ and $C_2$ can be realized by "LNodeEquivalent = True iff $c_1c_2 \vee \bar{c_1}\bar{c_2}$", which leads to the CPT in Table 4.6;

| C1 | C2 | True | False |
|---|---|---|---|
| True | True | 1.000 | 0.000 |
| True | False | 0.000 | 1.000 |
| False | True | 0.000 | 1.000 |
| False | False | 1.000 | 0.000 |

Table 4.6: **CPT of LNodeEquivalent**

4. **LNodeIntersection**: The relation that $C$ is the intersection of $C_1$ and $C_2$ can be realized by "LNodeIntersection = True iff $cc_1c_2 \vee \bar{c}\bar{c_1}c_2 \vee \bar{c}c_1\bar{c_2} \vee \bar{c}\bar{c_1}\bar{c_2}$", which leads to the CPT in Table 4.7. If $C$ is the intersection of $n > 2$ classes, the $2^{n+1}$ entries in its CPT can be determined analogously.

5. **LNodeUnion**: The relation that $C$ is the union of $C_1$ and $C_2$ can be realized by "LNodeUnion = True iff $cc_1c_2 \vee c\bar{c_1}c_2 \vee cc_1\bar{c_2} \vee \bar{c}\bar{c_1}\bar{c_2}$", which leads to the CPT in Table 4.8. Similarly, if $C$ is the union of $n > 2$ classes, then the $2^{n+1}$ entries in its CPT can be obtained analogously.

When the CPTs for L-Nodes are properly determined as above, and the states of all the L-Nodes are set to "True", the logical relations defined in the original ontology

| C1 | C2 | C | True | False |
|---|---|---|---|---|
| True | True | True | 1.000 | 0.000 |
| True | True | False | 0.000 | 1.000 |
| True | False | True | 0.000 | 1.000 |
| True | False | False | 1.000 | 0.000 |
| False | True | True | 0.000 | 1.000 |
| False | True | False | 1.000 | 0.000 |
| False | False | True | 0.000 | 1.000 |
| False | False | False | 1.000 | 0.000 |

Table 4.7: **CPT of LNodeIntersection**

| C1 | C2 | C | True | False |
|---|---|---|---|---|
| True | True | True | 1.000 | 0.000 |
| True | True | False | 0.000 | 1.000 |
| True | False | True | 1.000 | 0.000 |
| True | False | False | 0.000 | 1.000 |
| False | True | True | 1.000 | 0.000 |
| False | True | False | 0.000 | 1.000 |
| False | False | True | 0.000 | 1.000 |
| False | False | False | 1.000 | 0.000 |

Table 4.8: **CPT of LNodeUnion**

will be held in the translated BN, making the BN consistent with the OWL semantics. Denoting the situation in which all the L-Nodes in the translated BN are in "True" state as $\boldsymbol{\tau}$, the CPTs for the concept nodes in $X_C$ should be constructed in such a way that $P(X_C|\boldsymbol{\tau})$, the joint probability distribution of all concept nodes in the subspace of $\boldsymbol{\tau}$, is consistent with all the given prior and conditional probabilistic constraints. This task is difficult for two reasons. First, the constraints are usually not given in the form of CPT. For example, CPT for a concept node $C$ with two parents $A$ and $B$ is in the form of $P(C|A,B)$ but a constraint may be given as $Q(C|A)$ or even $Q(C)$. Secondly, CPTs are given in the general space of $X = X_C \cup X_L$ but constraints are for the subspace of $\boldsymbol{\tau}$ (the dependencies changes when going from the general space

to the subspace of $\boldsymbol{\tau}$). For example, for constraint $Q(C|A)$, $P(C|A,B)$, the CPT for $C$, should be constructed in such a way that $P(C|A,\boldsymbol{\tau}) = Q(C|A)$.

To overcome these difficulties, an algorithm is developed to approximate these CPTs for $X_C$ based on the ***SD-IPFP*** algorithm developed in Section 3.5.

**Constructing CPTs for Concept Nodes**

Let $X = \{X_1, X_2, ..., X_n\}$ be the set of binary variables in the translated BN. As stated earlier, $X$ is partitioned into two disjoint sets $X_C$ and $X_L$, for concept nodes, and L-Nodes, respectively. As a BN, by chain rule [121] we have $Q(X) = \prod_{X_i \in X} Q(X_i|\pi_{X_i})$. Now, given a set of probabilistic constraints in the form of either $P(C_i)$ or $P(C_i|O_{C_i})$ where $O_{C_i} \subseteq \pi_{C_i}$, $\pi_{C_i} \neq \emptyset$, $O_{C_i} \neq \emptyset$ for $C_i \in X_C$, our objective is to construct CPTs $Q(C_i|\pi_{C_i})$ for each $C_i$ in $X_C$ such that $Q(X_C|\boldsymbol{\tau})$, the joint probability distribution of $X_C$ in the subspace of $\boldsymbol{\tau}$, is consistent with all the given constraints. Moreover,we want $Q(X_C|\boldsymbol{\tau})$ to be as close as possible to the initial distribution, which may be set by human experts, by some default rules, or by previously available probabilistic information.

Note that all parents of $C_i$ are concept nodes, which are superclasses of $C_i$ defined in the original ontology. The superclass relation can be encoded by letting every entry in $Q(C_i|\pi_{C_i})$ be zero (i.e., $Q(c_i|\pi_{C_i}) = 0$ and $Q(\bar{c}_i|\pi_{C_i}) = 1$) if any of its parents is "**False**" in that entry. The only other entry in the table is the one in which all parents are "**True**". The probability distribution for this entry indicates the degree of inclusion of $C_i$ in the intersection of all its parents, and it should be filled in such a way that is consistent with the given probabilistic constraints relevant to $C_i$. Construction of CPTs for all concept nodes thus becomes a constraint satisfaction problem in the scope of ***SD-IPFP*** developed in Section 3.5 for local constraints. However, ***SD-IPFP*** need to be slightly modified to work under the subspace of $\boldsymbol{\tau}$.

Let $Q_{(k)}(X_C|\boldsymbol{\tau})$ be a distribution projected from $Q_{(k)}(X_C, X_L)$ with $X_L = \boldsymbol{\tau}$ (that

is, every L-Node $B_j$ in $X_L$ is set to $b_j$, the "True" state). Then by chain rule,

$$\begin{aligned} & Q_{(k)}(X_C|\boldsymbol{\tau}) \\ & = \frac{Q_{(k)}(X_C, \boldsymbol{\tau})}{Q_{(k)}(\boldsymbol{\tau})} \\ & = \frac{Q_{(k)}(C_i|\pi_{C_i}) \cdot \prod\limits_{B_j \in X_L} Q_{(k)}(b_j|\pi_{B_j}) \cdot \prod\limits_{V_j \in X_C, j \neq i} Q_{(k)}(V_j|\pi_{V_j})}{Q_{(k)}(\boldsymbol{\tau})} \end{aligned} \tag{4.1}$$

Since each probabilistic constraint is *local* to the CPT for some $C_i \in X_C$, it can just be represented as $R(C_i|O_{C_i} \subseteq \pi_{C_i})$. Apply Eq. 2.7 to $Q_{(k)}(X_C|\boldsymbol{\tau})$ with respect to constraint $R(C_i|O_{C_i})$ at step $k$,

$$Q_{(k)}(X_C|\boldsymbol{\tau}) = Q_{(k-1)}(X_C|\boldsymbol{\tau}) \cdot \frac{R(C_i|O_{C_i})}{Q_{(k-1)}(C_i|O_{C_i}, \boldsymbol{\tau})} \tag{4.2}$$

Then after substituting on both sides of Eq. 4.2 with Eq. 4.1 and cancelling out all CPTs other than $Q(C_i|\pi_{C_i})$, we get our modified ***SD-IPFP*** procedure under the subspace of $\boldsymbol{\tau}$ as:

$$Q_{(k)}(C_i|\pi_{C_i}) = Q_{(k-1)}(C_i|\pi_{C_i}) \cdot \frac{R(C_i|O_{C_i})}{Q_{(k-1)}(C_i|O_{C_i}, \boldsymbol{\tau})} \cdot \alpha_{(k-1)}(\pi_{C_i}) \tag{4.3}$$

where $\alpha_{(k-1)}(\pi_{C_i}) = Q_{(k)}(\boldsymbol{\tau})/Q_{(k-1)}(\boldsymbol{\tau})$ is the normalization factor.

The process starts with $Q_{(0)} = P_{init}(X)$, the initial distribution of the translated BN where CPTs for L-Nodes are set as described earlier in this section and CPTs for concept nodes in $X_C$ are set to some distributions consistent with the semantics of the subclass relation. At each iteration, $\boldsymbol{\tau}$ is specified as a set of hard evidences to the original BN, and only one table, $Q_{(k)}(C_i|\pi_{C_i})$, is modified. ***SD-IPFP*** by Eq. 4.3 converges because Eq. 4.3 realizes Eq. 4.2, a direct application of Eq. 2.7, which has been shown to converge in [31]. It will be more complicated if non-local constraints are provided, e.g., $P(A|B)$, where $A$, $B$ are non-empty subsets of $X_C$ involving variables

in multiple CPTs. Extending ***SD-IPFP*** to handle non-local constraints [123] of more general form can be found in Chapter 3.

Some other general optimization methods such as simulated annealing (SA) and genetic algorithm (GA) can also be used to construct CPTs of the concept nodes in the translated BN. However, they are much more expensive and the quality of results is often not guaranteed. Experiments show that ***SD-IPFP*** converges quickly (in seconds, most of the time in less than 30 iterative steps), despite its exponential time complexity in theoretical analysis. The space complexity of ***SD-IPFP*** is trivial since each time only one node's CPT, not the entire joint probability table, is manipulated. Experiments also verify that the order in which the constraints are applied do not affect the solution (but may affect the speed), and the values of the initial distribution $Q_{(0)}(X) = P_{init}(X)$ (but avoid 0 and 1) do not affect the convergence.

**Put It All Together: An Example**

Readers may get confused without given an illustration example. A simple taxonomy ontology about nature domain is used here to demonstrate the basic ideas and the validity of the approach (The ontology "nature.owl" is attached in "Appendix"). In this ontology, six concepts and their relations are defined as follows:

- "*Animal*" *is a primitive concept class*;
- "*Male*", "*Female*", "*Human*" *are* **subclasses** *of* "*Animal*";
- "*Male*" *and* "*Female*" *are* **disjoint** *with each other*;
- "*Man*" *is the* **intersection** *of* "*Male*" *and* "*Human*";
- "*Woman*" *is the* **intersection** *of* "*Female*" *and* "*Human*"; *and*
- "*Human*" *is the* **union** *of* "*Man*" *and* "*Woman*".

And the following local probabilistic constraints are attached to $X_C = \{$Animal, Male, Female, Human, Man, Woman$\}$:

- $P(Animal) = 0.5$
- $P(Male|Animal) = 0.5$
- $P(Female|Animal) = 0.48$
- $P(Human|Animal) = 0.1$
- $P(Man|Human) = 0.49$
- $P(Woman|Human) = 0.51$

When translating this ontology into BN, first the DAG of the BN is constructed (as described in Section 4.2), then the CPTs for L-Nodes in $X_L$ = {LNodeUnion_0, LNodeIntersection_0, LNodeIntersection_1, LNodeDisjoint_0} (as described in the first part of Section 4.3) are specified, and finally the CPTs of concept nodes in $X_C$ are approximated by running ***SD-IPFP*** from Eq. 4.3.

Fig. 4.5 shows the resulting BN, with the indices of L-Nodes start from zero. It can be seen that, when all L-Nodes are set to "**True**", the conditional probability of "Male", "Female", and "Human", given "Animal", are **0.5**, **0.48**, and **0.1**, respectively, the same as the given probabilistic constraints. All other constraints, which are ignored due to space limitation, are also satisfied.

The CPTs of concept nodes obtained by ***SD-IPFP*** from Eq. 4.3 are listed in Fig. 4.6. It can be seen that the values on the first rows in all CPTs have been changed to different values from their initial values of (0.5, 0.5).

## 4.4 Semantics of BayesOWL

The semantics of the Bayesian network obtained can be outlined as follows.

- The translated BN will be associated with a joint probability distribution $P'(X_C)$ over the set of concept nodes $X_C$, and $P'(X_C) = P(X_C|\boldsymbol{\tau})$ (which can be computed by first getting the product of all the CPTs in the BN, and then marginalizing it to the subspace of $\boldsymbol{\tau}$), on top of the standard description logic semantics.

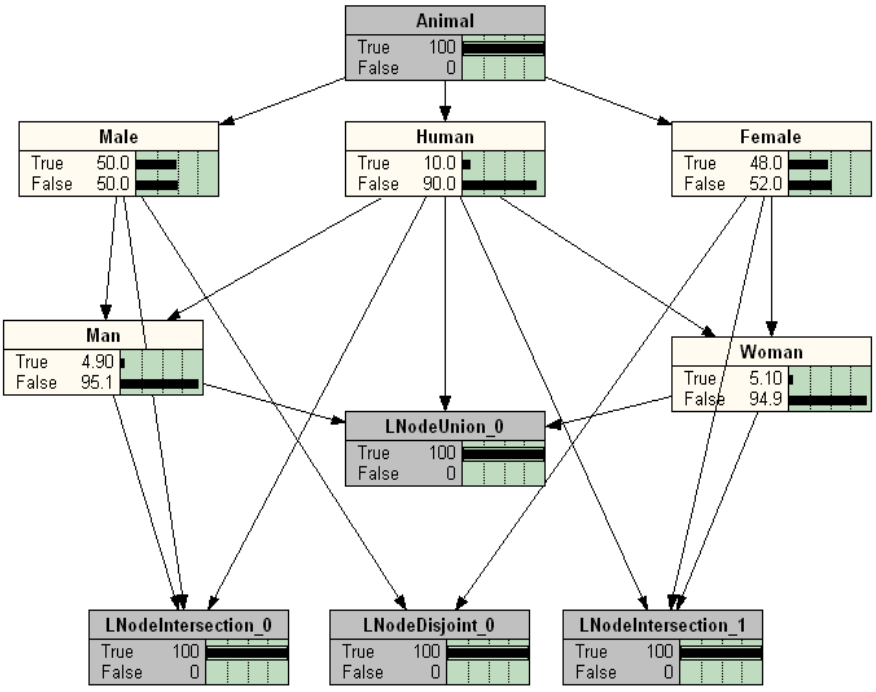



Fig. 4.5: **Example I - DAG of Translated BN**

| Animal | |
|---|---|
| **True** | **False** |
| 0.92752 | 0.07248 |

| Animal | Human | |
|---|---|---|
| | **True** | **False** |
| True | 0.18773 | 0.81227 |
| False | 0.0 | 1.0 |

| Animal | Female | |
|---|---|---|
| | **True** | **False** |
| True | 0.95469 | 0.04531 |
| False | 0.0 | 1.0 |

| Animal | Male | |
|---|---|---|
| | **True** | **False** |
| True | 0.95677 | 0.04323 |
| False | 0.0 | 1.0 |

| Male | Human | Man | |
|---|---|---|---|
| | | **True** | **False** |
| True | True | 0.47049 | 0.52951 |
| True | False | 0.0 | 1.0 |
| False | True | 0.0 | 1.0 |
| False | False | 0.0 | 1.0 |

| Female | Human | Woman | |
|---|---|---|---|
| | | **True** | **False** |
| True | True | 0.51433 | 0.48567 |
| True | False | 0.0 | 1.0 |
| False | True | 0.0 | 1.0 |
| False | False | 0.0 | 1.0 |

Fig. 4.6: **Example I - CPTs of Translated BN**

A description logic interpretation $\boldsymbol{I} = (\Delta^{\boldsymbol{I}}, .^{\boldsymbol{I}})$ consists of a non-empty domain of objects $\Delta^{\boldsymbol{I}}$ and an interpretation function $.^{\boldsymbol{I}}$. This function maps every concept to a subset of $\Delta^{\boldsymbol{I}}$, every role and attribute to a subset of $\Delta^{\boldsymbol{I}} \times \Delta^{\boldsymbol{I}}$, and every individual to an object of $\Delta^{\boldsymbol{I}}$. An interpretation $\boldsymbol{I}$ is a model for a concept $C$ if $C^{\boldsymbol{I}}$ is non-empty, and $C$ is said "satisfiable". Besides this description logic interpretation $\boldsymbol{I} = (\Delta^{\boldsymbol{I}}, .^{\boldsymbol{I}})$, in ***BayesOWL*** semantics, there is a function Pr to map each object $o \in \Delta^{\boldsymbol{I}}$ to a value between 0 and 1, $0 \leq \Pr(o) \leq 1$, and $\sum \Pr(o) = 1, \text{for all } o \in \Delta^{\boldsymbol{I}}$. This is the probability distribution over all the domain objects. For a class $C$: $P'(C) = \sum \Pr(o)$ for all $o \in C$. If $C$ and $D$ are classes and $C \subseteq D$, then $P'(C) \leq P'(D)$. Then, for a node $C_i$ in $X_C$, $P'(C_i) = P(C_i|\boldsymbol{\tau})$ represents the probability distribution of an arbitrary object belonging (and not belonging) to the concept represented by $C_i$.

- In the translated BN, when all the L-Nodes are set to "**True**", all the logical relations specified in the original OWL file will be held, which means:

  1. if $B$ is a subclass of $A$ then "$P'(b|\bar{a}) = 0 \wedge P'(a|b) = 1$";
  2. if $B$ is disjoint with $A$ then "$P'(b|a) = 0 \wedge P'(a|b) = 0$";
  3. if $A$ is equivalent with $B$ then "$P'(a) = P'(b)$";
  4. if $A$ is complement of $B$ then "$P'(a) = 1 - P'(b)$";
  5. if $C$ is the intersection of $C_1$ and $C_2$ then "$P'(c|c_1, c_2) = 1 \wedge P'(c|\bar{c_1}) = 0 \wedge P'(c|\bar{c_2}) = 0 \wedge P'(c_1|c) = 1 \wedge P'(c_2|c) = 1$"; and
  6. if $C$ is the union of $C_1$ and $C_2$ then "$P'(c|\bar{c_1}, \bar{c_2}) = 0 \wedge P'(c|c_1) = 1 \wedge P'(c|c_2) = 1 \wedge P'(c_1|\bar{c}) = 0 \wedge P'(c_2|\bar{c}) = 0$".

  Note it would be trivial to extend 5 and 6 to general case.

- Due to d-separation in the BN structure, additional conditional independencies may be imposed on the concept nodes in $X_C$ in the translated BN. These are

caused by the independence relations assumed in the three (serial, diverging, converging, as in Fig. 2.3) types of BN connections:

1. serial connection: consider $A$ is a parent superclass of $B$, $B$ is a parent superclass of $C$, then the probability of an object $o$ belonging to $A$ and belonging to $C$ is independent if $o$ is known to be in $B$;
2. diverging connection: $A$ is the parent superclass for both $B$ and $C$, then $B$ and $C$ is conditionally independent given $A$;
3. converging connection: both $B$ and $C$ are parent superclasses of $A$, then $B$ and $C$ are assumed to be independent if nothing about $A$ is known.

These independence relations can be viewed as a default relationship, which are compatible with the original ontology since there is no information to the contrary in the OWL file that defines this ontology.

## 4.5 Reasoning

The ***BayesOWL*** framework can support common ontology reasoning tasks as probabilistic reasoning in the translated BN. The follows are some of the example tasks.

- **Concept Satisfiability**: Test whether the concept represented by a description $e$ exists. This can be answered by determining if $P(e|\boldsymbol{\tau}) = 0$, which can be computed by applying the chain rule of BN.
- **Concept Overlapping**: Compute the degree of the overlap or inclusion of a description $e$ by a concept $C$. This can be measured by $P(e|c, \boldsymbol{\tau})$, which can be computed by applying general BN belief update algorithms. If $P(e|c, \boldsymbol{\tau}) = 0$, then $e$ and $C$ are disjoint with each other; if $P(e|c, \boldsymbol{\tau}) = 1$, then $e$ is a subsumer of $C$; otherwise, $P(e|c, \boldsymbol{\tau})$ will have a value between $\mathbf{0}$ and $\mathbf{1}$, and either $C$ is a subsumer of $e$, or $e$ and $C$ have some overlap with each other. Moreover, when

only considering subsumers of $e$ (i.e., $P(c|e,\boldsymbol{\tau}) = 1$), the $C$ with the greatest $P(e|c,\boldsymbol{\tau})$ value is a most specific subsumer of $e$.

- **Concept Subsumption**: Instead of finding the most specific subsumer of a given description $e$, find the concept $C$ that is most similar to $e$. This task cannot be done by simply computing the posterior $P(e|c,\boldsymbol{\tau})$, because any subsumee $C$ of $e$ will make its value be $\mathbf{1}$. Instead, a similarity measure $MSC(e,C)$ between $e$ and $C$ based on Jaccard Coefficient [149] is defined:

$$MSC(e,C) = P(e \cap C|\boldsymbol{\tau})/P(e \cup C|\boldsymbol{\tau}) \tag{4.4}$$

Since $P(e \cup C|\boldsymbol{\tau}) = P(e|\boldsymbol{\tau}) + P(C|\boldsymbol{\tau}) - P(e \cap C|\boldsymbol{\tau})$, Eq. 4.4 can be rewritten as:

$$MSC(e,C) = P(e \cap C|\boldsymbol{\tau})/(P(e|\boldsymbol{\tau}) + P(C|\boldsymbol{\tau}) - P(e \cap C|\boldsymbol{\tau})) \tag{4.5}$$

This measure is intuitive and easy-to-compute since now each of the components can be computed by applying general BN belief update algorithms. In particular, when only considering subsumers of $e$ (i.e., $P(c|e,\boldsymbol{\tau}) = 1$), this measure is reduced to $P(e|c,\boldsymbol{\tau})$, then the $C$ with the greatest $MSC$ value is a most specific subsumer of $e$.

In the previous example ontology (see Fig. 4.5), to find the concept that is most similar to the description $e = \neg Male \sqcap Animal$, we compute the similarity measure between $e$ and each of the nodes in $X_C$ = {Animal, Male, Female, Human, Man, Woman} using Eq. 4.5, and $e$ is applied as a set of hard evidences to the BN, then we have:

- $MSC(e, Animal) = 0.5004$
- $MSC(e, Male) = 0.0$
- $MSC(e, Female) = \mathbf{0.9593}$
- $MSC(e, Human) = 0.0928$

- $MSC(e, Man) = 0.0$
- $MSC(e, Woman) = 0.1019$

This leads us to conclude that "Female" is the most similar concept to $e$. When a traditional DL reasoner such as Racer [3] is used, the same description would have "Animal" as the most specific subsumer, a clear over generalization.

Reasoning with uncertain input descriptions can also be supported. As mentioned earlier in Subsection 2.2.1, BNs support three kinds of evidences: hard, soft, and virtual, so $e$ is not only restricted to hard evidences, it can also be a set of soft or virtual evidences, and $MSC(e, C)$ can still be easily computed as long as $e$ can be correctly applied to the BN. For example, an uncertain input description $e'$ containing two soft evidences $P(Male) = 0.1$ and $P(Animal) = 0.7$ can be processed by inputting these probabilities as virtual evidences to the BN. Pearl [122] has shown that a soft evidence $Q(X_i)$ to a binary node $X_i$ can be formally equivalent to add a virtual node $ve_i$ as a child of $X_i$ with the CPT of $ve_i$ given by the likelihood ratio:

$$L(X_i) = \frac{P(ve_i|x_i)}{P(ve_i|\overline{x_i})} = \frac{P(x_i)Q(\overline{x_i})}{Q(x_i)P(\overline{x_i})} \tag{4.6}$$

This method can be easily extended to multi-valued variables but only works for one such evidence. [117, 147] further extends it to handle multiple soft evidences simultaneously. Back to the above two soft evidences $P(Male) = 0.1$ and $P(Animal) = 0.7$, first they can be computed as equivalent to the following virtual evidences to the BN of Fig. 4.5 under the subspace of $\boldsymbol{\tau}$:

- $P(ve_1|Animal = True) = 1.0$
- $P(ve_1|Animal = False) = 0.25058582$
- $P(ve_2|Male = True) = 0.1669985$
- $P(ve_2|Male = False) = 1.0$

[3] http://www.racer-systems.com/index.phtml

This is illustrated in Fig. 4.7. Similarly, we compute the similarity measure between $e'$ and each of the nodes in $X_C$ = {Animal, Male, Female, Human, Man, Woman} using Eq. 4.5 and get:

- $MSC(e', Animal) = 0.4668$
- $MSC(e', Male) = 0.0667$
- $MSC(e', Female) = \mathbf{0.5753}$
- $MSC(e', Human) = 0.0676$
- $MSC(e', Man) = 0.0094$
- $MSC(e', Woman) = 0.0611$

It can be seen that class "Female" remains the most similar concept to $e'$, but its similarity value $MSC(e', Female)$ now decreases to **0.5753**.

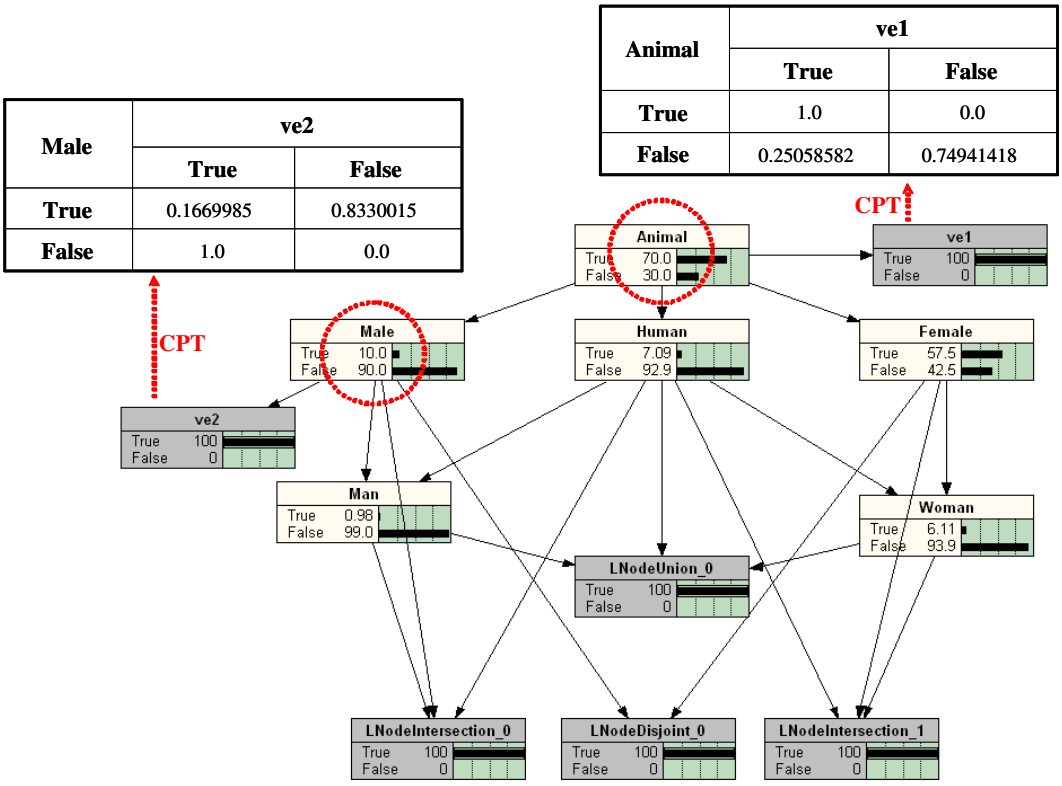



Fig. 4.7: **Example I - Uncertain Input to Translated BN**

## 4.6 The *OWL2BN* API

To support the actual usage of ***BayesOWL***, an early version of the prototype has been implemented in Java, which includes two major APIs (Fig. 4.8): *OWL2BN* for translating an OWL-DL taxonomy into a BN DAG, and *IPFP* for various ***IPFP*** algorithms as described in Section 3.6, some of which are used by *OWL2BN* for CPT construction.

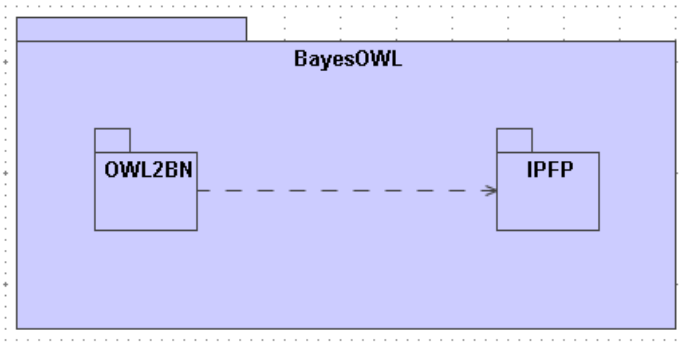



Fig. 4.8: **Package Overview Diagram**

Implementation of the *OWL2BN* API is much easier than the *IPFP* API, since there are many existing tools help to make the components. Basically, to translate an OWL taxonomy ontolgy into a BN DAG, first one needs to make sure that the provided ontology is both syntactically valid (using Jena [4], a Java framework for building semantic web applications which provides an RDF API, an OWL API, and a rule-based inference engine) and semantically consistent (using Pellet [5], a Java based OWL DL reasoner for species validation, consistency checking, concept classification, etc, which can be used in conjunction with Jena). Next, in the pre-processing step, by using the OWL API in Jena, for each concept class, one could collect information about its parent concept classes, its child subclasses, its equivalent classes, the classes it is disjoint with, as well as information related to union, intersection and complement relations among concept classes. Using the information collected and our translation

[4] `http://jena.sourceforge.net/index.html`
[5] `http://www.mindswap.org/2003/pellet/index.shtml`

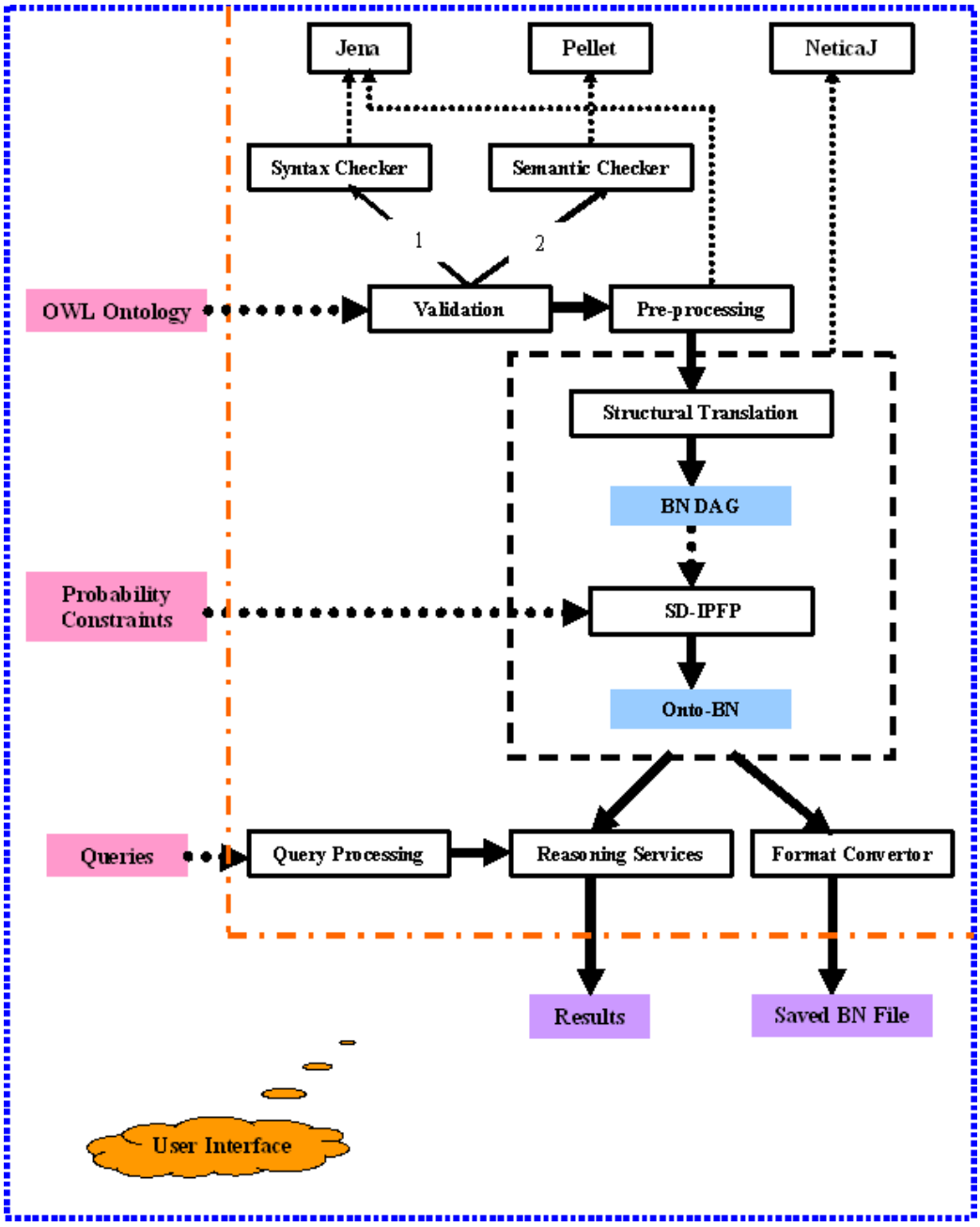



Fig. 4.9: **Architecture of the *OWL2BN* API**

rules, one can generate a BN DAG easily using the NeticaJ API, with the CPTs for L-Nodes assigned as discussed in Section 4.3. With this DAG, and a set of probabilistic constraints provided, one can use the ***SD-IPFP*** algorithm in the *IPFP* API to generate CPTs for each concept node. Later, one can use this translated BN in reasoning, and one could save it into a file. The architecture is shown in Fig. 4.9.

The example shown in Section 4.3 is obtained using this API. The index number of the L-Nodes starts from zero, and if the ontology provides several disconnected taxonomies, each will be translated into a BN, though they can be still included in one .dne file of Netica. Fig. 4.10 and Fig. 4.11 shows the translated BN of a larger ontology in the nature domain with 71 concept classes defined by "owl:Class" (2 of them are defined via "owl:intersectionOf", 1 of them are defined via "owl:unionOf"), 11 "disjoint" relations defined by "owl:disjointWith", 1 "equivalent" relation defined by "owl:equivalentClass" and 80 "subclass" relations defined by "rdfs:subClassOf". The translated BN, includes 71 concept nodes, 15 L-nodes, and a total number of 84 "superclass → subclass" arcs, the degree of connectivity of each concept node is same as the "subClassOf" relations [6] that the node is involved with.

The current APIs are provided with Javadocs to be used by developers or researchers who are familiar with Java. The goal of the next version of these APIs is to design and implement GUI interfaces, which can be used by novice users of Java or common users who do not know Java at all.

## 4.7 Comparison to Existing Works

The works closest to ***BayesOWL*** [40] are P-CLASSIC [76] and PTDL [159]. One major difference lies in CPTs. As mentioned earlier in Subsection 2.3.1, neither P-CLASSIC nor PTDL provides a method to construct CPTs. In contrast, one of

[6] Here it includes the implicit "subClassOf" relations imposed by "unionOf" and "intersectionOf" relations.

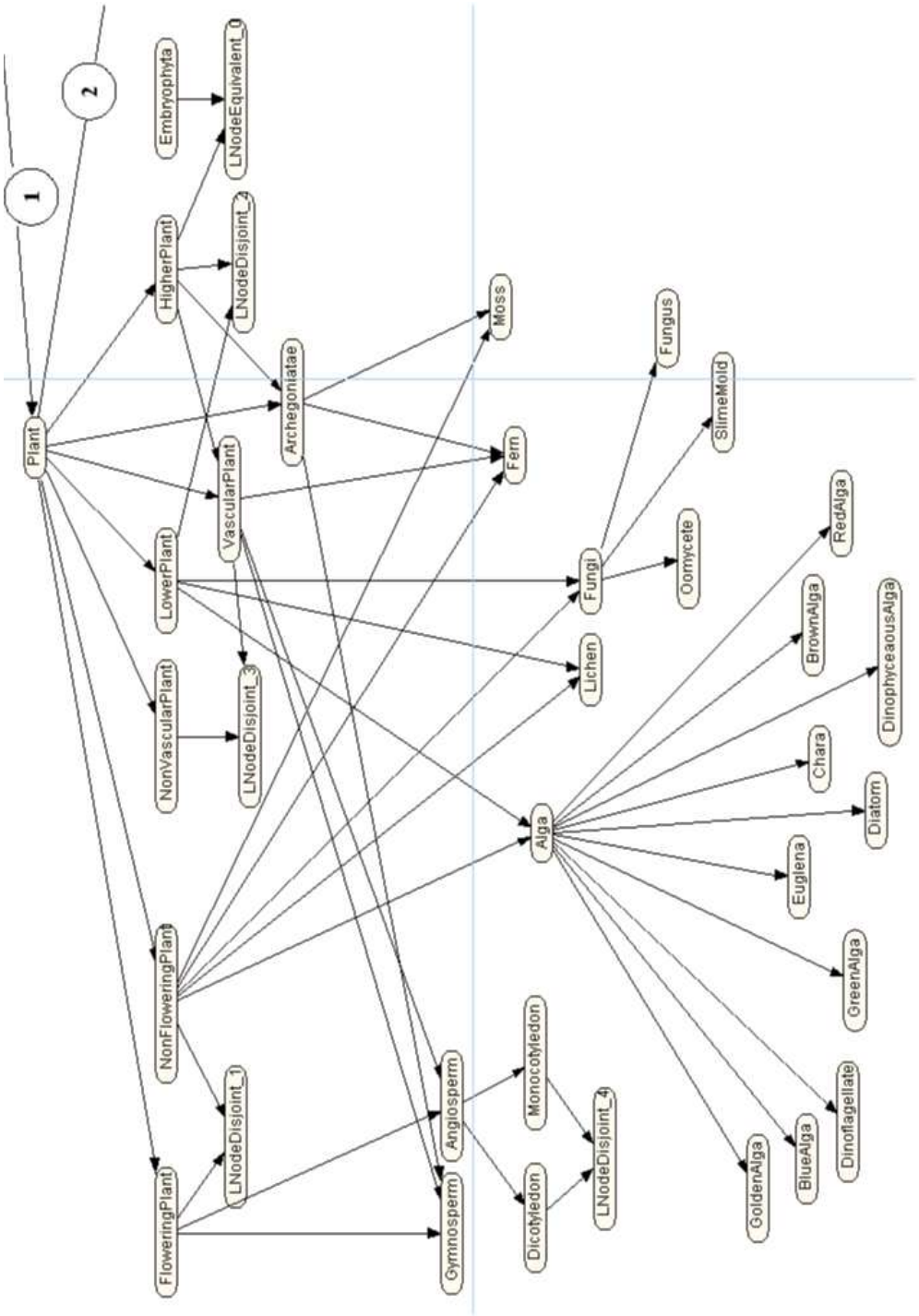



Fig. 4.10: **An Ontology with 71 Concept Classes, Part 1**

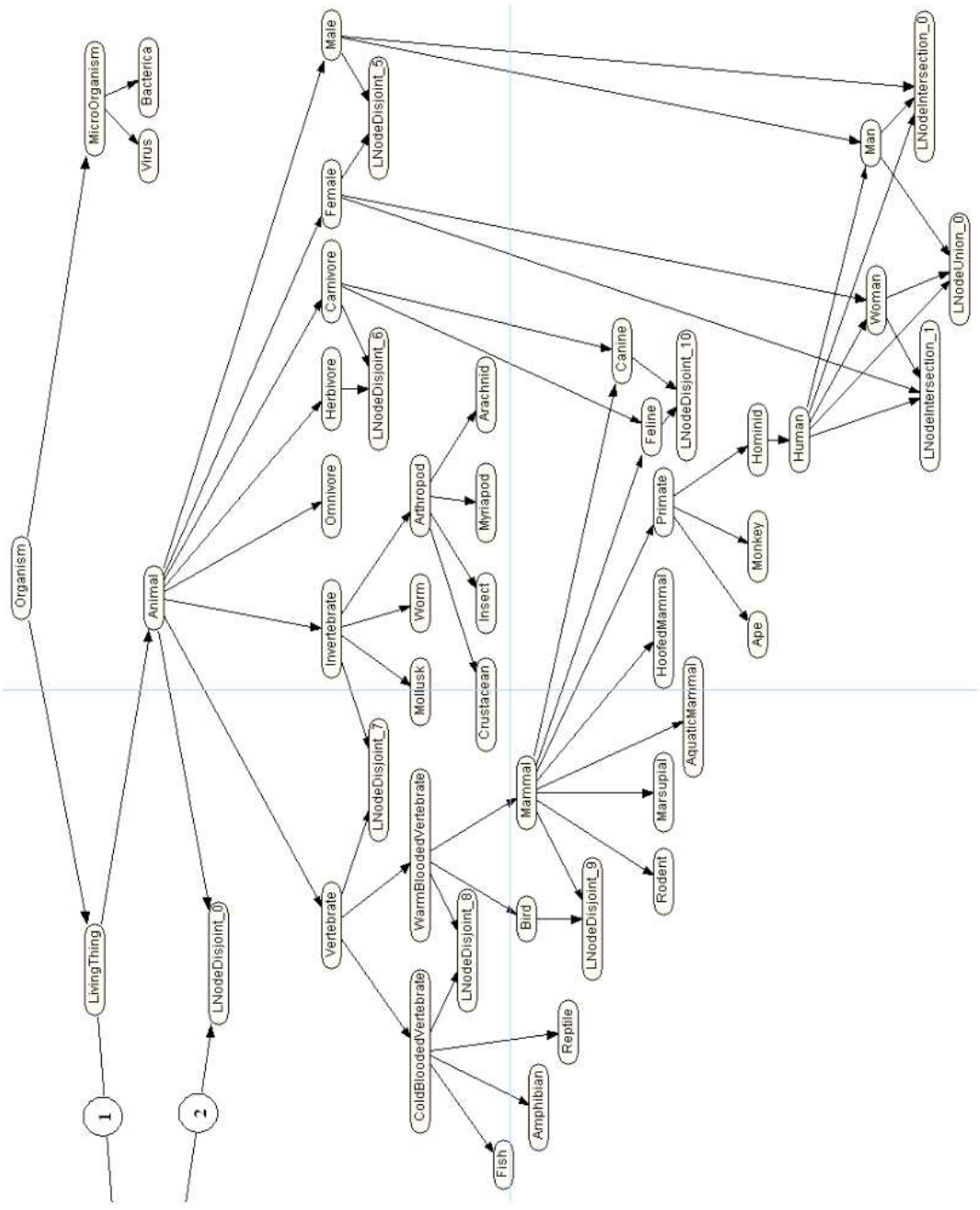



Fig. 4.11: **An Ontology with 71 Concept Classes, Part 2**

***BayesOWL***'s major contributions is its ***SD-IPFP*** mechanism to construct CPTs from given piece-wise probabilistic constraints. Moreover, in ***BayesOWL***, by using L-Nodes, the "rdfs:subclassOf" relations (or the subsumption hierarchy) are separated from other logical relations, so the in-arcs to a concept node $C$ will only come from its parent superclass nodes, which makes $C$'s CPT smaller and easier to construct than P-CLASSIC or PTDL, especially in a domain with rich logical relations.

Next we show two examples that both P-CLASSIC and PTDL can not handle but ***BayesOWL*** can do it easily using L-Nodes. First, consider four concepts $A$, $B$, $C$, and $D$ where $A$ is equivalent to $C$, $B$ is equivalent to $D$, and $C$ and $D$ are disjoint with each other. The translated BN according to our rules is depicted in Fig. 4.12, which realizes the given logical relations when all three L-nodes are set to "**True**". It also demonstrates that $A$ and $B$ are disjoint with each other as well.

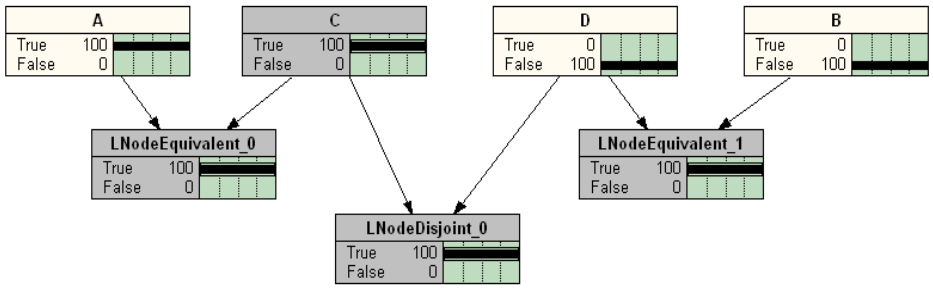



Fig. 4.12: **Example II: Usage of L-Nodes - 1**

L-Nodes can be used to model more complicated logical relations. In the second example, consider five concepts $A$, $B$, $C$, $D$ and $E$, where $C$ is the intersection of $A$ and $B$, $E$ is the intersection of $A$ and $D$, and $A$ is the union of $C$ and $E$, i.e., we have:

$$\left.\begin{array}{l} C \equiv A \sqcap B \\ E \equiv A \sqcap D \\ A \equiv C \sqcup E \end{array}\right\} \Rightarrow A \equiv (A \sqcap B) \sqcup (A \sqcap D) \Rightarrow A \equiv A \sqcap (B \sqcup D) \Leftrightarrow A \sqsubseteq (B \sqcup D)$$

That is, implicitly, $A$ is a subclass of $B \sqcup D$. It is shown that ***BayesOWL*** can handle this correctly, while systems such as P-CLASSIC fail on this. The translated BN according to our rules is depicted in Fig. 4.13, which fulfills all given logical relations when all the L-nodes are set to "**True**". And we can see that, when both $B$ and $D$ are "**False**", $A$ is also in "**False**", that means if an individual $o$ does not belong to concept $B$ or $D$, then it must not be an instance of $A$ either, i.e., this is consistent with $A$ is a subclass of $B \sqcup D$.

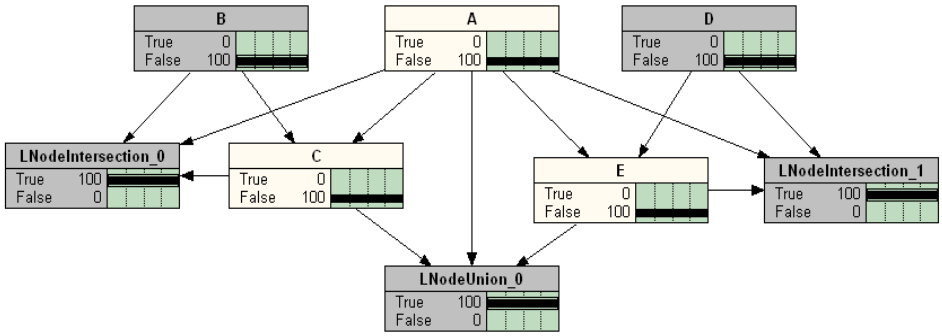



Fig. 4.13: **Example II: Usage of L-Nodes - 2**

Compared to PR-OWL [34] and OWL_QM [128], ***BayesOWL*** concerns explicitly more about the set or class memberships and logical relations rather than relationship among attributes. Also, same as P-CLASSIC and PTDL, ***BayesOWL*** uses the standard BN model, while PR-OWL and OWL_QM do not. ***BayesOWL*** trades the expressiveness with the simplicity.

In constrast to ***BayesOWL***, when modeling an RDF(S) concept subsumption, the arcs in the translated BN by the work of Holi and Hyvönen [67, 68] are pointed from from child subconcept nodes to parent superconcept nodes. And this work only deals with the "rdfs:subClassOf" relation.

Also, ***BayesOWL*** is not to extend or incorporate into OWL or any other ontology language or logics with probability theory, but to translate a given ontology to a BN in a systematic and practical way, and then treats ontological reasoning as probabilistic

inferences in the translated BNs. Several benefits can be seen with this approach. It is non-intrusive in the sense that neither OWL nor ontologies defined in OWL need to be modified. Also, it is flexible, one can translate either the entire ontology or part of it into BN depending on the needs. Moreover, it does not require availability of complete conditional probability distributions, pieces of probabilistic information can be incorporated into the translated BN in a consistent fashion. With these and other features, the cost of the approach is low and the burden to the user is minimal. One thing to emphasis is that ***BayesOWL*** can be easily extended to handle other ontology representation formalisms (syntax is not important, semantic matters), if not using OWL.

## 4.8 Summary

This chapter describes the research on developing a probabilistic framework for modeling uncertainty in semantic web taxonomy ontologies based on BNs. We have proposed a method to encode probabilistic constraints for ontology classes and relations in OWL. We have also defined a set of rules for translating an OWL taxonomy ontology into a BN DAG and provided a new algorithm ***SD-IPFP*** for efficient construction of CPTs. The translated BN is semantically consistent with the original ontology and satisfies all given probabilistic constraints. With this translation, ontology reasoning can be conducted as probabilistic inferences with potentially better, more accurate results. Future work includes extending the translation to include properties, instances and datatypes, and continuing work on ontology mapping based on ***BayesOWL*** which includes addressing the difficult issue of one-to-many mapping and its generalized form of many-to-many mapping where more than one concepts need to be mapped from one ontology to another at the same time. The ***BayesOWL*** framework presented in this chapter relies heavily on the availability of probabilis-

tic information for both ontology to BN translation and ontology mapping. This information is often not available (or only partially available) from domain experts. Learning these probabilities from data then becomes the only option for many applications. The current focus in this direction is the approach of text classification [32, 92]. The most important and also most difficult problem in this approach is to provide high quality sample documents to each ontology class. We are exploring ontology guided search of the web for such documents. Another interesting direction for future work is to deal with inconsistent probabilistic information. For example, in constructing CPTs for the translated BN, the given constraints may be inconsistent with each other, also, a set of consistent constraints may itself be inconsistent with the network structure. This issue involves detection of inconsistency, identification of sources of inconsistency, and resolution of inconsistency.

# Chapter 5

# Conclusion and Future Work

Dealing with uncertainty is crucial in ontology engineering tasks such as domain modeling, ontology reasoning, and concept mapping between ontologies. In this research we have developed ***BayesOWL***, a probabilistic extension to OWL that translates OWL taxonomy ontologies into BNs. We have defined new OWL classes ("PriorProb", "CondProb", and "Variable"), which can be used to representing in OWL the probabilistic constraints concerning the entities and relations in given ontologies. We have also defined a set of rules for translating OWL ontology taxonomy into Bayesian network DAG and provided a new algorithm ***SD-IPFP*** to construct CPTs for all concept nodes. ***SD-IPFP*** is further developed into ***E-IPFP*** and ***D-IPFP*** to modify the CPTs of Bayesian networks from low-dimensional probabilistic constraints. We have also implemented an early version of this framework, including an API for *OWL2BN* translation and an API for the various *IPFP* algorithms.

This probabilistic extension to OWL is compatible with OWL-DL semantics, and the translated BN is associated with a joint probability distribution over the application domain that is consistent with given probabilistic constraints.

However, as mentioned earlier in previous chapters, there are a number of issues remained to be addressed, which lead to several possible future research directions: 1) extending the translation to include properties and instances; 2) handling inconsistent probabilistic constraints in the various ***IPFP*** algorithms, especially in ***D-IPFP***; 3) investigating the scalability issues of ***BayesOWL*** in both translation and consequent reasoning; 4) developing methods to learn probabilities about concepts and their relations from existing web data; 5) the application of ***BayesOWL*** in supporting ontology mapping. We will briefly discuss each of these issues next.

**1. Dealing with Properties and Instances**

An ontology in OWL can define object properties and datatype properties, and there are also constructs available for properties about properties. Methods from P-CLASSIC can be directly adopted into our framework, but with a complicated probability computation mechanism across multiple BNs. However, our goal is to translate the whole ontology into one single standard Bayesian network so that standard belief updating algorithm could be used to do the reasoning. The difficulty comes from the fact that a single concept $C$ may be associated with more than one probability spaces when $C$ acts in different roles. For example, a concept "Animal" with an object property "hasParent" (which has "Animal" as its domain and range) links an individual "$a$" in "Animal" to another individual "b" in "Animal", thus, the probability space of "Animal" as a concept node is different from the probability space of "Animal" as the range of a concept node. How to connect these two spaces is the hinge to completely resolve this issue.

***BayesOWL*** is based on the model-theoretic semantics of OWL, so the modeling of uncertainty is in the granularity of concept classes. Methods from PRM [55] or DAPER [65] may be borrowed in building a BN based on instances.

**2. Dealing with Inconsistent Probabilistic Constraints**

The success of the algorithms presented in Chapter 3 relies on the quality of the probabilistic constraints provided. Among other thing, it is required that the probabilistic constraints must be consistent with each other, and there exists at least one distribution that can satisfy all the constraints. There are at least three theoretical issues related to the impact of the input constraint set's quality on the quality of solution: 1) Existence: Under what condition will the input constraint set specify a multivariate joint distribution? 2) Uniqueness: Assume such joint distribution exists, when will it be unique? 3) Quality of input set: How to deal with weakly consistent,

inconsistent or incomplete input constraint set which fails the current algorithms?

**3. Investigating Scalability**

Scalability is an important issue in both BN translation and consequent reasoning, when the application domain becomes large and complex. A real world ontology may involves hundreds or even thousands of concept definitions and the same scale of properties and concept relations, the translated BN thus becomes huge and very complex, and inference in it becomes increasingly more expensive or even practically intractable using standard exact BN inference algorithms. So the first issue of scalability is with computational complexity when the size of the translated BN becomes large. To address this issue, one may use some of the existing BN approximate algorithms such as loopy propagation and various stochastic sampling [60]. A more promising approach, however, would be to reduce the complexity by exploring the structure of the translated BN. For example, since the BN is translated from ontologies, interrelations between some or many parts of BN may be sparse, especially if the given ontology is a taxonomy. Then, as suggested by "Multiply Sectioned Bayesian Networks" [158] its may be relatively easy to break the BN into small parts or sections and perform inference distributively in individual modules while maintaining the coherence over the large BN.

Scalability is less an issue for the translation of a given ontology to BN, the number of nodes in BN is well controlled (it equals to the number of classes in the ontology plus the number of logical relations defined over these classes). As discussed in Chapter 3, ***SD-IPFP*** substantially reduces computational complexity for CPT construction by localizing the computation to one single CPT. However, it may become an issue when the ontology is expanding with additional classes and relations defined. For structural translation, ***BayesOWL*** can easily add new concept nodes and L-nodes into the DAG of the translated BN without modifying the rest of the

existing network structure. However, ***SD-IPFP***, cannot work incrementally to incorporate probabilistic constraints concerning newly added classes, we must re-run the whole process and obtain a new converged distribution based on all constraints provided (both old and new), so the second issue is to develop an incremental version of ***SD-IPFP*** (and in more general case, ***D-IPFP*** and ***E-IPFP***).

Also, compared to ***E-IPFP***, ***D-IPFP*** trades *I-divergence* for efficiency. One question is, what would be the upper bound of such a sacrifice in *I-divergence*? In what range the increase of *I-divergence* is reasonable or acceptable? This third issue is related to determining a reasonable $Y$ and $S$ at the technical level. If $Y$ is small, ***D-IPFP*** will in general be faster but the converged distribution is farther away from the original distribution, compared to that of ***E-IPFP***, the best we can obtained by both satisfying all probabilistic constraints and the structural constraint.

**4. Learning Probabilities from Web Data**

The CPT construction of ***BayesOWL*** requires prior probability distributions $P(C)$ to capture the uncertainty about concepts (i.e., how an arbitrary individual belongs to class $C$), and conditional probability distributions $P(C|D)$ for relations between $C$ and $D$ in the same ontology (e.g., how likely an arbitrary individual in class $D$ is also in $D$'s subclass $C$). Further, the framework for ontology mapping (to be discussed next) requires a set of joint probability distributions $P(C, D)$ for initial raw semantic similarity between concepts $C$ and $D$ from different ontologies. In many cases these kinds of probabilistic information are not available and are difficult to obtain from domain experts. Learning probabilities (i.e., priors about concepts, conditionals between subconcepts and superconcepts, and raw semantic similarities between concepts in two different ontologies) from existing web data maybe possible with the development of search engines such as Google [1], Swoogle [2], Ask Jeeves [3],

[1] `http://www.google.com`
[2] `http://swoogle.umbc.edu/`
[3] `http://ask.com/`

Answers.com [4], etc.

Our initial solution to learning these probabilities is to apply Naive Bayes text classification technique [32, 92] by explicitly associating a concept with a group of sample documents (called *exemplar*s) retrieved and selected automatically from World Wide Web (WWW). The idea is inspired by those machine learning based semantic integration approaches such as [44, 80, 130] where the meaning of a concept is implicitly represented by a set of exemplars that are relevant to it. The rationale is that the meaning of a concept can be described or defined in the way that it is used.

Learning the probabilities we need from these exemplars is straightforward. First, we build a model containing statistical information about each concept's exemplars in Ontology 1 using a text classifier such as Rainbow [5], and then classify each concept in Ontology 2 by their respective exemplars using the model of Ontology 1 to obtain a set of probabilistic scores showing the similarity between concepts. Ontology 1's exemplars can be classified in the same way by the model built using Ontology 2's exemplars. This cross-classification (Fig. 5.1) process helps find a set of raw mappings between Ontology 1 and Ontology 2 by setting some threshold values. Similarly, we can obtain prior or conditional probabilities related to concepts in a single ontology through self-classification with the model for that ontology.

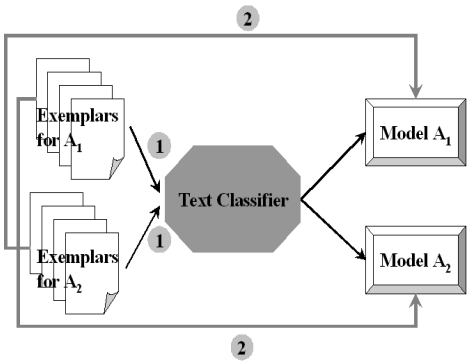



Fig. 5.1: **Cross-Classification using Rainbow**

[4] http://www.answers.com/

[5] http://www-2.cs.cmu.edu/~mccallum/bow/rainbow

How to obtain high quality exemplars (both positive and negative) automatically is a crucial issue. The quality of the learned probabilities is highly dependent on the quality of the exemplars (e.g., how relevant they are to the concept and how comprehensive they are in capturing all important aspects of the concept), and it would be a very time-consuming task for knowledge workers to choose high quality exemplars manually. The need to find sufficient relevant exemplars for a large quantity of concepts manually greatly reduces the attractiveness and applicability of these machine learn-ing based approaches. Our approach is to use search engines such as Google and Answers.com to retrieve exemplars for each concept node automatically from WWW, the richest information resource available nowadays. This again introduces several practical concerns such as how to form the query strings to these engines based on given ontologies, how to pre-processing the results crawled back from these engines to include only those most relevant documents?

Even if we obtained highly relevant exemplars successfully, there still remains one big theoretical issue: the semantics of a concept in a document represents more close to its meaning in natural language, while in ***BayesOWL***, the semantics of a concept is based on model-theoretics. For example, if "Woman" and "Man" are two disjoint concepts, in OWL semantics, they share no instances in common, thus makes "$P(Woman = True|Man = True) = 0$"; however, the concept "Woman" and "Man" in natural language are closely related to each other, using the exemplars associated with them, the learned probability "$P(Woman = True|Man = True)$" will never be zero. Is it possible to find a way to reconcile these two semantics? If it is yes, how?

**5. Supporting Ontology Mapping**

As surveyed in Section 2.5, semantic heterogeneity between two different applications or agents comes from their use of conflicted or mismatched terms about concepts. It has become increasingly clear that being able to map concepts between different,

independently developed ontologies is imperative to semantic web applications and other applications requiring semantic integration. Narrowly speaking, a mapping can be defined as a correspondence between concept $A$ in Ontology 1 and concept $B$ in Ontology 2 which share similar or the same semantics. [107] provides a brief survey on existing approaches for ontology-based semantic integration. Most of these works are either based on syntactic and semantic heuristics, machine learning (e.g., text classification techniques in which each concept is associates with a set of text documents that exemplify the meaning of that concept), or linguistics (spelling, lexicon relations, lexical ontologies, etc.) and natural language processing techniques.

It is often the case that, when mapping concept $A$ defined in Ontology 1 to Ontology 2, there is no concept in Ontology 2 that is semantically identical to $A$. Instead, $A$ is similar to several concepts in Ontology 2 with different degree of similarities. A solution to this so-called one-to-many problem, as suggested by [130] and [43], is to map $A$ to the target concept $B$ which is most similar to $A$ by some measure. This simple approach would not work well because 1) the degree of similarity between $A$ and $B$ is not reflected in Ontology2 and thus will not be considered in reasoning after the mapping; 2) it cannot handle the situation where $A$ itself is uncertain; and 3) potential information loss because other similar concepts are ignored in the mapping.

Different from their contributions, we propose a new methodology in supporting ontology mapping based on ***BayesOWL***. As can be seen from Fig. 5.2, the system includes four components: 1) a learner to obtain probabilistic ontological information and initial raw similarities using data obtained from web (as described earlier); 2) a representation mechanism for the learned uncertain information concerning the entities and relations in given ontologies (as described in Section 4.1); 3) a ***BayesOWL*** module to translate given taxonomy ontologies (together with the learned uncertain information) into BNs (as described in Chapter 4); and 4) a concept mapping module which takes a set of learned initial raw similarities as input and finds new mappings

between concepts from two different ontologies as an application of Rong Pan's formalized BN mapping framework [117] for belief propagation between different BNs that is based on probabilistic evidential reasoning across two BNs.

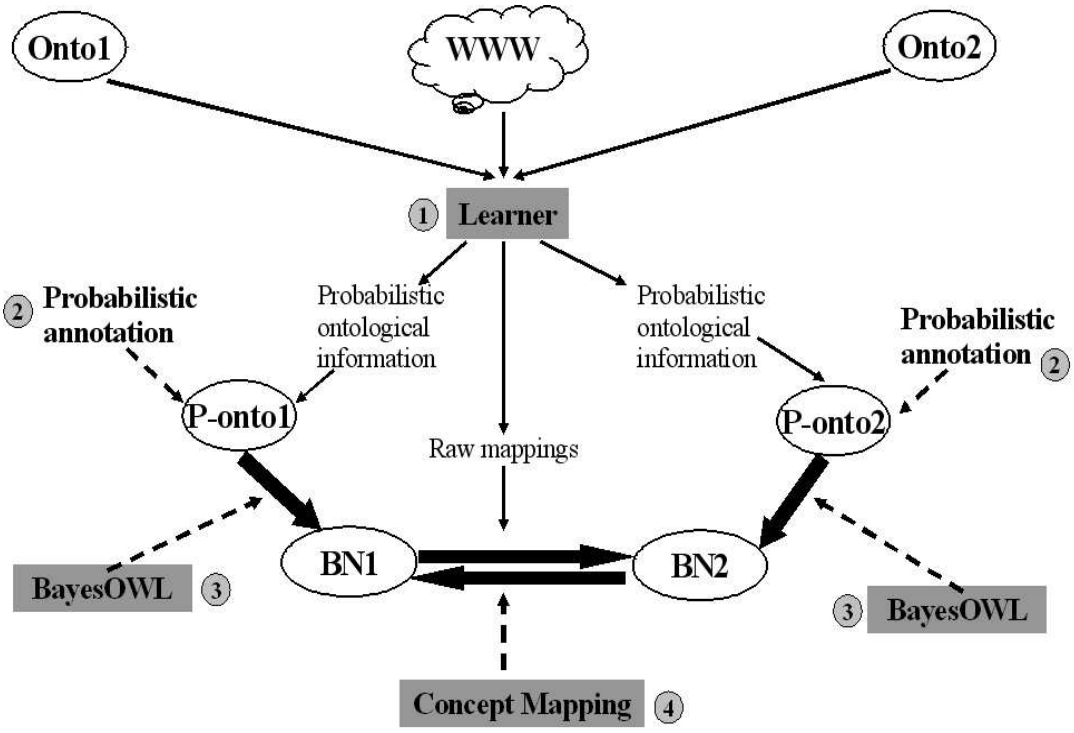



Fig. 5.2: **The Proposed Ontology Mapping Framework**

Our preliminary work along this direction and some initial experimental results can be found at [41, 117]. Here we briefly sketches the BN mapping framework [117] and its remaining issues to be addressed.

### The BN Mapping Framework

What we need in supporting mapping concepts is a framework that allows two BNs (translated from two ontologies) to exchange beliefs via variables that are similar but not identical. We illustrate our ideas by first describing how mapping shall be done for a pair of similar concepts ($A$ from Ontology 1 to $B$ in Ontology 2), and then discussing issues we face when generalizing such pair-wise mappings to network to network mapping. We assume the similarity information between $A$ and $B$ is captured

by the joint distribution $P(A, B)$. Now we are dealing with three probability spaces: $S_A$ and $S_B$ for BN1 and BN2, and $S_{AB}$ for $P(A, B)$. The mapping from $A$ to $B$ amounts to determining the distribution of $B$ in $S_B$, given the distribution $P(A)$ in $S_A$ under the constraint $P(A, B)$ in $S_{AB}$.

To propagate probabilistic influence across these spaces, we can apply Jeffrey's rule and treat the probability from the source space as soft evidence to the target space [122, 147]. This rule goes as follow. When the soft evidence on $X_i \in X$, represented as the distribution $Q(X_i)$, is presented, not only $P(X_i)$, the original distribution of $X_i$, is changed to $Q(X_i)$, all other variables $X_{j \neq i} \in X$ will change their distributions from $P(X_j)$ to $Q(X_j)$ according to Eq. 5.1

$$Q(X_j) = \sum_i P(X_j|x_i)Q(x_i) \tag{5.1}$$

if $P(X_j|X_i)$ is invariant with respect to $Q(X_i)$, where the summation is over all states $x_i$ of $X_i$.

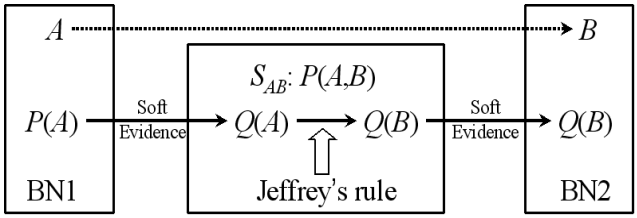



Fig. 5.3: **Mapping Concept $A$ in Ontology1 to $B$ in Ontology2**

As depicted in Fig. 5.3, mapping $A$ to $B$ is accomplished by applying Jeffrey's rule twice, first from $S_A$ to $S_{AB}$, then $S_{AB}$ to $S_B$. Since $A$ in $S_A$ is identical to $A$ in $S_{AB}$, $P(A)$ in $S_A$ becomes soft evidence $Q(A)$ to $S_{AB}$ and by applying Eq. 5.1 the distribution of $B$ in $S_{AB}$ is updated to

$$Q(B) = \sum_i P(B|a_i)Q(a_i) \tag{5.2}$$

$Q(B)$ is then applied as soft evidence from $S_{AB}$ to node $B$ in $S_B$, updating beliefs for

every other variable $V$ in $S_B$ by

$$\begin{aligned} Q(V) &= \sum_j P(V|b_j)Q(b_j) \\ &= \sum_j P(V|b_j) \sum_i P(b_j|a_i)Q(a_i) \\ &= \sum_j P(V|b_j) \sum_i P(b_j|a_i)P(a_i) \end{aligned} \tag{5.3}$$

Back to the example in Fig. 4.5, where the posterior distribution of "Human", given hard evidence $\neg Male \sqcap Animal$, is ($True$ 0.102, $False$ 0.898). Suppose we have another BN which has a variable "Adult" with marginal distribution ($True$ 0.8, $False$ 0.2). Suppose we also know that "Adult" is similar to "Human" with conditional distribution ("$T$" for "True", "$F$" for "False")

$$P(Adult|Human) = \begin{array}{c} \\ T \\ F \end{array} \begin{array}{c} \begin{array}{cc} T & F \end{array} \\ \begin{pmatrix} 0.7 & 0.3 \\ 0.0 & 1.0 \end{pmatrix} \end{array}$$

Mapping "Human" to "Adult" leads to a change of latter's distribution from ($True$ 0.8, $False$ 0.2) to ($True$ 0.0714, $False$ 0.9286) by Eq. 5.2. Such a change can then be propagated to further update believes of all other variables in the target BN by Eq. 5.3.

**Remaining Issues**

Usually, $A$ from Ontology1 maybe semantically similar to more than one concept in Ontology2. For example, if $A$ is fairly similar to $B$ in Ontology2, it would also be similar to all super concepts and also some sub-concepts of $B$, possibly with different similarity measures. The learned initial raw similarities may include multiple pair-wise mappings that initiate from $A$ in Ontology1 and end at each similar concept $B^J$ in Ontology2. Probabilistically, BN2 for Ontology2 can be seen as receiving $n$ soft evidences, one for a pair-wise mapping from $A$ to $B^J$ for each similar concept $B^J$ in Ontology2. This requires 1) all similarity measures $P(A, B^J)$ remain invariant,

and 2) conditional dependencies among variables in BN2 also remain invariant. How to extend the previous "1 to 1" mapping to this "1 to n" mapping is the first issue need to be addressed, that is, we need a mechanism to propagate multiple pair-wise raw mappings as soft evidences to BN2, and after propagation, all these "1 to 1" mappings should be held simultaneously across BN1 and BN2.

On the other hand, in theory, any pair of variables between two BNs can be linked, albeit with different degree of similarities. Therefore we may potentially have $n_1 \times n_2$ raw mappings ( $n_1$ and $n_2$ are the number of variables in BN1 and BN2, respectively). However, some of these raw mappings maybe be redundant since they can be satisfied by propagating other raw mappings.

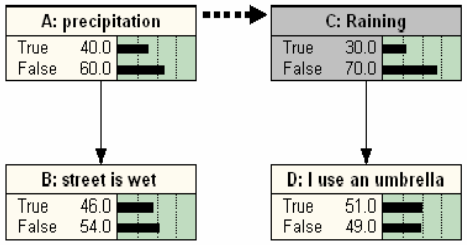



Fig. 5.4: **Example of Mapping Reduction**

As shown in Fig. 5.4, we have variables $A$ and $B$ in BN1, $C$ and $D$ in BN2, and raw similarities between every pair as below:

$$P(C,A) = \begin{pmatrix} 0.3 & 0.0 \\ 0.1 & 0.6 \end{pmatrix}, \qquad P(D,A) = \begin{pmatrix} 0.33 & 0.18 \\ 0.07 & 0.42 \end{pmatrix},$$

$$P(D,B) = \begin{pmatrix} 0.348 & 0.162 \\ 0.112 & 0.378 \end{pmatrix}, \qquad P(C,B) = \begin{pmatrix} 0.3 & 0.0 \\ 0.16 & 0.54 \end{pmatrix}.$$

However, we do not need to propagate for all these raw similarities. As Fig. 5.4 depicts, when we have a mapping from $A$ to $C$, all these raw similarities are satisfied (the other three mappings are thus redundant). This is because not only beliefs on $C$, but also beliefs on $D$ are properly updated by mapping $A$ to $C$. Several experiments

with large BNs have shown that only a very small portions of all $n_1 \times n_2$ mappings are needed in satisfying all raw similarities (or, name it "probabilistic constraints"). This, we suspect, is due to the fact that some of these constraints can be derived from others based on the probabilistic interdependencies among variables in the two BNs. So, how to identify and remove redundant mappings by examining the BN structures and CPTs is the second issue to face.

Given the above issues being successfully addressed, and all initial raw similarities be properly propagated from BN1 to BN2, we can conduct probabilistic reasoning to find the best concept matches between Ontology1 and Ontology2. However, sometimes the best match is not between two simple concepts (i.e., between two variables in BNs), but between a composite concept (i.e, a concept that is defined as a conjunction (intersection) or disjunction (union) of several variables or their negations) and a simple concept, or even between two composite concepts. So, the third big issue is how to calculate joint influence (from multiple variables) from pair-wise mappings to find this type of complex matches.

### 6. Other Comments

Besides the above theoretical issues. Another relatively easier but useful work is to design and develop GUI interfaces for the current prototype implementation and make it professional enough to be used by other researchers or common users. Also, it would be very interesting to develop an ontology for standard Bayesian networks, the development of semantic web lies in the authoring and publishing of as many useful ontologies as possible on the web.

With the research in these areas to be conducted in the next few years, the work in this dissertation is potentially useful in practical applications, especially in probabilistic concept subsumption in a single ontology and ontology mapping between two ontologies.

# Appendix

## A. Ontology for Representing Probabilistic Information

**Name: prob.owl**

```
<?xml version="1.0"?>
<rdf:RDF xmlns:rdf ="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
         xmlns:rdfs ="http://www.w3.org/2000/01/rdf-schema#"
         xmlns:xsd ="http://www.w3.org/2001/XMLSchema#"
         xmlns:owl ="http://www.w3.org/2002/07/owl#"
         xmlns:dt ="http://www.cs.umbc.edu/ zding1/owl/dt.xsd#"
         xmlns ="http://www.cs.umbc.edu/ zding1/owl/prob.owl#">
<owl:Ontology rdf:about="http://www.cs.umbc.edu/ zding1/owl/prob.owl#">
    <owl:versionInfo>v1.0</owl:versionInfo>
</owl:Ontology>
<owl:Class rdf:ID="Variable">
    <rdfs:subClassOf>
        <owl:Restriction>
            <owl:onProperty rdf:resource="#hasClass"/>
            <owl:cardinality rdf:datatype="&xsd;nonNegativeInteger">1
            </owl:cardinality>
        </owl:Restriction>
    </rdfs:subClassOf>
    <rdfs:subClassOf>
        <owl:Restriction>
            <owl:onProperty rdf:resource="#hasState"/>
            <owl:cardinality rdf:datatype="&xsd;nonNegativeInteger">1
```

```
                    </owl:cardinality>
                </owl:Restriction>
            </rdfs:subClassOf>
    </owl:Class>
    <owl:Class rdf:ID="States">
            <owl:oneOf rdf:parseType="Collection">
                <owl:Thing rdf:about="#True"/>
                <owl:Thing rdf:about="#False"/>
            </owl:oneOf>
    </owl:Class>
    <owl:Class rdf:ID="ProbObj"/>
    <owl:Class rdf:ID="PriorProb">
            <rdfs:subClassOf rdf:resource="#ProbObj"/>
            <rdfs:subClassOf>
                <owl:Restriction>
                    <owl:onProperty rdf:resource="#hasVariable"/>
                    <owl:cardinality rdf:datatype="&xsd;nonNegativeInteger">1
                    </owl:cardinality>
                </owl:Restriction>
            </rdfs:subClassOf>
            <rdfs:subClassOf>
                <owl:Restriction>
                    <owl:onProperty rdf:resource="#hasProbValue"/>
                    <owl:cardinality rdf:datatype="&xsd;nonNegativeInteger">1
                    </owl:cardinality>
                </owl:Restriction>
            </rdfs:subClassOf>
```

```
</owl:Class>
<owl:Class rdf:ID="CondProb">
        <rdfs:subClassOf rdf:resource="#ProbObj"/>
        <owl:disjointWith rdf:resource="#PriorProb"/>
        <rdfs:subClassOf>
            <owl:Restriction>
                <owl:onProperty rdf:resource="#hasCondition"/>
                <owl:minCardinality rdf:datatype="&xsd;nonNegativeInteger">1
                </owl:minCardinality>
            </owl:Restriction>
        </rdfs:subClassOf>
        <rdfs:subClassOf>
            <owl:Restriction>
                <owl:onProperty rdf:resource="#hasVariable"/>
                <owl:cardinality rdf:datatype="&xsd;nonNegativeInteger">1
                </owl:cardinality>
            </owl:Restriction>
        </rdfs:subClassOf>
        <rdfs:subClassOf>
            <owl:Restriction>
                <owl:onProperty rdf:resource="#hasProbValue"/>
                <owl:cardinality rdf:datatype="&xsd;nonNegativeInteger">1
                </owl:cardinality>
            </owl:Restriction>
        </rdfs:subClassOf>
</owl:Class>
<owl:ObjectProperty rdf:ID="hasCondition">
```

<rdfs:domain rdf:resource="#CondProb"/>

<rdfs:range rdf:resource="#Variable"/>

</owl:ObjectProperty>

<owl:ObjectProperty rdf:ID="hasVariable">

<rdfs:domain rdf:resource="#ProbObj"/>

<rdfs:range rdf:resource="#Variable"/>

</owl:ObjectProperty>

<owl:ObjectProperty rdf:ID="hasClass">

<rdfs:domain rdf:resource="#Variable"/>

</owl:ObjectProperty>

<owl:ObjectProperty rdf:ID="hasState">

<rdfs:domain rdf:resource="#Variable"/>

<rdfs:range rdf:resource="#States"/>

</owl:ObjectProperty>

<owl:DatatypeProperty rdf:ID="hasProbValue">

<rdf:type rdf:resource="&owl;FunctionalProperty"/>

<rdfs:domain rdf:resource="#ProbObj"/>

<rdfs:range rdf:resource="&dt;between0and1"/>

</owl:DatatypeProperty>

</rdf:RDF>

**Name: dt.xsd**

<?xml version="1.0"?>

<xsd:schema xmlns:xsd="http://www.w3.org/2001/XMLSchema">

<xsd:simpleType name="between0and1">

<xsd:restriction base="xsd:real">

<xsd:minInclusive value="0.0"/>

<xsd:maxInclusive value="1.0"/>

```
        </xsd:restriction>
</xsd:simpleType>
</xsd:schema>
```

## B. An Example Taxonomy Ontology

**Name: nature.owl**

```
<?xml version="1.0"?>
<rdf:RDF xmlns:rdf ="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
         xmlns:rdfs ="http://www.w3.org/2000/01/rdf-schema#"
         xmlns:xsd ="http://www.w3.org/2001/XMLSchema#"
         xmlns:owl ="http://www.w3.org/2002/07/owl#"
         xmlns ="http://www.cs.umbc.edu/ zding1/owl/nature.owl#">
<owl:Ontology rdf:about="http://www.cs.umbc.edu/ zding1/owl/nature.owl#">
        <owl:versionInfo>v1.0</owl:versionInfo>
</owl:Ontology>
<owl:Class rdf:ID="Animal"/>
<owl:Class rdf:ID="Male">
        <rdfs:subClassOf rdf:resource="#Animal"/>
</owl:Class>
<owl:Class rdf:ID="Female">
        <rdfs:subClassOf rdf:resource="#Animal"/>
        <owl:disjointWith rdf:resource="#Male"/>
</owl:Class>
<owl:Class rdf:ID="Human">
        <rdfs:subClassOf rdf:resource="#Animal"/>
</owl:Class>
<owl:Class rdf:ID="Man">
```

```
        <owl:intersectionOf rdf:parseType="Collection">
            <owl:Class rdf:about="#Human"/>
            <owl:Class rdf:about="#Male"/>
        </owl:intersectionOf>
</owl:Class>
<owl:Class rdf:ID="Woman">
        <owl:intersectionOf rdf:parseType="Collection">
            <owl:Class rdf:about="#Human"/>
            <owl:Class rdf:about="#Female"/>
        </owl:intersectionOf>
</owl:Class>
<owl:Class rdf:about="#Human">
        <owl:unionOf rdf:parseType="Collection">
            <owl:Class rdf:about="#Man"/>
            <owl:Class rdf:about="#Woman"/>
        </owl:unionOf>
</owl:Class>
</rdf:RDF>
```

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