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Integration of Logic and Probability in Terminological and Inductive Reasoning

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Part I

Introduction

Chapter 1

Context

Early work on Machine Learning (ML) often focused on learning *deterministic logical* concepts. This approach of machine learning fell out of vogue for many years because of problems in handling noise and large-scale data. During that time, the ML community shifted attention to *statistical* methods that ignored relational aspects of the data (e.g., neural networks, decision trees, and generalized linear models). These methods led to major boosts in accuracy in many problems in low-level vision and natural language processing. However, their focus was on the *propositional* or attribute-value representation.

The major exception has been the inductive logic programming (ILP) community. Specifically, ILP is a research field at the intersection of machine learning and logic programming. The ILP community has concentrated its efforts on learning (deterministic) first-order rules from *relational* data (Lavrac and Dzeroski, 1994). Initially the ILP community focused its attention solely on the task of program synthesis from examples and background knowledge. However, recent research has tackled the discovery of useful rules from larger databases. The ILP community has had successes in a number of application areas including discovery of 2D structural alerts for mutagenicity/carcinogenicity (Srinivasan et al., 1997, 1996), 3D pharmacophore discovery for drug design (Finn et al., 1998) and analysis of chemical databases (Turcotte et al., 1998). Among the strong motivations for using a *relational model* is its ability to model dependencies between related instances. Intuitively, we would like to use our information about one object to help us reach conclusions about other, related objects. For example, in web data, we should be able to propagate information about the topic of a document to documents it has links to and documents that link to it. These, in turn, would propagate information to yet other documents.

Recently, both the ILP community and the statistical ML community have begun to incorporate aspects of their complementary technology. Many ILP researchers are developing stochastic and probabilistic representations and algorithms (Cussens, 1999; Kersting et al., 2001; Muggleton, 2000). In more traditional ML circles, researchers who have in the past focused on attribute-value or propositional learning algorithms are exploring methods for incorporating relational information.

We refer to this emerging area of research as **statistical relational learning (SRL)**. SRL research attempts to represent, reason, and learn in domains with **complex relational** and rich **probabilistic structure**. Other terms that have been used recently include *probabilistic logic learning*. **Learning** is the third fundamental component in any SRL approach: the aim of SRL is to build rich representations of domains including objects, relations and uncertainty, that one can effectively learn and carry out inference with. Over the last 25 years there has been a considerable body of research to close the gap between *logical* and *statistical* Artificial Intelligence (AI).

We overview in the following the foundations of the SRL area - learning, logic and probability - and give some research problems, representations and applications of SRL approaches.

1.1 Learning

Machine learning and data mining techniques essentially search a space of possible patterns, models or regularities. Depending on the task, different search algorithms and principles apply.

Data mining is the process of computing the set of patterns $Th(Q, D, \mathcal{L})$ (Mannila and Toivonen, 1997). The search space consists of all patterns expressible within a language of patterns $\mathcal{L}$; the data set D consists of the examples that need to be generalized; and, finally, the constraint Q specifies which patterns are of interest.

A slightly different perspective is given by the machine learning view, which is often formulated as that of finding a particular function h (again belonging to a language of possible functions $\mathcal{L}$) that minimizes a loss function $l(h, D)$ on the data. An adequate loss function is the accuracy, that is, the fraction of database queries that is correctly predicted. The machine learning and data mining views can be reconciled, for instance, by requiring that the constraint $Q(h, D)$ succeeds only when $l(h, D)$ is minimal.
Machine learning algorithms are described as either 'supervised' or 'unsupervised'. The distinction is drawn from how the learner classifies data. In supervised algorithms, the classes

are predetermined. These classes can be conceived of as a finite set, previously arrived at by a human. In practice, a certain segment of data will be labeled with these classifications. Unsupervised learners are not provided with classifications. In fact, the basic task of unsupervised learning is to develop classification labels automatically. Unsupervised algorithms seek out similarity between pieces of data in order to determine whether they can be characterized as forming a group. These groups are termed clusters.

The computation of the solutions proceeds typically by searching the space of possible patterns or hypotheses $\mathcal{L}$ according to *generality*. One pattern or hypothesis is more general than another if all examples that are covered by (satisfy) the latter pattern are also covered by the former.

1.2 Logic

Using logical description languages provides not only a high expressivity in representation, useful in *relational* domains, but also an excellent theoretical foundation for *learning*.

Logical learning typically employs a form of reasoning known as *inductive inference*. This form of reasoning generalizes specific facts into general laws. The idea is that knowledge can be obtained by careful experimenting, observing, generalizing and testing of hypotheses. Relational learning has investigated *computational* approaches to inductive reasoning, i.e. general-purpose inductive reasoning systems that could be applied across different application domains. Supporting the discovery process across different domains requires a solution to two important computational problems. First, an expressive formalism is needed to represent many learned theories. Second, the inductive reasoning process should be able to employ the available background knowledge to obtain meaningful hypotheses. These two problems can be solved to a large extent by using *logical* representations for learning. For logical learning the set of patterns expressible in the language $\mathcal{L}$ will typically be a set of clauses.

Since the mid-1960s a number of researchers proposed to use (variants of) *predicate logic* as a formalism for machine learning. Theoretical properties of generalization and specialization were also studied by various researchers. In the 1990s inductive logic programming (ILP) developed firm theoretical foundations, built on logic programming concepts, for logical learning and various well-known inductive logic programming systems (Muggleton, 1987, 1995; Muggleton and Buntine, 1988; Muggleton and Feng, 1990).

The vast majority of statistical learning literature assumes the data is represented by points in a high-dimensional space. For many task, such as learning to detect a face in an image or classify an email message as spam or not, we can usually construct the relevant low-level features (e.g., pixels, filters, words, URLs) and solve the problem using standard tools for the vector representation. This abstraction hides the rich logical structure of the underlying data that is crucial for solving more general and complex problems. We may like to detect that an email message is not only not-spam but is a request for a meeting tomorrow with three colleagues, etc. We are ultimately interested in not just answering an isolated yes/no question, but in producing structured representations of the data, *involving objects described by attributes and participating in relationships*, actions, and events. The challenge is to develop formalisms, models, and algorithms that enable effective and robust reasoning about this type of object-relational structure of the data.

Logic is inherently relational, expressive, understandable, and interpretable, and it is well understood. It provides solid theoretical foundations for many developments within artificial intelligence and knowledge representation. At the same time, it enables one to specify and employ background knowledge about the domain, which is often also a key factor in many applications of artificial intelligence. Predicate logic adds relations, individuals and quantified variables, allowing to treat cases where the values in the database are names of individuals, and it is the properties of the individuals and the relationship between the individuals that are modeled. We often want to build the models before we know which individuals exist in a domain, so that the models can be applied to diverse populations. Moreover, we would like to make probabilistic predictions about properties and relationships among individuals; this issue is tackled under probability theory, see next Section.

1.3 Probability

Probability theory provides an elegant and formal basis for reasoning about uncertainty.

Dealing with real data, like images and text, inevitably requires the ability to handle the *uncertainty* that arises from noise and incomplete information (e.g., occlusions, misspellings). In relational problems, uncertainty arises on many levels. Beyond uncertainty about the attributes of an object, there may be uncertainty about an object's type, the number of objects, and the identity of an object (what kind, which, and how many entities are depicted or written about), as well as relationship membership, type, and number (which entities are related, how, and how many times). Solving interesting relational learning tasks robustly requires sophisticated treatment of uncertainty at these multiple levels of representation.

In the past few decades, several probabilistic knowledge representation formalisms have been developed to cope with uncertainty, and many of these formalisms can be learned from data. Unfortunately, most such formalisms are propositional, and hence they suffer from the same limitations as traditional propositional learning systems. In the 1990s a development took place also in the uncertainty in artificial intelligence community. Researchers started to develop expressive probabilistic logics and to study learning in these frameworks soon afterward, see next Section.

1.4 Probabilistic Logic Learning Formalisms

Probability-logic formalisms have taken one of two routes to defining probabilities.

In the *directed* approach there is a nonempty set of formulae all of whose probabilities are explicitly stated: they are called probabilistic facts, similarly to Sato (Sato, 1995). Other probabilities are defined recursively with the probabilistic facts acting as base cases. A probability-logic model using the directed approach will be closely related to a recursive graphical model (Bayesian net).

Most probability-logic formalisms fall into this category: for example, probabilistic logic programming (PLP) by Ng and Subrahmanian (Ng and Subrahmanian, 1992); probabilistic Horn abduction (PHA) by Poole (Poole, 1993) and its later expansion the independent choice logic (ICL) (Poole, 1997); probabilistic knowledge bases (PKBs) by Ngo and Haddawy (Ngo and Haddawy, 1996); Bayesian logic programs (BLPs) by Kersting and De Raedt (Kersting and Raedt, 2001); relational Bayesian networks (RBNs) by (Jaeger, 1997); stochastic logic programs (SLPs) by Muggleton (Muggleton, 2000); the PRISM system by Sato (Sato and Kameya, 2001); Logic Programs with Annotated Disjunctions (LPADs) by (Vennekens et al., 2004); ProbLog by (De Raedt et al., 2007) and CP-logic by (Vennekens et al., 2009). This wide variety of probabilistic logics that are available today are described in two recent textbooks (Getoor and Taskar, 2007; Raedt, 2008).

In order to upgrade logic programs to a probabilistic logic, two changes are necessary:

1. The most basic requirement of such formalisms is to explicitly state that a given ground atomic formula has some probability of being true: clauses are annotated with probability values;

2. the “covers” relation (a rule covers an example, if the example satisfies the body of the rule) becomes a probabilistic one: rather than stating in absolute terms whether the example is covered or not, a probability will be assigned to the example being covered. The logical coverage relation can be re-expressed as a probabilistic one by stating that the probability is 1 or 0 of being covered.

In all these cases, *possible worlds* semantics are explicitly invoked: these programs define a probability distribution over normal logic programs (called instances or possible worlds). They differ in the way they define the distribution over logic programs.

The second approach is *undirected*, where no formula has its probability explicitly stated. Relational Markov networks (RMNs) (Taskar et al., 2002) and Markov Logic networks (MLNs) (Richardson and Domingos, 2006) are examples of this approach. In the undirected approach, the probability of each possible world is defined in terms of its “features” where each feature has an associated real-valued parameter.

To understand the needs for such a combination between predicate logic and probability, consider learning from the two datasets in Figure 1.1 (taken from (Poole and Mackworth, 2010)).

Example	*Author*	*Thread*	*Length*	*WhereRead*	*UserAction*
e_1	*known*	*new*	*long*	*home*	*skips*
e_2	*unknown*	*new*	*short*	*work*	*reads*
e_3	*unknown*	*follow_up*	*long*	*work*	*skips*
e_4	*known*	*follow_up*	*long*	*home*	*skips*
...	...	...	...	...	...

(a)

Individual	Property	Value
joe	*likes*	*resort_14*
joe	*dislikes*	*resort_35*
...	...	...
resort_14	*type*	*resort*
resort_14	*near*	*beach_18*
beach_18	*type*	*beach*
beach_18	*covered_in*	*ws*
ws	*type*	*sand*
ws	*color*	*white*
...	...	...

(b)

Figure 1.1: Two examples of datasets from which one may want to capture characteristics of interest of the unknown underlying probability distribution.

Dataset (a) can be used by supervised learning algorithms to learn a decision tree, a neural network, or a support vector machine to predict *UserAction*. A belief network learning algorithm can be used to learn a representation of the distribution over all of the features. Dataset (b), from which we may want to predict what Joe likes, is different. Many of the values in the table cannot be used directly in supervised learning. Instead, it is the relationship among the individuals in the world that counts: for example, we may want to learn that Joe likes resorts that are near sandy beaches.

Reasoning tasks

One typically distinguishes two problems within the statistical learning community:

- **Learning**: there are two variants of the learning task: parameter estimation and structure learning. In the parameter estimation task, we assume that the qualitative structure of the SRL model is known; in this case, the learning task is simply to fill in the parameters characterizing the model. In the structure learning task, there is no additional required input (although the user can, if available, provide prior knowledge about the structure, e.g., in the form of constraints). The goal is to extract structure as well as parameters, from the training data (database) alone; the search can make use of certain biases defined over the model space.

- **Inference**: having defined a probability distribution in a logic-based formalism there remains the problem of computing probabilities to answer specific queries, such as "What's the probability that Tweety flies?". The major problem is the computational complexity of probabilistic inference. For a large number of models, in fact, exact inference is intractable and we resort to approximations.

Applications

Statistical relational models have been used for estimating the result size of complex database queries, for clustering gene expression data, and for discovering cellular processes from gene expression data. They have also been used for understanding tuberculosis epidemiology. Probabilistic relational trees have discovered publication patterns in high-energy physics. They have also been used to learn to rank brokers with respect to the probability that they would commit a serious violation of securities regulations in the near future. Relational Markov networks have been used for semantic labeling of 3D scan data. They have also been used to compactly represent object maps and to estimate trajectories of people. Relational hidden Markov models have been used for protein fold recognition. Markov logic networks have been proven to be successful for joint unsupervised coreference resolution and unsupervised semantic parsing. for classification, link prediction and for learning to rank search results.

1.5 Ontologies and Probability

Ontology in Computer Science is a way of representing a common understanding of a domain. Informally, an ontology consists of a hierarchical description of important and precisely defined concepts in a particular domain, along with the description of the properties (of the instances) of each concept and the relations among them. In the AI perspective, an ontology refers to the specification of knowledge in a bounded universe of discourse only. As a result, a number of bounded-universe ontologies have been created over the last decade: the Chemicals ontology in the chemistry area, the Enterprise ontologies for enterprise modeling, an ontology of air campaign planning in the defense area, the GALEN ontology in the medical informatics area. Data that are reliable and people care about, particularly in the sciences, are being represented using the vocabulary defined in formal ontologies (Fox et al., 2006).

The next stage in this line of research is to represent scientific hypotheses as formal ontologies that are able to make *probabilistic predictions* that can be judged against data (Poole et al., 2008).

Ontologies play also a crucial role in the development of the *Semantic Web* as a means for defining shared terms in web resources. Semantic Web aims at an extension of the current Web by standards and technologies that help machines to understand the information on the Web so that they can support richer discovery, data integration, navigation, and automation of tasks. Ontologies in the Semantic Web are formulated in web ontology languages (such as OWL), which are based on expressive Description Logics (DL). Description logics aim at providing a decidable first-order formalism with a simple well-established declarative semantics to capture the meaning of structured representations of knowledge.

However, classical ontology languages and Description Logics are less suitable in all those domains where the information to be represented comes along with (quantitative) *uncertainty*. Formalisms for dealing with uncertainty and vagueness have started to play an important role in research related to the Web and the Semantic Web. For example, the order in which Google returns the answers to a web search query is computed by using probabilistic techniques. Furthermore, formalisms for dealing with uncertainty in ontologies have been successfully applied in ontology matching, data integration, and information retrieval. Vagueness and imprecision also abound in multimedia information processing and retrieval. To overcome this deficiency, approaches for integrating *probabilistic logic and fuzzy logic* into Description Logics have been proposed.

Reasoning tasks: inference

In addition to the ability to describe (uncertain) concepts formally, one also would like to employ the description of a set of concepts to ask questions about the concepts and instances described. The most common inference problems are basic questions like instance checking (is a particular instance a member of a given concept?) and relation checking (does a relation/role hold between two instances?), and global questions like subsumption (is a concept a subset of another concept?), and concept consistency (the concept is necessarily empty?).

These works combine all of the issues of relational probabilistic modeling as well as the problems of describing the world at multiple level of abstraction and detail and handling multiple heterogeneous data sets.

Applications

As pointed out, there is a plethora of applications with an urgent need for handling probabilistic knowledge in ontologies, especially in areas like web, medicine, biology, defense, and astronomy. Some of the arguments for the critical need of dealing with probabilistic uncertainty in ontologies are:

- in addition to being logically related, the concepts of an ontology are generally also probabilistically related. For example, two concepts either may be logically related via a subset or disjointness relationship, or they may show a certain degree of overlap. Probabilistic ontologies allow for quantifying these degrees of overlap, reasoning about them, and using them in semantic-web applications. The degrees of concept overlap may also be exploited in personalization and recommender systems;

- like the current Web, the Semantic Web will necessarily contain ambiguous and controversial pieces of information in different web sources. This can be handled via probabilistic data integration by associating a probability describing the degree of reliability with every web source;

- an important application for probabilistic ontologies is information retrieval: fuzzy description logics, that are not treated in this thesis, have first been proposed for logic-based information retrieval, for multimedia data, in the medical domain, for the improvement of search and comparison of products in electronic markets, etc.

Chapter 2

Thesis Aims

Statistical relational learning is a young field. There are many opportunities to develop new methods and apply the tools to compelling real-world problems. Today, the challenges and opportunities of dealing with structured data and knowledge have been taken up by the artificial intelligence community at large and form the motivation for a lot of ongoing research.

First, this thesis addresses the two problems of **parameter estimation and structure learning** for the probabilistic logic language of **Logic Programs with Annotated Disjunctions** (LPADs) (Vennekens and Verbaeten, 2003), a formalism based on disjunctive logic programs and the distribution semantics. The basis provided by *disjunctive logic programs* makes LPADs particularly suitable when reasoning about actions and effects, where we have causal independence among the possible different outcomes for a given action. In this formalism, each of the disjuncts in the head of a logic clause is annotated with a probability, for instance: $heads(Coin) : 0.6 \vee tails(Coin) : 0.4 \leftarrow toss(Coin), biased(Coin).$ states that a biased coin lands on heads with probability 0.6 and on tails with probability 0.4. Viewing such set of probabilistic disjunctive clauses as a probabilistic disjunction of normal logic programs allows to derive a possible world semantics. This semantics offers a natural way of describing complex probabilistic knowledge in terms of a number of simple choices.

The *distribution semantics* is one of the most prominent approaches to define the semantics of probabilistic logic languages, in fact it underlies Probabilistic Logic Programs, Probabilistic Horn Abduction, PRISM, Independent Choice Logic (ICL), pD, Logic Programs with Annotated Disjunctions, ProbLog and CP-logic. The approach is particularly appealing for its intuitiveness and because efficient inference algorithms have been developed, which use Binary Decision Diagrams (BDDs) for the computation of the probability of queries.

LPADs are not a radically new formalism with respect to other probabilistic logic languages, but, although they may be similar in terms of theoretical expressive power, they are quite different in their practical modeling properties. For example, ICL (Poole, 1997) is suited for problem domains such as diagnosis or theory revision, where we express uncertainty on the causes of certain effects; the more flexible syntax of LPADs makes them also suited for modeling indeterminate actions, in which it is most natural to express uncertainty on the effects of certain causes. The algorithms developed for LPADs are also applicable to other probabilistic programming languages, since there are transformations with linear complexity that can convert each one into the others. We exploit the graphical structures of BDDs for efficient inference.

The goal of the thesis is also to show how techniques of Logic Programming for inference and learning of probabilistic logic languages following the distribution semantics can compete with the techniques for inference and learning of Markov Logic Networks. MLNs combine probabilistic graphical models and first-order logic but are not logic programming-based.

The effectiveness of the algorithms developed for LPADs is tested on several machine learning tasks: text classification, entity resolution, link prediction, information extraction, recommendation systems.

Second, the thesis addresses the issues of (1) **integrating probability** in $\mathcal{SHOIN}^{(\mathbf{D})}$ Description Logic and (2) performing efficient inference in probabilistic ontologies expressed in this language. $\mathcal{SHOIN}^{(\mathbf{D})}$ is an expressive description logic which plays an important role in the Semantic Web, being the theoretical counterparts of OWL DL, a sublanguage of the Web Ontology Language for the Semantic Web.

Both issues draw inspiration from the SRL field in terms of semantics and inference techniques. To our knowledge, there are no other approaches to probabilistic DLs based on the distribution semantics.

Chapter 3

Structure of the text

The thesis is divided into six parts: Introduction, preliminaries of Logic and Probability, Statistical Relational Learning, where our algorithms for Logic Programs with Annotated Disjunctions are described, preliminaries on Description Logics and Semantic Web, Probabilistic Description Logics, where a new semantics and inference algorithm are proposed, Summary and Future works.

Part I starts with an introductory chapter clarifying the nature, motivations and goals of this thesis. Chapter 4 lists the publications related to the themes treated herein.

Part II recalls basic concepts required in the course of this thesis. In particular, Chapter 5 provides an introduction to logic and logic programming, which will be used throughout the thesis as the representation language. Chapter 6 provides an introduction to probability theory to understand the probabilistic component of SRL formalisms. Chapter 7 reviews Decision Diagrams and in particular the Binary ones (BDDs) that are used by LPADs inference techniques. Chapter 8 describes the Expectation Maximization (EM) algorithm, which is the core of our learning algorithms, since it is the basis of parameter optimization in LPAD's clauses.

Part III covers statistical relational learning and the new contributions promoted by this thesis. Chapter 9 illustrates the probabilistic logic language of LPADs and its semantic basis, the so-called Distribution Semantics. Chapters 10 and 11 present one parameter estimation algorithm (`EMBLEM`) and two structure learning algorithms (`SLIPCASE` and `SLIPCOVER`) for LPADs, respectively; detailed descriptions of the algorithms are provided, together with the descriptions of the real world datasets used for testing, the performance estimation measures and an extensive comparison among these algorithms and many state-of-the-art learning systems. Chapters 10 compares `EMBLEM`'s performance with the following systems: Relational Information Bottleneck (RIB), created for a sub-class of SRL languages that can be converted to Bayesian networks, CEM, an implementation of EM based on the cplint inference library (Riguzzi, 2007b, 2009), a learning algorithm for Causal Probabilistic-Logic (CP-Logic), LeProblog and LFI-Problog for the ProbLog language, Alchemy for Markov Logic Networks. Chapter 11 compares SLIPCASE and SLIPCOVER with the following systems: Aleph, SEM-CP-Logic, which applies structural EM to CP-Logic, LSM for Learning MLNs using Structural Motifs, ALEPH++ExactL1, which incorporates Aleph for structure learning and an evolution of the basic algorithm in Alchemy for weight learning.

Part IV recalls basic concepts on ontologies and their languages (DLs). Chapter 12 begins with a forecast on the future of the current Web. Chapter 13 summarizes the meaning of the word ‘ontology’ in Computer Science, its building blocks, the languages for Semantic Web ontologies and application fields. Chapter 14 covers knowledge representation in description logics in terms of syntax, semantics and inference.

Part V is dedicated to probabilistic approaches to description logics and the new contributions presented by this thesis. In particular, after an introduction regarding previous probabilistic extensions in Chapter 15, Chapter 16 illustrates how, inspired by the work of (Halpern, 1990) about the different interpretations of the meaning of probability, a probabilistic framework based on the distribution semantics for probabilistic logic languages can be built for the $\mathcal{SHOIN}^{(\mathcal{D})}$ DL. Chapter 17 presents a probabilistic reasoner (BUNDLE) built upon this framework for computing the probability of queries. It also presents experimental evaluations of inference performances in comparison with another state-of-the-art system for $\mathcal{P} - \mathcal{SHIQ}^{(\mathcal{D})}$ DL on a real world probabilistic ontology.

Part VI summarizes the research work conducted in this dissertation and presents directions for future work.

Implementation

The parameter learning algorithm EMBLEM and the structure learning algorithm SLIPCASE are available in the cplint package in the source tree of Yap Prolog, which is open source; user manuals can be found at http://sites.google.com/a/unife.it/ml/emblem and http://sites.unife.it/ml/slipcase.

The structure learning algorithm `SLIPCOVER` will be available in the source code repository of the development version of Yap. More information on the system, including a user manual and the datasets used, will be published at `http://sites.unife.it/ml/slipcover`.

As regards the SRL algorithms, the BDDs are manipulated by means of the CUDD library [1] and the experiments were conducted by means of the YAP Prolog system (COSTA et al., 2012).

As regards the probabilistic DL reasoner, the BDDs are manipulated by means of the CUDD library through JavaBDD[2], which is used as an interface to it; the system was built upon the Pellet reasoner (Sirin et al., 2007), which is written in Java. `BUNDLE` is available for download from `http://sites.unife.it/ml/bundle` together with the datasets used in the experiments.

[1]`http://vlsi.colorado.edu/~fabio/`

[2]`http://javabdd.sourceforge.net/`

Chapter 4

Publications

Papers containing the work described in this thesis were presented in various venues:

- **Journals**
  - Bellodi, E. and Riguzzi, F. (2012a). Expectation Maximization over binary decision diagrams for probabilistic logic programs. Intelligent Data Analysis, 16(6).
  - Bellodi, E. and Riguzzi, F. (2012b). Experimentation of an expectation maximization algorithm for probabilistic logic programs. Intelligenza Artificiale, 8(1):3-18.
  - Riguzzi, F. and Bellodi, E. (submitted). Structure learning of probabilistic logic programs by searching the clause space. Theory and Practice of Logic Programming.
- **Conferences**
  - Bellodi, E. and Riguzzi, F. (2011a). EM over binary decision diagrams for probabilistic logic programs. In Proceedings of the 26th Italian Conference on Computational Logic (CILC2011), Pescara, Italy, 31 August 31-2 September, 2011.
  - Bellodi, E. and Riguzzi, F. (2011b). Learning the structure of probabilistic logic programs. In Inductive Logic Programming, 21th International Conference, ILP 2011, London, UK, 31 July-3 August, 2011.
  - Bellodi, E., Riguzzi, F., and Lamma, E. (2010a). Probabilistic declarative process mining. In Bi, Y. and Williams, M.-A. editors, Proceedings of the 4th International Conference on Knowledge Science, Engineering & Management (KSEM 2010),

Belfast, UK, September 1-3, 2010, volume 6291 of Lecture Notes in Computer Science, pages 292-303, Heidelberg, Germany. Springer.

  - Bellodi, E., Riguzzi, F., and Lamma, E. (2010b). Probabilistic logic-based process mining. In Proceedings of the 25th Italian Conference on Computational Logic (CILC2010), Rende, Italy, July 7-9, 2010, number 598 in CEUR Workshop Proceedings, Aachen, Germany. Sun SITE Central Europe.
  - Riguzzi, F., Bellodi, E., and Lamma, E. (2012). Probabilistic ontologies in Datalog+/-. In Proceedings of the 27th Italian Conference on Computational Logic (CILC2012), Roma, Italy, 6-7 June 2012, number 857 in CEUR Workshop Proceedings, pages 221-235, Aachen, Germany. Sun SITE Central Europe.

- **Workshops**
  - Bellodi, E., Lamma, E., Riguzzi, F., and Albani, S. (2011). A distribution semantics for probabilistic ontologies. In Proceedings of the 7th International Workshop on Uncertainty Reasoning for the Semantic Web, Bonn, Germany, 23 October, 2011, number 778 in CEUR Workshop Proceedings, Aachen, Germany. Sun SITE Central Europe.
  - Bellodi, E. and Riguzzi, F. (2011). An expectation maximization algorithm for probabilistic logic programs. In Workshop on Mining Complex Patterns (MCP2011), Palermo, Italy, 17 September, 2011.
  - Riguzzi, F., Bellodi, E., and Lamma, E. (2012a). Probabilistic Datalog+/- under the distribution semantics. In Kazakov, Y.,Lembo, D., and Wolter, F., editors, Proceedings of the 25th International Workshop on Description Logics (DL2012), Roma, Italy, 7-10 June 2012, number 846 in CEUR Workshop Proceedings, Aachen, Germany. Sun SITE Central Europe.
  - Riguzzi, F., Bellodi, E., Lamma, E., and Zese, R. (2012b). Epistemic and statistical probabilistic ontologies. In Proceedings of the 8th International Workshop on Uncertainty Reasoning for the Semantic Web, Boston, USA, 11 November, 2012, number 900 in CEUR Workshop Proceedings, Aachen, Germany. Sun SITE Central Europe.
  - Riguzzi, F., Lamma, E., Bellodi, E., and Zese, R. (2012c). Semantics and inference for probabilistic ontologies. In Baldoni, M., Chesani, F., Magnini, B., Mello,

P., and Montai, M., editors, Popularize Artificial Intelligence. Proceedings of the AI*IA Workshop and Prize for Celebrating 100th Anniversary of Alan TuringŠs Birth (PAI 2012), Rome, Italy, June 15, 2012, number 860 in CEUR Workshop Proceedings, pages 41-46, Aachen, Germany. Sun SITE Central Europe.

Part II

Foundations of Logic and Probability

Chapter 5

Logic

This chapter is dedicated to introducing the language of logic. In particular Section 5.1 presents propositional logic, Section 5.2 first order logic, Section 5.3 logic programming and finally Section 5.4 Inductive Logic Programming. For a detailed coverage of these aspects see (Nilsson and Maluszynski, 1990), (Lobo et al., 1992).

5.1 Propositional Logic

In this section, we introduce propositional logic, a formal system whose original purpose, dating back to Aristotle, was to model reasoning. In more recent times, this system has proved useful as a design tool. Many systems for automated reasoning, including theorem provers, program verifiers, and applications in the field of artificial intelligence, have been implemented in logic-based programming languages. These languages generally use *predicate logic*, a more powerful form of logic that extends the capabilities of propositional logic. We shall meet predicate logic in the next Section.

Syntax

In propositional logic there are atomic assertions (or atoms, or propositional symbols) and compound assertions built up from the atoms. The atomic facts stand for any statement that can have one of the truth values, true or false. Compound assertions express logical relationships between the atoms and are called propositional formulae.

The **alphabet** for propositional formulae consists of:

1. A countable set **PS** of propositional symbols or variables: P_0, P_1, P_2,...;

2. The *logical connectives*: $\wedge$ (and), $\vee$ (or), $\rightarrow$ or $\supset$ (implication), $\neg$ (not), $\equiv$ or $\leftrightarrow$ (equivalence) and the constant $\perp$ (false);

3. *Auxiliary symbols*: "("(left parenthesis), ")"(right parenthesis).

The set *PROP* of propositional formulae (or "propositions") is defined inductively as the smallest set of strings over the alphabet, such that:

1. Every proposition symbol P_i and $\perp$ are in *PROP*; these are the atomic operands;

2. Whenever A is in *PROP*, $\neg$ A is also in *PROP*;

3. Whenever A, B are in *PROP*, (A $\vee$ B), (A $\wedge$ B), (A $\rightarrow$ B) and (A $\equiv$ B) are also in *PROP*.

4. A string is in *PROP* only if it is formed by applying the rules (1),(2),(3).

The proposition (A $\wedge$ B) is called conjunction and A,B conjuncts. The proposition (A $\vee$ B) is called disjunction and A,B disjuncts. The proposition (A $\rightarrow$ B) is called implication, A (to the left of the arrow) is called the antecedent and B (to the right of the arrow) is called the consequent.

Example 1 *The following strings are propositions.*

$$\begin{array}{ccc} P1 & P2 & (P1 \vee P2) \\ ((P1 \rightarrow P2) \equiv (\neg P1 \vee P2)) & (\neg P1 \equiv (P1 \rightarrow \perp)) & (P1 \vee \neg P1) \end{array}$$

On the other hand, strings such as $(P1 \vee P2)\wedge$ are not propositions, because they cannot be constructed from PS and $\perp$ and the logical connectives.

In order to minimize the number of parentheses, a precedence is assigned to the logical connectives and it is assumed that they are left associative. Starting from highest to lowest precedence we have:

$$\neg$$

$$\wedge$$

$$\vee$$

$$\rightarrow, \equiv$$

Semantics

The semantics of propositional logic assigns a truth function to each proposition in *PROP*. First, it is necessary to define the meaning of the logical connectives. The set of truth values is the set *BOOL* = **{T,F}**. Each logical connective is interpreted as a function with range *BOOL*. The logical connectives are interpreted as follows.

P	Q	$\neg P$	$P \wedge Q$	$P \vee Q$	$P \rightarrow Q$	$P \equiv Q$
T	T	F	T	T	T	T
T	F	F	F	T	F	F
F	T	T	F	T	T	F
F	F	T	F	F	T	T

The logical constant $\perp$ is interpreted as **F**.

The above table is what is called a *truth table*. A *truth assignment* or *valuation* is a function assigning a truth value in *BOOL* to all the propositional symbols. Once the symbols have received an interpretation, the truth value of a propositional formula can be computed, by means of truth tables. A function that takes truth assignments as arguments and returns either TRUE or FALSE is called *Boolean function*.

If a propositional formula A contains *n* propositional letters, one constructs a truth table in which the truth value of A is computed for all valuations depending on n arguments. Since there are 2^n such valuations, the size of this truth table is 2^n.

Example 2 *The expression A =* $P \wedge (P \vee Q)$*, for the truth assignment P =* ***T*** *and Q =* ***F****, evaluates to* ***T****. One can evaluate A for the other three truth assignments, and thus build the entire Boolean function that A represents.*

A proposition is *satisfiable* if there is a valuation (or truth assignment) *v* such that *v(A)* = **T**. A proposition is *unsatisfiable* if it is not satisfied by any valuation. The proposition A in example 2 is satisfied with the given assignment.

5.2 First Order Logic

Propositional logic is not powerful enough to represent all types of assertions that are used in computer science and mathematics, or to express certain types of relationship between propositions.

If one wants to say in general that, if a person knows a second person, then the second person knows the first, propositional logic is inadequate; it gives no way of encoding this more general belief. *Predicate Logic* solves this problem by providing a finer grain of representation. In particular, it provides a way of talking about individual objects and their interrelationships. It introduces two new features: *predicates* and *quantifiers*. In particular we shall introduce *First Order* predicate *logic*.

Syntax

The syntax of First Order Logic is based on an alphabet.

Definition 1 *A first order alphabet Σ consists of the following classes of symbols:*

1. *variables, denoted by alphanumeric strings starting with an uppercase character;*
2. *function symbols (or functors), denoted by alphanumeric strings starting with a lowercase character;*
3. *predicate symbols, alphanumeric strings starting with a lowercase character;*
4. *propositional constants, true and false;*
5. *logical connectives (negation, disjunction, conjunction, implication and equivalence;*
6. *quantifiers, $\exists$ (there exists or existential quantifier) and $\forall$ (for all or universal quantifier);*
7. *punctuation symbols, '(' and ')' and ','.*

Associated with each predicate symbol and function symbol there is a natural number called *arity*. If a function symbol has arity 0 it is called a *constant*. If a predicate symbol has arity 0 it is called a *propositional symbol*.

A *term* is either a variable or a functor applied to a tuple of terms of length equal to the arity of the functor.

Definition 2 *A (well-formed) formula (wff) is defined as follows:*

1. *If p in an n-ary predicate symbol and $t_1, ...t_n$ are terms, then $p(t_1, ...t_n)$ is a formula (called atomic formula or more simply atom);*
2. *true and false are formulas;*

3. *If F and G are formulas, then so are ($\neg F$), ($F \wedge G$), ($F \vee G$), ($F \rightarrow G$), ($F \leftarrow G$) and ($F \leftrightarrow G$);*

4. *If F is a formula and X is a variable, then so are ($\exists XF$) and ($\forall XF$).*

Definition 3 *A First Order language is defined as the set of all well-formed formulas constructible from a given alphabet.*

A *literal* is either an atom a or its negation $\neg a$. In the first case it is called a *positive literal*, in the latter case it is called a *negative literal*.

An occurrence of a variable is *free* if and only if it is not in the scope of a quantifier of that variable. Otherwise, it is *bound*. For example, Y is free and X is bound in the following formula: $\exists Xp(X, Y)$.

A formula is *open* if and only if it has free variables. Otherwise, it is *closed*. For example, the formula $\forall X \forall Y path(X, Y)$ is closed.

The following precedence hierarchy among the quantifiers and logical connectives is used to avoid parentheses in a large formula:

$$\neg, \forall, \exists$$

$$\vee$$

$$\wedge$$

$$\rightarrow, \leftarrow, \leftrightarrow$$

A *clause* is a formula C of the form

$$\forall X h_1 \vee \ldots \vee h_n \leftarrow b_1, \ldots, b_m$$

where X is the set of variables appearing in C, $h_1, \ldots, h_n$ and $b_1, \ldots, b_m$ are atoms, whose separation by means of commas represents a ; usually the quantifier is omitted. A clause can be seen as a set of literals, e.g., C can be seen as

$$\{h_1, \ldots, h_n, \neg b_1, \ldots, \neg b_m\}.$$

In this representation, the disjunction among the elements of the set is left implicit.

Which form of a clause is used in the following will be clear from the context. $h_1 \vee \ldots \vee h_n$ is called the *head* of the clause and $b_1, \ldots, b_m$ is called the *body*. We will use $head(C)$ to indicate either $h_1 \vee \ldots \vee h_n$ or $\{h_1, \ldots, h_n\}$, and $body(C)$ to indicate either $b_1, \ldots, b_m$ or $\{b_1, \ldots, b_m\}$, the exact meaning will be clear from the context.

When $m = 0$ and $n = 1$, C is called a *fact*. When $n = 1$, C is called a *definite clause* and represents a clause with exactly one positive literal. When $n = 0$ - that is, the head is empty - C is called a *goal*; each $b_i (i = 1, ...m)$ is called a *subgoal* of the goal clause. The empty clause, denoted as $\Box$, is a clause with both head and body empty; it is interpreted as false. A *query* is a formula of the form

$$\exists (A_1 \wedge ... \wedge A_n)$$

where $n \geq 0$ and $A_1, ...A_n$ are atoms with all variables existentially quantified. Observe that a goal clause

$$\leftarrow A_1, ...A_n$$

is the negation of the query defined above. The logical meaning of a goal can be explained by referring the equivalent universally quantified formula:

$$\forall X_1 ... \forall X_n \neg (A_1 \wedge ... \wedge A_n)$$

where $X_1, ..., X_n$ are all variables that occur in the goal. This is equivalent to:

$$\neg \exists X_1 ... \exists X_n (A_1 \wedge ... \wedge A_n)$$

This, in turn, can be seen as an existential question and the system attempts to deny it by constructing a counter-example. That is, it attempts to find terms $t_1, ..., t_n$ such that the formula obtained from $A_1 \wedge ... \wedge A_n$ when replacing the variable X_i by t_i $(1 \leq i \leq n)$, is true in any model of the program, i.e. to construct a logical consequence of the program which is an instance of a conjunction of all subgoals in the goal.

A clause is *range restricted* if all the variables that appear in the head appear as well in positive literals in the body.

A term, atom, literal, goal, query or clause is *ground* if it does not contain variables. A *substitution* θ is an assignment of variables to terms: $\theta = \{V_1/t_1, \ldots, V_n/t_n\}$. The *application of a substitution to a term, atom, literal, goal, query or clause* C, indicated with $C\theta$, is the replacement of the variables appearing in C and in θ with the terms specified in θ.

A *theory* P is a set of clauses. A *definite theory* is a finite set of definite clauses.

The *Herbrand universe* $H_U(P)$ of a theory P is the set of all the ground terms that can be built from functors and constants appearing in P. The *Herbrand base* $H_B(P)$ is the set of all the ground atomic formulas. It is assumed that the theory contains at least one constant (since otherwise, the domain would be empty). A *Herbrand interpretation* of P is a set of ground atoms, i.e. a subset of $H_B(P)$. A *Herbrand model* of a set of (closed) formulas is a Herbrand interpretation which is a model of every formula in the set. In order to determine if a Herbrand interpretation I is a model of a universally quantified formula $\forall F$ it is necessary to check if all ground instances of F are true in I. For the restricted language of definite theories, in order to determine whether an atomic formula A is a logical consequence of a definite theory P it suffices to check that every Herbrand model of P is also a Herbrand model of A. The *least Herbrand model* M_P of a definite theory P is the set of all ground atomic logical consequences of the theory. That is, $M_P = \{A \in H_B(P) \mid P \models A\}$. In the following, we will omit the word 'Herbrand'.

A *grounding* of a clause C is obtained by replacing the variables of C with terms from $H_U(P)$. The grounding $g(P)$ of a theory P is the program obtained by replacing each clause with the set of all of its groundings.

Semantics

The semantics of a First Order theory provides the meaning of the theory based on some interpretation. Interpretations provide specific meaning to the symbols of the language and are used to provide meaning to a set of well-formed formulas. They also determine a domain of discourse that specifies the range of the quantifiers. The result is that each term is assigned to an object, and each formula is assigned to a truth value.

The domain of discourse *D* is a nonempty set of "objects" of some kind. Intuitively, a First Order formula is a statement about these objects; for example, $\exists X p(X)$ states the existence of an object *X* such that the predicate *p* is true. The domain of discourse is the set of considered objects. For example, one can take it to be the set of integer numbers. The interpretation of a function symbol is a function. For example, if the domain of discourse consists of integers, a function symbol *f* of arity 2 can be interpreted as the function that gives the sum of its arguments. In other words, the symbol *f* is associated with the function *I(f)* which, in this interpretation, is addition.

An interpretation *I* is a *model* of a closed formula ϕ if ϕ evaluates to *true* with respect to *I*. Let us now define the truth of a formula in an interpretation.
Let I be an interpretation and ϕ a formula, ϕ is true in I, written $I \models \phi$ if

- $a \in I$, if ϕ is a ground atom a;
- $a \notin I$, if ϕ is a ground negative literal $\neg a$;
- $I \models a$ and $I \models b$, if ϕ is a conjunction $a \wedge b$;
- $I \models a$ or $I \models b$, if ϕ is a disjunction $a \vee b$;
- $I \models \psi\theta$ if $\phi = \forall \mathbf{X}\psi$ for all θ that assign a value to all the variables of $\mathbf{X}$;
- $I \models \psi\theta$ if $\phi = \exists \mathbf{X}\psi$ for a θ that assigns a value to all the variables of $\mathbf{X}$.

Let *S* be a set of closed formulas, then *I* is a model of *S* if *I* is a model of each formula of *S*. This is denoted as $I \models S$. Let *S* be a set of closed formulas and *F* a closed formula. *F* is a *logical consequence of S* if for each model *M* of *S*, *M* is also a model of *F*. This is denoted as $S \models F$.

A clause C of the form

$$h_1 \vee \ldots \vee h_n \leftarrow b_1, \ldots, b_m$$

is a shorthand for the formula

$$\forall \mathbf{X}\; h_1 \vee \ldots \vee h_n \leftarrow b_1, \ldots, b_m$$

where $\mathbf{X}$ is a vector of all the variables appearing in C. Therefore, C is true in an interpretation I iff, for all the substitutions θ grounding C, if $I \models \mathit{body}(C)\theta$ then $I \models \mathit{head}(C)\theta$, i.e., if $(I \models \mathit{body}(C)\theta) \rightarrow (\mathit{head}(C)\theta \cap I \neq \emptyset)$. Otherwise, it is false. In particular, a definite clause is true in an interpretation I iff, for all the substitutions θ grounding C, $(I \models \mathit{body}(C)\theta) \rightarrow h \in I$.

A theory P is true in an interpretation I iff all of its clauses are true in I and we write

$$I \models P.$$

If P is true in an interpretation I we say that I is a *model* of P. It is sufficient for a single clause of a theory P to be false in an interpretation I for P to be false in I.

We usually are interested in deciding whether a query Q is a logical consequence of a theory P, expressed as

$$P \models Q$$

This means that Q must be true in every model $M(P)$ of P that is assigned to P as its meaning by one of the semantics that have been proposed for normal logic programs (e.g. (Clark, 1978; Gelfond et al., 1988; Van Gelder et al., 1991)).

For theories, we are interested in deciding whether a given theory or a given clause is true in an interpretation I. This will be explained in the next paragraph.

5.3 Logic Programming

The idea of logic programming is to use a computer for drawing conclusions from declarative descriptions. Thus, the idea has its roots in research on *automatic theorem proving*. The first programs based on logic were developed in 1972 at the University of Marseilles where the logic programming language Prolog was developed. Kowalski (Kowalski, 1974) published the first paper that formally described logic as a programming language in 1974. Van Emden and Kowalski laid down the theoretical foundation for logic programming.

Disjunctive logic programming is an extension of logic programming and is useful in representing and reasoning with indefinite information.
A *disjunctive logic program* consists of a finite set of implicitly quantified universal clauses of the form

$$a_1, \ldots, a_n \leftarrow b_1, \ldots, b_m \;\; n > 0 \; and \; m \geq 0 \tag{5.1}$$

where the a_i and the b_j are atoms. The formula is read as "a_1 or a_2 or ... or a_n if b_1 and b_2 and ... and b_m." If the body of the formula is empty and the head is not, it is referred to as a *fact*. If both are not empty the formula is referred to as a *procedure*. A procedure of a fact is also referred to as a *logic program clause*. A finite set of such logic program clauses constitutes a *disjunctive* logic program. If clauses of the form 5.1 contain *literals* in the body (the b_i), they are referred to as *normal* (when the head is an atom) or *general disjunctive* logic program clauses.

A definite logic program is a special case of disjunctive logic program, where the head of a logic program clause consists of a single atom. This is stated by the following definitions.

Definition 4 *A definite logic program clause is a program clause of the form:*

$$a \leftarrow b_1, \ldots, b_m (m \geq 0)$$

where a is an atom and $b_1, \ldots, b_m$ are literals. Looking at these clauses in conjunctive normal form one can see that each clause has only one positive literal.

Definition 5 *A definite logic program (or Horn program) is a finite set of definite logic program clauses.*

Such a delineation provides a declarative meaning for a clause in that the consequent is true when the antecedent is true. It also translates into a procedural meaning where the consequent can be viewed as a problem which is to be solved by reducing it to a set of sub-problems given by the antecedent. This is tackled in the next section.

Definite Logic Programming

In 1976 paper, van Emden and Kowalski (van Emden and Kowalski, 1976) defined different semantics for a definite logic program. These are referred to as model-theoretic, proof theoretic (or procedural) and fixpoint (or denotational) semantics. Since we are dealing with logic, a natural semantics is to state that the meaning of a definite logic program is given by a Herbrand model of the theory. Hence, the meaning of the logic program is the set of atoms that are in the model. However, this definition is too broad as there may be atoms in the Herbrand model that one would not want to conclude to be true. For example, in the logic program given in Example 3, M_2 includes atoms $edge(c,c), path(b,a), path(a,a)$. It is clear that the logic program does not state that any of these atoms are true.

Example 3 *Consider the following definite logic program P:*

$path(X,Y) \leftarrow edge(X,Y).$
$path(X,Y) \leftarrow edge(X,Z), path(Z,Y).$
$edge(a,b).$
$edge(b,c).$
$M_1 = \{edge(a,b), edge(b,c), path(a,b), path(b,c), path(a,c)\}$
$M_2 = \{edge(a,b), edge(b,c), edge(c,c), path(a,b), path(b,c), path(a,c), path(b,a),$
$path(a,a)\}$

are two Herbrand models of P.

The authors showed that for definite logic programs, the intersection of all Herbrand models of a logic program is a Herbrand model of the logic program. This property is called the Herbrand model intersection property: the intersection is the *least Herbrand model* as it is contained within all models. The least model captures all the ground atomic logical consequences of the logic program and represents the least amount of information that can be specified as true.

Example 4 *Consider the definite logic program P given in Example 3. The least Herbrand model of P is given by $M_P = \{edge(a,b), edge(b,c), path(a,b), path(b,c), path(a,c)\}$. These are the only ground atoms which are logical consequences of P.*

A second semantics that can be associated with logic programs is a *procedural semantics*. Gödel showed that one obtains the same results with proof theory as one does from model theory. Van Emden and Kowalski showed that if one uses a proof procedure called *linear resolution with selection function for definite logic programs (SLD-resolution)*, the ground atoms that are derivable using SLD from the logic program, forming the SLD-success set of the logic program, are exactly the same atoms in the least Herbrand model M_P. SLD-resolution is a reduction type of processing and derives a sequence of queries, starting from a query.

A third semantics is obtained by defining a mapping, T, from Herbrand interpretations to Herbrand interpretations. By a *fixpoint* of a mapping T, we mean an element I of the domain of T that satisfies the formula $T(I) = I$. The least fixpoint of T exists if the domain over which T is defined is a complete lattice and the mapping is continuous, in fact it is computed by applying T on the lattice. Herein we are not interested in this kind of semantics.

The major result is that the model theoretic, the procedural and fixpoint semantics, all capture the same meaning to a logic program: the set of ground atoms that are logical consequences of the logic program.

SLD resolution principle

Reasoning can be seen as the process of manipulating formulas, which from a given set of formulas, called the premises, produces a new formula called the conclusion. One of the objectives is to formalize reasoning principles as formal re-write rules that can be used to generate new formulas from given ones. These rules are called *inference rules*. It is required that the inference rules correspond to correct ways of reasoning - whenever the premises are true in any world under consideration, any conclusion obtained by the application of an inference rule should also be true in this world. The transition from experimental theorem proving to applied logic programming requires improved efficiency of the system. This is achieved by introducing restrictions on the language of formulas, restrictions that make it possible to use the powerful inference rule called *SLD-resolution principle*.

Logic programs consist of logical formulas and computation is the process of deduction or proof construction. One of the main ingredients in this inference mechanism is the process of making two atomic formulas syntactically equivalent. This process is called *unification*.

Definition 6 *(Unifier) Let* s *and* t *be terms. A substitution θ such that $s\theta$ and $t\theta$ are identical (denoted $s\theta$ = $t\theta$) is called a unifier of* s *and* t.

For instance, the substitution $\{X/a, Y/a\}$ is a unifier of terms $f(X, g(Y)), f(a, g(X))$.

Definition 7 *(Generality of substitutions) A substitution θ is said to be more general than a substitution σ (denoted $\sigma \preceq \theta$) iff there exists a substitution ω such that $\sigma = \theta\omega$.*

Definition 8 *(Most general unifier) A unifier θ is said to be a most general unifier (mgu) of two terms iff θ is more general than any other unifier of the terms.*

Definition 9 *(Renaming) A substitution $\{X_1/Y_1, ..., X_n/Y_n\}$ is called a* renaming substitution *iff $Y_1, ..., Y_n$ are new variables.*

Such a substitution always preserves the structure of a term.

The reasoning method at the base of *SLD-resolution* is summarized as the following inference rule (using logic programming notation):

$$\frac{\leftarrow a_1, ...a_{i-1}, a_i, a_{i+1}, ..., a_m \qquad b_0 \leftarrow b_1, ..., b_n}{\leftarrow (a_1, ...a_{i-1}, b_1, ..., b_n, a_{i+1}, ..., a_m)\theta}$$

where

1. $a_1, ..., a_m$ are atomic formulas;
2. $b_0 \leftarrow b_1, ..., b_n$ is a (renamed) definite clause in *P* ($n \geq 0$);
3. mgu(a_i, b_0) = θ.

The rule has two premises - a goal clause and a definite clause. The goal clause may include several atomic formulas which unify with the head of some clause in the program. In this case it may be desirable to introduce some deterministic choice of the selected atom a_i for unification.

In what follows it is assumed that this is given by some function which for a given goal selects the subgoal for unification. This function is called *selection function* or *computation rule*. For example, Prolog's computation rule always selects the leftmost subgoal.

This is a version of the inference rule called *resolution principle*, which was introduced by J. A. Robinson in 1965. The resolution principle applies to clauses. Since definite clauses are restricted clauses the corresponding restricted form of resolution presented is called *SLD-resolution* (Linear resolution for Definite clauses with Selection function).

In the following the use of the SLD-resolution principle is discussed for a given definite program *P*. The starting point is a definite goal clause G_0 of the form:

$$\leftarrow a_1, ..., a_m (m \geq 0)$$

From this goal a subgoal a_i is selected by the computation rule. A new goal clause G_1 is constructed by selecting (if possible) some renamed program clause $b_0 \leftarrow b_1, ..., b_n$ whose head unifies with a_i (resulting in an mgu θ). If so, G_1 will be of the form:

$$(a_1, ...a_{i-1}, b_1, ..., b_n, a_{i+1}, ..., a_m)\theta_1$$

(the variables of the program clause are being renamed so that they are different from those of G_0). Now it is possible to apply the resolution principle to G_1 thus obtaining G_2, etc. This process may or may not terminate. There are two cases when it is not possible to obtain G_{i+1} from G_i:

- when the selected subgoal cannot be resolved (i.e. is not unifiable) with the head of any program clause;
- when $G_i = \square$ (i.e. the empty goal).

A goal G_{i+1} is said to be *derived* (directly) from G_i and C_i via the computation rule (or alternatively, G_i and C_i resolve into G_{i+1}).

Definition 10 *(SLD-derivation) Let G_0 be a definite goal,* P *a definite program and* R *a computation rule. An* SLD-derivation *of G_0 (using* P *and* R*) is a finite or infinite sequence of goals:*

$$G_0 \leadsto^{C_0} G_1 \cdots G_{n-1} \leadsto^{C_{n-1}} G_n ...$$

where each G_{i+1} is derived directly from G_i and a renamed program clause C_i via R.

A finite SLD-derivation where $G_{n+1} = \Box$ is called an *SLD-refutation* of G_0. SLD-derivations that end in the empty goal (and the bindings of variables in the initial goal of such derivations) are of special importance since they correspond to refutations of (and provide answers to) the initial goal. If the initial goal is seen as a *query*, the computed substitutions θ of the refutation restricted to its variables is an answer to this query.

Not all SLD-derivations lead to refutations. If the selected subgoal cannot be unified with any clause, it is not possible to extend the derivation any further and the derivation is called *failed*.

By a *complete derivation* we mean a *refutation*, a *failed derivation* or an *infinite derivation*. A given initial goal clause G_0 may have many complete derivations via a given computation rule *R*. This happens if the selected subgoal of some goal can be resolved with more than one program clause. All such derivations may be represented by a possibly infinite tree called the *SLD-tree* of G_0 (using *P* and *R*).

Example 5 *Consider the following definite program:*

$1 : grandfather(X, Z) \leftarrow father(X, Y), parent(Y, Z).$
$2 : parent(X, Y) \leftarrow father(X, Y).$
$3 : parent(X, Y) \leftarrow mother(X, Y).$
$4 : father(a, b).$
$5 : mother(b, c).$

The SLD-tree of the goal $\leftarrow grandfather(a, X)$ *is depicted in Figure 5.1.*

The SLD-trees of a goal clause G_0 are often distinct for different computation rules. It may even happen that the SLD-tree for G_0 under one computation rule is finite whereas the SLD-tree of the same goal under another computation rule is infinite. A refutation corresponds to a complete path in the SLD-tree that end in $\Box$. Thus the problem reduces to a systematic search of the SLD-tree. Existing Prolog systems often exploit some ordering on the program clauses, e.g. the textual ordering in the source program (Prolog). This imposes the ordering on the outgoing edges of the SLD-tree. The tree is then traversed in a depth-first manner following this ordering. Whenever a leaf node of the SLD-tree is reached the traversal continues by backtracking to the last preceding node of the path with unexplored branches. If it is the empty goal the answer substitution of the completed refutation is reported.

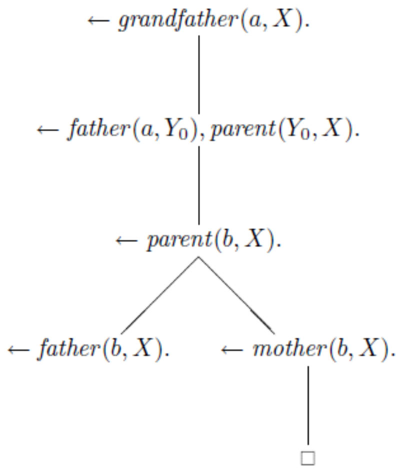


Figure 5.1: SLD-tree of $\leftarrow grandfather(a, X)$ (using Prolog's computation rule).

The *soundness* of SLD-resolution is an essential property which guarantees that the conclusions produced by the system are correct. Correctness in this context means that they are logical consequences of the program. That is, that they are true in every model of the program. Moreover the refutation *completeness* of resolution can be demonstrated, that is, if a goal *G* can be solved by a program *P*, then there is a refutation of $P \cup \{G\}$ by resolution.

Prolog is incomplete, since even if a formula is a logical consequence of the program, the interpreter may go into an infinite loop on infinite SLD-trees, because of depth-first traversal and not because of resolution. Consider for example the definite program:

$sibling(X, Y) : -sibling(Y, X).$
$sibling(b, a).$

When trying to answer *sibling(a,X)* the subgoal is unified with the rule yielding a new goal, identical to the initial one, which is again resolved with the rule yielding the same initial goal. This process will obviously go on forever. The misbehavior can, to some extent, be avoided by moving the rule textually after the fact. By doing so it is possible to find all refutations before going into an infinite loop.

5.4 Inductive Logic Programming

Inductive Logic Programming (ILP) has been defined by (Muggleton and De Raedt, 1994) as a research field at the intersection of Machine Learning and Logic Programming. It is concerned with the development of learning algorithms that adopt logic programs for representing the input data and learn a general theory from specific examples (*induction*). Logic proved to be a powerful tool for representing the complexity that is typical of the real world. In particular, logic can represent in a compact way domains in which the entities of interest are composed of subparts connected by a network of relationships. Logic has some important advantages over other approaches used in machine learning:

- Logic in general, and First Order Logic in particular, is a very well developed mathematical field, providing ILP with a large stock of concept, techniques and results.
- Logic provides a uniform and very expressive means of representation: the background knowledge, the examples and the induced theory can all be represented as formulas in a clausal language. Theory and background knowledge just derive from different sources: the first comes from inductive learning, the second in provided by the user of the system.

See (Nienhuys-Cheng and de Wolf, 1997) for an introduction to ILP.
The problem that is faced by ILP can be expressed as follows:
Given:

- a space of possible theories $\mathcal{H}$;
- a set E^+ of positive examples;
- a set E^- of negative examples;
- a background theory B.

Find a theory $H \in \mathcal{H}$ such that

- all the positive examples are covered by H (completeness);
- no negative example is covered by H (consistency).

If a theory does not cover an example we say that it rules the example out so the last condition can be expressed by saying the "all the negative examples are ruled out by H".

Learning settings The general form of the problem can be instantiated in different ways by choosing appropriate forms for the theories in input and output, for the examples and for the covering relation (Raedt, 1997).

1. In the *learning from entailment* setting, the theories are normal logic programs, the examples are (most often) ground facts and the coverage relation is entailment, i.e., a theory H covers an example e iff
$$H \cup B \models e.$$

   Example 6 *Let us consider the domain of animals and assume that we have a blackbird that flies. This bird could be represented using the following clause* e*:*
$$flies \leftarrow black, bird, hasFeathers, hasWings, normal, laysEggs$$

   Let H be the theory:
   $flies \leftarrow bird, normal$
   $flies \leftarrow insect, hasWings, normal$

   Because $H \models e$, the hypothesis H *covers the example* e*.*

2. In the *learning from interpretations* setting, the theories are composed of clauses, the examples are Herbrand interpretations and the coverage relation is truth in an interpretation, i.e., a theory H covers an example interpretation I iff
$$I \models H.$$

   Similarly, we say that a clause C covers an example interpretation I iff $I \models C$.

   In this setting examples are a kind of partial interpretations I (set of facts) and are completed by taking the minimal Herbrand model $M(B \cup I)$ of background theory B plus I. The minimal Herbrand model of a definite clause theory contains the set of all ground facts that are logically entailed by that theory. The formal and specific definition for learning from interpretations is the following.

   Given:

   - a space of possible theories $\mathcal{H}$;
   - a set E^+ of positive interpretations;

- a set E^- of negative interpretations;
- a background theory (normal logic program) B,

Find a clausal theory $H \in \mathcal{H}$ such that;

- for all $P \in E^+$, H is true in the interpretation $M(B \cup P)$ (completeness);
- for all $N \in E^-$, H is false in the interpretation $M(B \cup N)$ (consistency).

The background knowledge B is used to encode each interpretation parsimoniously, by storing separately the rules that are not specific to a single interpretation but are true for every interpretation.

The truth of a range restricted clause C on a finite interpretation I can be tested by asking the goal ?-$body(C), \neg head(C)$ on a database containing the atoms of I as facts, using a theorem prover (such as Prolog). By $\neg head(C)$ we mean $\neg h_1, \ldots, \neg h_m$. If the query finitely fails, C is true in I, otherwise C is false in I. When we are not given an interpretation I completely but only a partial one, if B is composed only of range restricted clauses one can test the truth of a clause C on $M(B \cup I)$ by running the query ?-$body(C), \neg head(C)$ against a Prolog database containing the atoms of I as facts together with the rules of B. If the query fails, C is true in $M(B \cup I)$, otherwise C is false in $M(B \cup I)$.

Example 7 *The previous example can be represented using the interpretation* I*:*

$$\{flies, black, bird, hasFeathers, hasWings, normal, laysEggs\}$$

This interpretation is a model for the theory H *shown in the previous example.*

There is a subtle difference in meaning between the two representations (Raedt, 2008). By representing the bird using an interpretation, it is assumed that all propositions not in the interpretation are false. Thus, in the example, the interpretation implies that the proposition *insect* is known to be false. This assumption is not made using the clausal representation of the bird. A further difference is that in the clausal representation, there is a distinguished predicate, the predicate flies, that is entailed by the set of conditions. In contrast, using interpretations, all predicates are treated uniformly. The former representation can be more natural when learning a specific concept as a predicate definition, such as the concept of flying things: positive

examples describe the desired input-output behavior of the unknown target program, and negative ones specify a wrong output for a given input; the latter representation is more natural to describe a set of characteristics of the examples.
Learning from entailment setting is more popular than the learning from interpretations, and represents the setting adopted in Part III for the development of learning algorithms.

Structuring the Search Space

Within this view, the goal is to discover those hypotheses in the search space that satisfy desiderable properties and that provide information about the examples. Finding a satisfactory theory means that we have to search among the permitted clauses: learning is searching for a correct theory.

The two basics steps in the search for a correct theory are specialization and generalization. If the current theory together with the background knowledge does not imply all positive examples, one needs to weaken the theory, finding a more general theory such that all positive examples are implied. This is called generalization. On the other hand, if the current theory together with the background knowledge contradicts the negative examples, one needs to strengthen it, finding a more specific theory such that is consistent with respect to the negative examples. This is specialization. In general, finding a correct theory amounts to repeatedly adjusting the theory to the examples by means of steps of both kinds. If we start with an initial non-empty theory to be corrected, the learning task is also called *theory revision*.

One natural way to structure the search space is to employ the *generality* relation. Let the set of examples covered by hypothesis h be denoted as $\mathbf{c}(h)$. The generality relation is defined as follows:

Definition 11 *Let $h_1, h_2 \in \mathcal{H}$. Hypothesis h_1 is* more general *than hypothesis h_2, notation $h_1 \preceq h_2$, if and only if all examples covered by h_2 are also covered by h_1, that is, $\mathbf{c}(h_2) \subseteq \mathbf{c}(h_1)$.*

We also say that h_2 is a specialization of h_1, h_1 is a generalization of h_2. Furthermore, when $h_1 \preceq h_2$ but h_1 covers examples not covered by h_2, we say that h_1 is a proper generalization of h_2, and we write $h_1 \prec h_2$. The hypotheses can be single clauses or sets of clauses (that is, clausal theories).

When *learning from entailment*, the following property holds:

Definition 12 *A hypothesis D is more general than a hypothesis C iff D logically entails C, that is, $D \models C$.*

Indeed, D is more general than C iff $\mathbf{c}(C) \subseteq \mathbf{c}(D)$, if and only if for all examples e: $(C \models e) \rightarrow (D \models e)$, and this happens iff $D \models C$.

However, using logical implication as a generality relation is impractical because of its high computational cost. Therefore, the syntactic relation of θ-*subsumption* is used in place of implication.

Definition 13 *D θ-*subsumes *C (written $D \geq C$) if there exist a substitution θ such that $D\theta \subseteq C$. If $D \geq C$ then $D \models C$ and thus D is more general than C.*

The opposite, however, is not true, so θ-subsumption is only an approximation of the generality relation.

Example 8 *The clause*

$$father(X, john) \leftarrow male(X), male(john), parent(X, john)$$

is θ-subsumed (with substitution $\{Y/X, Z/john\}$) by

$$father(Y, Z) \leftarrow male(Y), parent(Y, Z)$$

The clause

$$p(X, Y, X) \leftarrow q(Y)$$

θ-subsumes (with substitution $\{X/U, Y/U\}$)

$$p(U, U, U) \leftarrow q(U), r(a)$$

Refinements Operators Refinements operators generate a set of specializations (or generalizations) of a given hypothesis for traversing the search space.

Definition 14 *A generalization operator $\rho_g : \mathcal{H} \rightarrow 2^{\mathcal{H}}$ is a function such that*

$$\forall h \in \mathcal{H} : \rho_g(h) \subseteq \{k \in \mathcal{H} \mid k \succeq h\}$$

This operator maps a hypothesis onto a set of its generalizations.

From the definition of θ-subsumption, it follows that a *clause can be generalized* by applying one of the following operations:

- deleting antecedents from the body, such that the remaining literals are linked;
- adding a new atom to the head;
- turning constants into variables.

Example 9 *Generalizations of*

$$student(S) :- advisedBy(S, ford), professor(ford)$$

include

$$student(S) \vee assistant(S) :- advisedBy(S, ford), professor(ford)$$

by adding a new atom to the head,

$$student(S) :- advisedBy(S, P), professor(P)$$

by turning constants into variables,

$$student(S) :- advisedBy(S, ford)$$

by deleting a literal.

Definition 15 *A specialization operator $\rho_s : \mathcal{H} \to 2^{\mathcal{H}}$ is a function such that*

$$\forall h \in \mathcal{H} : \rho_s(h) \subseteq \{k \in \mathcal{H} \mid h \succeq k\}$$

This operator maps a hypothesis onto a set of its specializations.

A *clause can be specialized* by applying one of the following operations:

- adding a literal to the body of a clause;
- removing an atom from the head;
- grounding variables.

Example 10 *Specializations of*

$$student(S) :- advisedBy(S, P)$$

include

$$student(S) :- advisedBy(S, ford)$$

by grounding variables,

$$student(S) :- advisedBy(S, P), professor(P)$$

by adding a literal.

While *top-down approaches* successively specialize a very general starting hypothesis, *bottom-up approaches* successively generalize a very specific hypothesis.
Thus, ILP approaches iteratively modify the current hypothesis syntactically and test it repeatedly against the examples and background theory. The syntactic modifications are done using the refinement operators.

Biases Practical ILP systems fight the inherent complexity of the problem by imposing constraints, mostly of syntactic in nature. Such constraints include *language* and *search biases*, and are sometimes summarized as **declarative biases**. Bias is typically defined as anything other than the training instances that influences the results of the learner.

The **language bias** imposes syntactic or semantic restrictions on the hypotheses to be induced. The syntactic ones define the well-formed elements in the language of hypotheses by employing some type of grammar. A great variety of formalisms to specify such grammars has been developed in the inductive logic programming literature, but there exist a few principles that underlie all syntactic biases employed. These include the use of predicate, type and mode declarations.

The predicate declarations specify the predicates to be used, the type declarations the corresponding types of the arguments of the predicates, the modes declarations the restrictions on the order of literals in clauses. The first two are written as $\mathtt{type}(\mathtt{pred}(\mathtt{type_1}, ..., \mathtt{type_n}))$, where `pred` denotes the name of the predicate and $\mathtt{type_i}$s denote the names of the types. Mode declarations are used to describe the input-output behaviour of predicate definitions through the form $\mathtt{mode}(\mathtt{pred}(\mathtt{m_1}, ..., \mathtt{m_n}))$, where the $\mathtt{m_i}$ are different modes. Three modes are distinguished: input (denoted by '+'), output (denoted by '-') and ground (denoted by '#'). The input mode specifies that at the time of calling the predicate the corresponding argument must be instantiated, the output mode specifies that the argument will be instantiated after a successful call to the predicate, and the constant mode specifies that the argument must be ground (and possibly belong to a specified type). A clause $h \leftarrow b_1, \ldots, b_n$ is mode-conform if and only if

1. any input variable in a literal b_i appears as an output variable in a literal b_j (with $j < i$) or as an input variable in the literal h,

2. any output variable in h appears as an output variable in some b_i,

3. any arguments of predicates required to be ground are ground.

The following example show mode-conform clauses.

Example 11 *Given the declarations:*

```
mode(molecule(-)). mode(atom(+,-,#,#)). mode(bond(+,+,-,#)).
type(molecule(m)). type(atom(m,a,at,r)). type(bond(m,a,a,bt)).
```

Then the clauses

```
molecule(M) :- atom(M,A,c,3).
molecule(M) :- atom(M,A,c,3), bond(M,A,B,double).
```

are mode-conform.

There are also syntactic biases in which the language of hypotheses is defined as a function of a set of parameters: for instance, one can restrict the number of literals, variables or simply the size of clauses.

Search bias has to do with the way a system searches its space of permitted clauses. One extreme is exhaustive search, which searches the space completely, but it would take far too much time, so the search has to be guided by certain *heuristics*. These indicate which parts of the space are searched, and which are ignored: this may cause the system to overlook some good theories, so here there is a trade-off between efficiency and the quality of the final theory. If a system has found that a correct theory is not available using its present language and search bias, it can try again using a more general language and/or a more thorough search procedure. This is called a *bias shift*.

Progol Aleph

Aleph[1] is an acronym for *A Learning Engine for Proposing Hypotheses* and is an Inductive Logic Programming (ILP) system. Earlier incarnations (under the name P-Progol) originated in 1993 at Oxford University. The main purpose was to understand ideas of inverse entailment which eventually appeared in Stephen Muggleton's 1995 paper: *Inverse Entailment and Progol* (Muggleton, 1995). Since then, the implementation has evolved to emulate some of the functionality of several other ILP systems. Some of these of relevance to Aleph are: CProgol, FOIL, FORS, Indlog, MIDOS, SRT, Tilde, and WARMR.

Aleph follows a very simple procedure that can be described in 4 steps:

[1]http://www.cs.ox.ac.uk/activities/machlearn/Aleph/aleph.html

1. *Select example.* Select an example to be generalized. If none exist, stop, otherwise proceed to the next step.

2. *Build most-specific-clause.* Construct the most specific clause that entails the example selected, and is within language restrictions provided. This is usually a definite clause with many literals, and is called the "bottom clause". This step is sometimes called the *saturation* step.

3. *Search.* Find a clause more general than the bottom clause. This is done by searching for some subset of the literals in the bottom clause that has the best score. Two points should be noted. First, confining the search to subsets of the bottom clause does not produce all the clauses more general than it, but is good enough for this thumbnail sketch. Second, the exact nature of the score of a clause is not really important here. This step is sometimes called the *reduction* step.

4. *Remove redundant.* The clause with the best score is added to the current theory, and all examples made redundant are removed. This step is sometimes called the *cover removal* step. Note here that the best clause may make clauses other than the examples redundant. Again, this is ignored here. Return to Step 1.

A more advanced use of Aleph allows alteration to each of these steps.

Background knowledge is in the form of Prolog clauses that encode information relevant to the domain. Also language and search restrictions have to be specified for Aleph. The most basic amongst these refer to modes, types and determinations.

Mode declarations These declare the mode of call for predicates that can appear in any clause hypothesized by Aleph. They take the form:

```
mode(RecallNumber,PredicateMode).
```

where `RecallNumber` bounds the non-determinacy of a form of predicate call, and `PredicateMode` specifies a legal form for calling a predicate.

`RecallNumber` can be either (a) a number specifying the number of successful calls to the predicate; or (b) *, specifying that the predicate has bounded non-determinacy. It is usually easier to specify `RecallNumber` as *. `PredicateMode` is a template of the form:

```
p(ModeType, ModeType,...)
```

Each `ModeType` is either (a) simple or (b) structured. A *simple* ModeType is one of: (a) $+T$ specifying that when a literal with predicate symbol p appears in a hypothesized clause, the corresponding argument should be an input variable of type T; (b) $-T$ specifying that the argument is an output variable of type T; or (c) $\#T$ specifying that it should be a constant of type T. A *structured* ModeType is of the form $f(..)$ where f is a function symbol, each argument of which is either a simple or structured `ModeType`.

With these directives Aleph ensures that for any hypothesized clause of the form $H : -B_1, B_2, ..., B_m$:

1. Input variables. Any input variable of type T in a body literal B_i appears as an output variable of type T in a body literal that appears before B_i, or appears as an input variable of type T in H.

2. Output variables. Any output variable of type T in H appears as an output variable of type T in B_i.

3. Constants. Any arguments denoted by $\#T$ in the modes have only ground terms of type T.

Type specifications Types have to be specified for every argument of all predicates to be used in constructing a hypothesis. This specification is done within a `mode`(..., ...) statement (see previous paragraph). For Aleph types are just names, and no type-checking is done. Variables of different types are treated distinctly, even if one is a sub-type of the other.

Determinations Determination statements declare the predicates that can be used to construct a hypothesis. They take the form:

```
determination(TargetName/Arity,BackgroundName/Arity).
```

The first argument is the name and arity of the target predicate, that is, the predicate that will appear in the head of hypothesized clauses. The second argument is the name and arity of a predicate that can appear in the body of such clauses. Typically there will be many determination declarations for a target predicate, corresponding to the predicates thought to be relevant in constructing hypotheses. If no determinations are present Aleph does not construct any clauses. Determinations are only allowed for 1 target predicate on any given run of Aleph: if multiple target determinations occur, the first one is chosen.

Positive and negative examples of a concept to be learned with Aleph are provided as input. Aleph is capable of learning from positive examples only. This is done using a Bayesian evaluation function.

Earlier incarnations of Aleph (called P-Progol) have been applied to a number of real-world problems. Prominent amongst these concern the construction of structure-activity relations for biological activity. In particular, the results for mutagenic and carcinogenic activity have received some attention. Also prominent has been the use for identifying pharmacophores – the three-dimensional arrangement of functional groups on small molecules that enables them to bind to drug targets. Applications to problems in natural language processing have been also done.

Chapter 6

Probability Theory

Causality connotes lawlike necessity, whereas probabilities connote exceptionality, doubt, and lack of regularity. There are two compelling reasons for probabilistic analysis of causality:

- The first reason rests on the observation that causal expressions are often used in situations that are plagued with uncertainty: for example, if we say "you will fail the course because of your laziness", we know quite well that the antecedents merely tend to make the consequences more likely, *not absolutely certain*. Any theory of causality that aims at accommodating such expressions must use a language that distinguishes various shades of likelihood - namely, the language of probabilities, which accounts for the relative strengths of those causal connections;

- Even the most assertive causal expressions in natural language are subject to exceptions, for instance "My neighbor's roof gets wet whenever mine does, except when it is covered with plastic, or when my roof is hosed, etc.". Probability theory is able to tolerate unexplicated exceptions.

This chapter discusses the basic concepts and terminology of probability theory. For a detailed view see (Pearl, 2000), (Neapolitan, 2003) and (Koller and Friedman, 2009).

6.1 Event Spaces

Before discussing the representation of probability, we need to define what the events are to which a probability is assigned. Probability theory has to do with experiments that have a set of distinct outcomes: the different outcomes of throwing a die, the outcome of a horse race, etc. The collection of all outcomes is called the *sample space*, denoted as Ω; for example, if we consider dice, $\Omega = \{1, 2, 3, 4, 5, 6\}$. In addition, there is a set of measurable events $\mathcal{S}$ to which assigning probabilities. Each event $\alpha \in \mathcal{S}$ is a subset of Ω; in the die example, the event $\{6\}$ represents the outcome 6. The event space satisfies three basic properties:

- It contains the empty event $\emptyset$ and the trivial event Ω;
- If $\alpha, \beta \in \mathcal{S}$, then so is $\alpha \cup \beta$ (union);
- If $\alpha \in \mathcal{S}$, then so is $\Omega - \alpha$ (complementation).

6.2 Probability Distributions

Definition 16 *A probability distribution P over* $(\Omega, \mathcal{S})$ *is a mapping from events in* $\mathcal{S}$ *to real values that satisfies the following conditions:*

- $P(\alpha) \geq 0$ *for all* α *in* $\mathcal{S}$
- $P(\Omega) = 1$
- *If* $\alpha, \beta \in \mathcal{S}$ *and* $\alpha \cap \beta = \emptyset$, *then* $P(\alpha \cup \beta) = P(\alpha) + P(\beta)$.

Probabilities are not negative. The maximal possible probability is 1. The probability that one of two mutually disjoint events will occur is the sum of their probabilities. These conditions imply that $P(\emptyset) = 0$ and $P(\alpha \cup \beta) = P(\alpha) + P(\beta) - P(\alpha \cap \beta)$.

6.3 Interpretations of Probability

There are two common interpretations for probabilities.

The *frequentist interpretation* views probabilities as frequencies of events: the probability of an event is the fraction of times the event occurs if we repeat the experiment indefinitely. If we consider the outcome of a particular die roll, the statement $P(\alpha) = 0.3$ for $\alpha = \{1, 3, 5\}$ states that if we repeatedly roll this die and record the outcome, the limit of the sequence of fractions of times the outcomes in α will occur is 0.3. This interpretation fails when we consider events such as "It will rain tomorrow", since we expect it to occur exactly once.

An alternative interpretation views probabilities as *subjective degrees of belief*: the statement $P(\alpha) = 0.3$ represents one's own degree of belief that the event α will come about, although the event occurs only once.

Both interpretations lead to the same mathematical rules, so the technical definitions hold for both.

6.4 Conditional Probability

Example 12 *Consider a distribution over a population of students taking a certain course. The space of outcomes is the set of all students. We define the event α to denote "all students with grade A" and event β to denote "all students with high intelligence". Using the distribution, one can consider the probability of these events and the probability of $\alpha \cap \beta$ (the set of intelligent students who got grade A).*

If new evidence α is given - a student has received grade A - we want to update our belief about her intelligence (β). The answer is given by conditional probability*:*

$$P(\beta \mid \alpha) = \frac{P(\alpha \cap \beta)}{P(\alpha)}$$

The probability that β is true given that we know α is the relative proportion of outcomes satisfying β among these that satisfy α.

From the definition of the conditional distribution, it results that

$$P(\alpha \cap \beta) = P(\alpha)P(\beta \mid \alpha)$$

known as the *chain rule* of conditional probabilities. More generally, if $\alpha_1, ..., \alpha_k$ are events, one can write

$$P(\alpha_1 \cap ... \cap \alpha_k) = P(\alpha_1)P(\alpha_2 \mid \alpha_1) \cdots P(\alpha_k \mid \alpha_1 \cap ... \cap \alpha_{k-1})$$

The probability of a combination of several events is expressed in terms of the probability of the first, the probability of the second given the first, etc. This expression may be expanded using any order of events.

Another immediate consequence of the definition of conditional probability is *Bayes' rule*

$$P(\alpha \mid \beta) = \frac{P(\beta \mid \alpha)P(\alpha)}{P(\beta)}$$

This operation takes one distribution and returns another over the same probability space.
A more general conditional version of this rule, where all our probabilities are conditioned on some background event γ, also holds:

$$P(\alpha \mid \beta \cap \gamma) = \frac{P(\beta \mid \alpha \cap \gamma)P(\alpha \mid \gamma)}{P(\beta \mid \gamma)}.$$

Example 13 *Consider the student population, and let $Smart$ denote smart students and $GradeA$ denote students who got grade A. We believe (perhaps based on estimates from past statistics) that $P(GradeA \mid Smart) = 0.6$, and now we learn that a particular student received grade A. Estimating the probability that the student is smart, according to Bayes' rule, depends on our* prior *probability for students being smart (before we learn anything about them) and the prior probability of students receiving high grades. For example, suppose that $P(Smart) = 0.3$ and $P(GradeA) = 0.2$, then we have that $P(Smart \mid GradeA) = 0.6 \star 0.3/0.2 = 0.9$. That is, an A grade strongly suggests that the student is smart. On the other hand, if the test was easier and high grades were more common, say $P(GradeA) = 0.4$, then we would get that $P(Smart \mid GradeA) = 0.6 \star 0.3/0.2 = 0.45$.*

6.5 Random Variables and Distributions

Random Variables

In many cases, it would be more natural to consider *attributes* of the outcome of an event. In the example of a distribution over a population of students in a course, one can use an event such as 'GradeA' to denote the subset of students who received the grade A; however it becomes rather cumbersome if we also want to consider students with grade B, grade C, and so on. The formal way for discussing attributes and their values in different outcomes are *random variables*, so called because their value is subject to variations due to chance. For example, if a random variable *Grade* reports the final grade of a student, than the statement $P(Grade = A)$ is another notation for $P(GradeA)$.

A random variable is a function that associates with each outcome in Ω a value. For example, $Grade$ is defined by a function f_{Grade} that maps each person in Ω to his/her grade (say, one of A, B, C). The event $Grade = A$ is a shorthand for the event $\{\omega \in \Omega : f_{Grade}(\omega) = A\}$. Random variables can be classified as either discrete (i.e. may assume any of a specified list of exact values) or as continuous (i.e. may assume any numerical value in an interval or collection of intervals). The mathematical function describing the possible values of a random variable and their associated probabilities is the *probability distribution*. *Val(X)* denotes the set of discrete values that a random variable *X* can take. Uppercase letters *X, Y, Z* are used to denote random variables; lowercase letters refer to a value of a random variable. Thus, we use *x* to refer to a generic value of *X*. The distribution over such a variable is called a *multinomial*. In the case of a binary-valued random variable *X*, where *Val(X)={false, true}*, the distribution is called a *Bernoulli distribution*. Sets of random variables are denoted by boldface type (***X*,**

Y, Z). $P(x)$ is a shorthand for $P(X = x)$; $\sum_x$ refers to a sum over all possible values that *X* can take. Finally, with conjunction, rather than write $P((X = x) \cap (Y = y))$ we write $P(X = x, Y = y)$ or just $P(x, y)$.

When we want to reason about continuous quantities such as weight, height, duration that take real numbers, in order to define probability over a *continuous random variable* we have to define probability density functions.

Definition 17 *A function $p : \mathbb{R} \mapsto \mathbb{R}$ is a probability density function or PDF for a random variable X if it is a non negative integrable function such that*

$$\int_{Val(X)} p(x)dx = 1$$

The integral over the set of possible values of X is 1.

The PDF defines a distribution for X as follows:

$$P(X \leq a) = \int\limits_{-\infty}^{a} p(x)dx.$$

Marginal and Joint Distributions

The distribution over events that can be described using a random variable *X* is referred to as the *marginal distribution over X*; it is denoted by $P(X)$.

Example 14 *Consider the random variable* Intelligence *for the student population example, taking the discrete values* {high,low}. *The marginal distribution over* Intelligence *assigns probability to specific events $P(Intelligence = high)$ and $P(Intelligence = low)$, as well as to the trivial event $P(Intelligence \in \{high, low\})$. The marginal distribution is a probability distribution satisfying the properties of definition 16.*

When we are interested in questions that involve values of several random variables, for example "*Intelligence* = *high* and *Grade* = *A*", we need to consider the joint distribution over these two random variables. The *joint distribution* over a set $\chi = \{X_1, ..., X_n\}$ is denoted by $P(X_1, ..., X_n)$ and assigns probabilities to events that are specified in terms of these random variables. ξ refers to a full assignment to the variables in χ. The marginal distribution $P(x)$ can be computed from the joint distribution of two random variables as:

$$P(x) = \sum_y P(x, y).$$

Given a joint distribution over the variables χ and a choice of values $x_1, ..., x_n$ for all the variables, the *outcome space* is a space where each outcome corresponds to a joint assignment to $X_1, ..., X_n$. For example, if $\chi = \{Intelligence, Grade\}$ and *Grade* takes values in *{A,B,C}* there are six atomic outcomes (all combinations of intelligence and grade).

The notion of conditional probability seen above for events extends to induced distributions over random variables. The following notations are often used:

- $P(X \mid Y)$: a set of conditional probability distributions. For each value of Y, this object assigns a probability to values of X;
- chain rule: $P(X, Y) = P(X)P(Y \mid X)$;
- chain rule for multiple variables: $P(X_1, ..., X_k) = P(X_1)P(X_2 \mid X1) \cdots P(X_k \mid X_1, ..., X_{k-1})$;
- Bayes' rule:
$$P(X \mid Y) = \frac{P(X)P(Y \mid X)}{P(Y)}$$

Note that the conditional distribution over a random variable given an observation of the values of another one is not the same as the marginal distribution. The latter represents our *prior* knowledge before learning anything else, while the conditional distribution represents our more informed distribution after learning something. There is a particular case in which the two probabilities coincide, as it is explained in the next subsection.

Independence

Definition 18 *An event α is* independent *of an event β in P, denoted $P \models (\alpha \perp \beta)$, if $P(\alpha \mid \beta) = P(\alpha)$ or if $P(\beta) = 0$.*

Definition 19 *Let $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ be sets of random variables. $\mathbf{X}$ is* conditionally independent *of $\mathbf{Y}$ given $\mathbf{Z}$ in a distribution P if $P(\mathbf{X} = \mathbf{x}, \mathbf{Y} = \mathbf{y} \mid \mathbf{Z} = \mathbf{z}) = P(\mathbf{X} \mid \mathbf{Z})P(\mathbf{Y} \mid \mathbf{Z})$ for all values of $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$. The variables in the set $\mathbf{Z}$ are said to be* observed. *If the set $\mathbf{Z}$ is empty, then $(\mathbf{X} \perp \mathbf{Y})$ and we say that* $\mathbf{X}$ and $\mathbf{Y}$ are marginally independent.

An independence statement over random variables is a universal quantification over all possible values of the random variables.

The distribution P satisfies $(\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z})$ iff $P(\mathbf{X}, \mathbf{Y} \mid \mathbf{Z}) = P(\mathbf{X} \mid \mathbf{Z})P(\mathbf{Y} \mid \mathbf{Z})$. The following properties must also hold in the distribution.

- *Simmetry*: $(\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}) \Rightarrow (\mathbf{Y} \perp \mathbf{X} \mid \mathbf{Z})$
- *Decomposition*: $(\mathbf{X} \perp \mathbf{Y}, \mathbf{W} \mid \mathbf{Z}) \Rightarrow (\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z})$
- *Weak union*: $(\mathbf{X} \perp \mathbf{Y}, \mathbf{W} \mid \mathbf{Z}) \Rightarrow (\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}, \mathbf{W})$
- *Contraction*: $(\mathbf{X} \perp \mathbf{W} \mid \mathbf{Z}, \mathbf{Y}) \& (\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}) \Rightarrow (\mathbf{X} \perp \mathbf{Y}, \mathbf{W} \mid \mathbf{Z})$

6.6 Querying a Distribution

Often a joint distribution over multiple random variables is used to answer queries of interest.

Probability Queries

A common query type is the probability query. It consists of two parts:

- The *evidence*: a subset $\mathbf{E}$ of random variables in the model, and an instantiation $\mathbf{e}$ to these variables;
- the *query variables*: a subset $\mathbf{Y}$ of random variables.

The task is to compute

$$P(\mathbf{Y} \mid \mathbf{E} = \mathbf{e})$$

that is, the *posterior probability distribution* over the values $\mathbf{y}$ of $\mathbf{Y}$, conditioned on the fact that $\mathbf{E} = \mathbf{e}$.

MAP Queries

A second type of task is that of finding a high-probability joint assignment to some subset of variables. This is called the *MAP* (Maximum A Posteriori) query (also *most probable explanation (MPE)*), whose aim is to find the most likely assignment to all of the non-evidence variables.

If $\mathbf{W} = \chi - \mathbf{E}$, the task is to find the most likely assignment to the variables in $\mathbf{W}$ given the evidence $\mathbf{E} = \mathbf{e}$:

$$MAP(\mathbf{W} \mid \mathbf{e}) = argmax_{\mathbf{w}} P(\mathbf{w}, \mathbf{e})$$

where in general $argmax_x f(x)$ represents the value of *x* for which *f(x)* is maximal.

In a MAP query one is finding the most likely *joint* assignment to $\mathbf{W}$. To find the most likely assignment to a single variable A, one could simply compute $P(A \mid \mathbf{e})$ and then pick the most likely value. However, the assignment where each variable individually picks its most likely value can be quite different from the most likely joint assignment to all variables simultaneously.

Example 15 *Consider two binary variables A and B and the assumed values as a^x and b^x, with $x = \{0, 1\}$. Assume that:*

a^0	a^1
0.4	0.6

A	b^0	b^1
a^0	0.1	0.9
a^1	0.5	0.5

$P(a^1) > P(a^0)$, *so that* $MAP(A) = a^1$. *However,* $MAP(A, B) = (a^0, b^1)$*: both values of B have the same probability given* a^1. *Thus, the most likely assignment containing* a^1 *has probability* $0.6 \cdot 0.5 = 0.3$. *On the other hand, the distribution over values of B is more skewed given* a^0*, and the most likely assignment* (a^0, b^1) *has probability* $0.4 \cdot 0.9 = 0.36$. *Thus,* $argmax_{a,b}P(a, b) \neq (argmax_a P(a), argmax_b P(b))$.

Marginal MAP Queries

Consider a medical diagnosis problem, where the most likely disease has multiple possible symptoms, each of which with some not overwhelming probability. On the other hand, a somewhat rare disease might have only a few symptoms, each of which is very likely given the disease. The MAP assignment to the data and the symptoms might be higher for the second disease than for the first one. The solution here is to look for the most likely assignment to the disease variable(s) only, rather than to both the disease and symptom variables.

In the *marginal MAP query* there is a subset of variables $\mathbf{Y}$ that forms the query. The task is to find the most likely assignment to the variables in $\mathbf{Y}$ given the evidence $\mathbf{E} = \mathbf{e}$:

$$MAP(\mathbf{Y} \mid \mathbf{e}) = argmax_{\mathbf{y}} P(\mathbf{y} \mid \mathbf{e}).$$

If $\mathbf{Z} = \chi - \mathbf{Y} - \mathbf{E}$ the marginal MAP task is to compute:

$$MAP(\mathbf{Y} \mid \mathbf{e}) = argmax_{\mathbf{Y}} \sum_{\mathbf{Z}} P(\mathbf{Y}, \mathbf{Z} \mid \mathbf{e}).$$

It contains elements of both a conditional probability query and a MAP query.

6.7 Expectation of a Random Variable

Let X be a discrete random variable that takes numerical values; **the expectation of X** under the distribution P is

$$E_P[X] = \sum_x x \cdot P(x)$$

For example, if X is the outcome of rolling a fair die with probability 1/6 for each outcome, then $E[X] = 1 \cdot 1/6 + 2 \cdot 1/6 + \cdots + 6 \cdot 1/6 = 3.5$. On the other hand, if we consider a biased die where $P(X = 6) = 0.5$ and $P(X = x) = 0.1$ for $x < 6$, then $E[X] = 1 \cdot 0.1 + \cdots + 5 \cdot 0.1 + 6 \cdot 0.5 = 4.5$.

Often we are interested in expectations of a function of a random variable, such as a function that map values of one or more random variables to numerical values: one such function used quite often is the indicator function, denoted by $\mathbf{I}\{\mathbf{X} = \mathbf{x}\}$, which takes value 1 when $X = x$ and 0 otherwise.

Some properties of expectations of a random variable hold:

- $E[a \cdot X + b] = aE[X] + b$;
- $E[X + Y] = E[X] + E[Y]$: the expectation of a sum of two random variables is the sum of expectations (linearity); this is true even when the variables are not independent, and is key in simplifying many complex problems;
- $E[X \cdot Y] = E[X] \cdot E[Y]$, if X and Y are independent.

The *conditional expectation* of X given some evidence $\mathbf{y}$ is

$$E_P[X \mid \mathbf{y}] = \sum_x x \cdot P(x \mid \mathbf{y}).$$

Chapter 7

Decision Diagrams

Decision diagrams are graphical structures that have been extensively used for representing and manipulating logic functions in varied areas. This chapter describes first Multivalued and then Binary Decision Diagrams, that are used by the inference and learning algorithms on LPADs.

7.1 Multivalued Decision Diagrams

A Multivalued Decision Diagram (MDD) (Thayse et al., 1978) is able to represent a function $f(\mathbf{X})$ taking Boolean values on a set of multivalued variables $\mathbf{X}$ by means of a rooted, directed acyclic graph that has one level for each variable. Each node is associated with the variable of its level and has one child for each possible value of the variable. The leaves store either 0 (false) or 1 (true). Given values for all the variables $\mathbf{X}$, one can compute the value of $f(\mathbf{X})$ by traversing the graph starting from the root and returning the value associated with the leaf that is reached. MDDs can be built by combining simpler MDDs using Boolean operators. While building MDDs, simplification operations can be applied that delete or merge nodes. Merging is performed when the diagram contains two identical sub-diagrams, while deletion is performed when all arcs from a node point to the same node. In this way a reduced MDD is obtained, often with a much smaller number of nodes with respect to the original MDD.

Most packages for the manipulation of decision diagrams are however restricted to work on Binary Decision Diagrams (BDD).

7.2 Binary Decision Diagrams

A Binary Decision Diagram is a rooted, directed acyclic graph with

- two terminal nodes of out-degree zero labeled 0 or 1, and
- a set of variables nodes of out-degree two. Given a variable node *n*, the two outgoing edges are given by two functions $low(n)$ and $high(n)$ (in pictures, these are shown as dotted and solid lines, respectively). A variable *var(n)* is associated with each variable node.

A BDD is *Ordered* (OBDD) if on all paths through the graph the variables respect a given linear order $X_1 < X_2 < \cdots < X_n$. An (O)BDD is *Reduced* (R(O)BDD) if

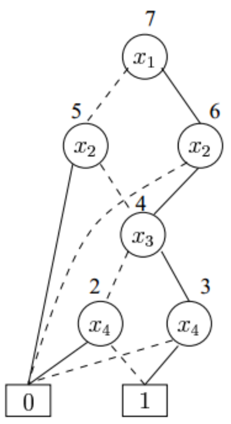
- (uniqueness) no two distinct nodes u and v have the same variable name and low- and high child, and
- (non-redundancy tests) no variable node u has identical low- and high- child

ROBDDs have some interesting properties. They provide compact representations of Boolean functions, and there are efficient algorithms for performing all kinds of logical operations on them. They are all based on the crucial fact that for any function $f : \mathbb{B}^n \rightarrow \mathbb{B}$ there is exactly one ROBDD representing it.

The ordering of variables chosen when constructing an (RO)BDD has a great impact on the size of the (RO)BDD. State-of-the-art BDD implementations therefore employ heuristics to automatically reorder the variables during BDD construction, which help to control the combinatorial explosion and make it representable in memory.

Since BDDs represent a Boolean formula as a decision graph, one can compute the value of the function given an assignment to the Boolean variables by navigating the graph from the root to a leaf. The next node is chosen on the basis of the value of the variable associated to that level: if the value is 1 the high child is chosen, if the value is 0 the low child is. When a leaf is reached the value stored there is returned.

An example of ROBDD is shown in Figure 7.1, representing the Boolean function $(X_1 \Leftrightarrow X_2) \wedge (X_3 \Leftrightarrow X_4)$. The logical equivalence is true if the operands are both true or if they are both false. Nodes are represented as numbers 0,1,2,...with 0 and 1 reserved for the terminal nodes. The variables in the ordering $X_1 < X_2 < \cdots < X_n$ are represented by their indexes. The ROBDD is stored in a table $T : n \mapsto (i, l, h)$ which maps a node n to its three attributes var(n) = i, low(n) = l, high(n) = h.



$T : u \mapsto (i, l, h)$

u	*var*	*low*	*high*
0	5		
1	5		
2	4	1	0
3	4	0	1
4	3	2	3
5	2	4	0
6	2	0	4
7	1	5	6

Figure 7.1: Representing an ROBDD with ordering $x_1 < x_2 < x_3 < x_4$. The numbers in the *var* column show the index of the variables in the ordering. The constants are assigned an index which is the number of variables in the ordering plus one (4+1=5).

Chapter 8

Expectation Maximization Algorithm

The Expectation-Maximization (EM) algorithm is a broadly applicable approach to the iterative computation of maximum likelihood (ML) estimates, useful in a variety of incomplete data problems. On each iteration of the EM algorithm, there are two steps - called the Expectation step or the E-step and the Maximization step or the M-step. Because of this, the algorithm is called the EM algorithm. This name was given by Dempster, Laird, and Rubin (1977) in their fundamental paper. The situations where the EM algorithm is profitably applied can be described as incomplete-data problems, where ML estimation is made difficult by the absence of some part of data. The basic idea of the EM algorithm is to associate the given incomplete-data problem with a complete-data problem for which ML estimation is computationally more tractable; for instance, the complete-data problem chosen may yield a closed form solution to the maximum likelihood estimate (MLE) or may be amenable to ML computation with a standard computer package. Even when a problem does not at first appear to be an incomplete-data one, computation of the MLE is often greatly facilitated by artificially formulating it to be as such. In ML estimation, *we wish to estimate the model parameter(s) for which the observed data are the most likely*.

The E-step consists in manufacturing data for the complete-data problem, using the observed data set of the incomplete-data problem and the current value of the model parameters, so that the simpler M-step computation can be applied to this “completed data set”. More precisely, it is the log likelihood of the complete-data problem that is “manufactured” in the E-step. As it is based partly on unobservable data, it is replaced by its conditional *expectation* given the observed data, where this E-step is effected using the current fit for the unknown parameters. In the M-step, the likelihood function is maximized under the assumption that the missing data are known. Starting from suitable initial parameter values, the E- and M-steps are repeated until convergence.

In the next two Sections we formally define the algorithm and its main properties. See (McLachlan and Krishnan, 1996) and (Dempster et al., 1977) for a detailed introduction.

8.1 Formulation of the algorithm

Let $\mathbf{Y}$ be a *p*-dimensional random vector with probability density function (p.d.f.) $g(\mathbf{y};\boldsymbol{\Psi})$ on $\mathbb{R}^p$, corresponding to the observed data $\mathbf{y}$, where $\boldsymbol{\Psi} = (\Psi_1, ..., \Psi_d)^T$ is the vector containing the unknown parameters with parameter space $\boldsymbol{\Omega}$.

For example, if $\mathbf{w_1}, ..., \mathbf{w_n}$ denotes an observed random sample of size *n* on some random vector $\mathbf{W}$ with p.d.f $f(\mathbf{w};\boldsymbol{\Psi})$, then

$$\mathbf{y} = (\mathbf{w_1^T}, ..., \mathbf{w_n^T})^\mathbf{T}$$

and

$$g(\mathbf{y};\boldsymbol{\Psi}) = \prod_{j=1}^{n} f(\mathbf{w}_j;\boldsymbol{\Psi})$$

The vector $\boldsymbol{\Psi}$ is to be estimated by maximum likelihood. The likelihood function for $\boldsymbol{\Psi}$ formed from the observed data $\mathbf{y}$ is given by

$$L(\boldsymbol{\Psi}) = g(\mathbf{y};\boldsymbol{\Psi}).$$

An estimate $\hat{\boldsymbol{\Psi}}$ of $\boldsymbol{\Psi}$ can be obtained as a solution of the likelihood equation

$$\partial L(\boldsymbol{\Psi})/\partial\boldsymbol{\Psi} = \mathbf{0},$$

or equivalently,

$$\partial log L(\boldsymbol{\Psi})/\partial\boldsymbol{\Psi} = \mathbf{0}.$$

The aim of ML estimation is to determine an estimate $\hat{\boldsymbol{\Psi}}$, so that it defines a sequence of roots of the likelihood equation corresponding to local maxima in the interior of the parameter space.

The observed data vector $\mathbf{y}$ is viewed as being incomplete and is regarded as an observable function of the so-called complete data. The notion of 'incomplete data' includes the conventional sense of missing data, but it also applies to situations where the complete data represent what would be available from some hypothetical experiment. In the latter case, the complete data may contain some variables that are never observable in a data sense. Within this framework, we let $\mathbf{x}$ denote the vector containing the *augmented* or so-called complete data, and we let $\mathbf{z}$ denote the vector containing the additional data, referred to as the unobservable or *missing* data. $g_c(\mathbf{x}; \boldsymbol{\Psi})$ will denote the p.d.f. of the random vector $\mathbf{X}$ corresponding to the complete-data vector $\mathbf{x}$. Then the complete-data log likelihood function that could be formed for $\boldsymbol{\Psi}$ if $\mathbf{x}$ were fully observable is given by

$$log\ L_c(\boldsymbol{\Psi}) = log\ g_c(\mathbf{x}; \boldsymbol{\Psi}).$$

Formally, we have two samples spaces $\mathcal{X}$ and $\mathcal{Y}$ and a many-to-one mapping from $\mathcal{X}$ to $\mathcal{Y}$. Instead of observing the complete-data vector $\mathbf{x}$ in $\mathcal{X}$, we observe the incomplete-data vector $\mathbf{y} = \mathbf{y}(\mathbf{x})$ in $\mathcal{Y}$.

The EM algorithm approaches the problem of solving the incomplete-data likelihood equation indirectly by proceeding iteratively in terms of the complete-data log likelihood function, log $L_c(\boldsymbol{\Psi})$. As it is unobservable, it is replaced by its conditional expectation given $\mathbf{y}$, using the current fit for $\boldsymbol{\Psi}$.

More specifically, let $\boldsymbol{\Psi}^{(0)}$ be some initial value for $\boldsymbol{\Psi}$. Then on the first iteration, the E-step requires the calculation of

$$Q(\boldsymbol{\Psi}; \boldsymbol{\Psi}^{(0)}) = E_{\boldsymbol{\Psi}^{(0)}}[log\ L_c(\boldsymbol{\Psi}) \mid \mathbf{y}].$$

The M-step requires the maximization of $Q(\boldsymbol{\Psi}; \boldsymbol{\Psi}^{(0)})$ with respect to $\boldsymbol{\Psi}$ over the parameter space $\boldsymbol{\Omega}$. That is, we choose $\boldsymbol{\Psi}^{(1)}$ such that

$$Q(\boldsymbol{\Psi}^{(1)}; \boldsymbol{\Psi}^{(0)}) \geq Q(\boldsymbol{\Psi}; \boldsymbol{\Psi}^{(0)})$$

for all $\boldsymbol{\Psi} \in \boldsymbol{\Omega}$. The E- and M-steps are then carried out again, but this time with $\boldsymbol{\Psi}^{(0)}$ replaced by the current fit $\boldsymbol{\Psi}^{(1)}$. On the (*k*+1)th iteration, the E- and M-steps are defined as follows:

E-step. Calculate $Q(\boldsymbol{\Psi}; \boldsymbol{\Psi}^{(k)})$, where

$$Q(\boldsymbol{\Psi}; \boldsymbol{\Psi}^{(k)}) = E_{\boldsymbol{\Psi}^{(k)}}[log\ L_c(\boldsymbol{\Psi}) \mid \mathbf{y}].$$

M-step. Choose $\boldsymbol{\Psi}^{(k+1)}$ to be any value of $\boldsymbol{\Psi} \in \boldsymbol{\Omega}$ that maximizes $Q(\boldsymbol{\Psi}; \boldsymbol{\Psi}^{(k)})$; that is,

$$Q(\boldsymbol{\Psi}^{(k+1)}; \boldsymbol{\Psi}^{(k)}) \geq Q(\boldsymbol{\Psi}; \boldsymbol{\Psi}^{(k)})$$

for all $\boldsymbol{\Psi} \in \boldsymbol{\Omega}$.

The E- and M-steps are alternated repeatedly until the difference

$$L(\boldsymbol{\Psi}^{(k+1)}) - L(\boldsymbol{\Psi}^{(k)})$$

changes by an arbitrarily small amount.

Another way of expressing M-step is to say that $\boldsymbol{\Psi}^{(k+1)}$ belongs to

$$\mathcal{M}(\boldsymbol{\Psi}^{(k)}) = arg\ max_{\boldsymbol{\Psi}} Q(\boldsymbol{\Psi}; \boldsymbol{\Psi}^{(k)}),$$

which is the set of points that maximize $Q(\boldsymbol{\Psi}; \boldsymbol{\Psi}^{(k)})$.

In the case of a *discrete* random vector, we wish to find $\boldsymbol{\Psi}$ such that P($\mathbf{Y} \mid \boldsymbol{\Psi}$) is a maximum, and the log likelihood function is defined as

$$L(\boldsymbol{\Psi}) = log\ P(\mathbf{Y} \mid \boldsymbol{\Psi}).$$

P($\mathbf{Y} \mid \boldsymbol{\Psi}$) may be written in terms of the hidden variables $\mathbf{z}$ as

$$P(\mathbf{Y} \mid \boldsymbol{\Psi}) = \sum_{\mathbf{z}} P(\mathbf{Y} \mid \mathbf{z}, \boldsymbol{\Psi}) P(\mathbf{z} \mid \boldsymbol{\Psi}).$$

Since we want to maximize the difference

$$L(\boldsymbol{\Psi}) - L(\boldsymbol{\Psi}^{(k)}) = \ P(\mathbf{Y} \mid \boldsymbol{\Psi}) - P(\mathbf{Y} \mid \boldsymbol{\Psi}^{(k)}),$$

we may substitute $P(\mathbf{Y} \mid \boldsymbol{\Psi})$ with the above equivalence. It can be shown that the following expression for the E-step is reached:

$$Q(\boldsymbol{\Psi}; \boldsymbol{\Psi}^{(k)}) = \sum_{\mathbf{z}} P(\mathbf{z} \mid \mathbf{Y}, \boldsymbol{\Psi}^{(k)}) log\ P(\mathbf{Y}, \mathbf{z} \mid \boldsymbol{\Psi}) = E_{\mathbf{Z}|\mathbf{Y},\boldsymbol{\Psi}^{(\mathbf{k})}}[log\ P(\mathbf{Y}, \mathbf{z} \mid \boldsymbol{\Psi})].$$

All that is necessary is the specification of the complete-data vector $\mathbf{x}$ and the conditional probability density of $\mathbf{X}$ given the observed data vector $\mathbf{y}$. Specification of this conditional probability density is needed in order to carry out the E-step. As the choice of the complete-data vector $\mathbf{x}$ is not unique, it is chosen for computational convenience with respect to carrying out the E- and M-steps.

8.2 Properties of the algorithm

- The EM algorithm is numerically stable, with each EM iteration increasing the likelihood (except at a fixed point of the algorithm); since log(x) is a strictly increasing function, the value of $\mathbf{\Psi}$ which maximizes $\mathbf{g}$ or P also maximizes L.
- The EM algorithm is typically easily implemented, because it relies on complete-data computations: the E-step of each iteration only involves taking expectations over complete data conditional distributions and the M-step of each iteration only requires complete data ML estimation, which is often in simple closed form.
- The EM algorithm is generally easy to program, since no evaluation of the likelihood nor its derivatives is involved.
- The cost per iteration is generally low, which can offset the larger number of iterations needed for the EM algorithm compared to other competing procedures.
- By watching the monotone increase in likelihood (if evaluated easily) over iterations, it is easy to monitor convergence.
- The EM algorithm can be used to provide estimated values of the missing data.
- The EM algorithm does not guarantee convergence to the global maximum when there are multiple maxima. Further, in this case, the estimate obtained depends upon the initial value $\mathbf{\Psi}^{(0)}$.

Part III

Statistical Relational Learning

Chapter 9

Distribution Semantics and Logic Programs with Annotated Disjunctions

This chapter reviews LPADs, the probabilistic logic programming language used in this thesis. We begin by outlining the basic concepts of its semantics in Section 9.1, and then describing syntax, semantics and inference in this language in Section 9.2.

9.1 Distribution Semantics

The concept of Distribution Semantics has been introduced by (Sato, 1995), with the objective to provide basic components for a unified symbolic-statistical information processing system in the framework of logic programming. It provides a semantic basis for probabilistic computation: the possibility of learning the parameters of a distribution.

A definite clause program $DB = F \cup R$ in a first order language is composed of a set of facts F and a set of rules R. It is assumed that DB is ground (if not, it is reduced to the set of all possible ground instantiations of clauses), infinite and no atom in F unifies with the head of a rule in R (disjoint condition). A ground atom A is treated as a random variable taking value 1 (when A is true) or 0 (when A is false).

A *basic distribution for F* P_F is a probability measure on the algebra of the sample space Ω_F of all possible interpretations ω (assignments of truth values) for F. The corresponding distribution function if $P_F^{(n)}(A_1 = x_1, ..., A_n = x_n)$, where x_i is the truth value of A_i. ω, by assigning x_i to atoms A_i, identifies a Herbrand model. Each interpretation $\omega \in \Omega_F$ determines a set $F_\omega \subset F$ of true ground atoms. So the logic program is $F_\omega \cup R$ and its least model $M_{DB}(\omega)$.

Example 16 *We show $M_{DB}(\omega)$ for a finite program DB_1.*

$$DB_1 = F_1 \cup R_1$$

$$F_1 = \{A_1, A_2\}$$

$$R_1 = \{B_1 \leftarrow A_1, B_1 \leftarrow A_2, B_2 \leftarrow A_2\}$$

$\Omega_{F_1} = \{0,1\}_1 \times \{0,1\}_2$ and $\omega = (x_1, x_2) \in \Omega_{F_1}$ means A_i takes $x_i (i = 1, 2)$ as its truth value. The M_{DB} is:

ω	F_{1_ω}	$M_{DB_1}(\omega)$
(0,0)	$\{\}$	$\{\}$
(1,0)	$\{A_1\}$	$\{A_1, B_1\}$
(0,1)	$\{A_2\}$	$\{A_2, B_1, B_2\}$
(1,1)	$\{A_1, A_2\}$	$\{A_1, A_2, B_1, B_2\}$

To move from P_F to P_{DB}, the distribution over the logic program, we do not have to consider the atoms $A_i \in F$ anymore, but all the atoms $A_i \in DB$. P_F can be extended to a probability measure P_{DB} over Ω_{DB}, the set of all possible interpretations for ground atoms appearing in DB. If $\omega_{F'}$ is a sample from P_F and F' the set of atoms made true by $\omega_{F'}$, it is possible to construct the least Herbrand model $M_{DB}(\omega)_{F'}$ of the definite program $F' \cup R$. It determines the truth value of every ground atom and by construction every ground atom is a measurable function of $\omega_{F'}$ with respect to P_F. It follows that P_F can be extended to P_{DB} on the set of possible Herbrand models for DB. If P_F puts the probability mass on a single interpretation, P_{DB} puts the probability mass on the least model $M_{DB}(\omega)_{F'}$ also. Intuitively, P_{DB} is identified with an infinite joint distribution $P_{DB} = (A_1 = x_1, A_2 = x_2, ...)$ on the probabilistic ground atoms $A_1, A_2, ...$ in the Herbrand base of DB where $x_i \in \{0, 1\}$ (Sato, 2009). This way, a program denotes a distribution in this semantics.

If G is an arbitrary formula whose predicates are among DB, $[G] = \{\omega \in \Omega_{DB} \mid \omega \models G\}$. Then the probability of G is defined as $P_{DB}([G])$. Intuitively, $P_{DB}([G])$ represents the probability mass assigned to the set of interpretations (possible worlds) satisfying G.

Example 17 *Considering example 16 again,* $\omega = (x_1, x_2, y_1, y_2) \in \Omega_{DB_1}$ *indicates that* x_i $(i = 1, 2)$ *is the value of* A_i *and* y_j $(j = 1, 2)$ *is the value of* B_j*, respectively.*

$P_{DB_1}(x_1, x_2, y_1, y_2)$ *can be computed from* $P_{F_1}(x_1, x_2)$*.*

9.2 LPADs

This section presents Logic Programs with Annotated Disjunctions (LPADs), the probabilistic logic programming language used in this thesis, which was introduced by J. Vennekens and S. Verbaeten in (Vennekens and Verbaeten, 2003; Vennekens et al., 2004).

Causality

The formalism of LPADs is based on disjunctive logic programming where probabilistic elements are added; for this reason it is referred as a "probabilistic logic programming language". These languages are the natural way of representing causal knowledge about *probabilistic* processes. The choice of disjunctive logic programs itself, i.e. of sets of rules $h_1 \vee \cdots \vee h_n \leftarrow \phi$, allows to represent a kind of uncertainty. They are highly inspired by the concept of *experiment*:

- a simple experiment (a "part" of the program) is represented by a single logical disjunction in which the disjuncts correspond to all its possible outcomes; by adding preconditions ϕ to the disjunctions through logical implication, the relationship between causes and indeterminate results of the experiment is established;
- these simple experiments are combined into a more complex one: the meaning of an entire program.

The fundamental idea is that a reason is represented for some event E by a formula ϕ, by writing "ϕ causes E" as: $r = E \leftarrow \phi$ (Vennekens et al., 2006). This is called a *Causal Probabilistic event (CP-event)*. The head E of r is a disjunction of effects h_i, so that its intuitive reading is "ϕ causes a non-deterministic event, that causes *precisely one of* $h_1, ..., h_n$. Many events might be involved in determining the truth of the same proposition, that is, the same effect might have a number of *independent* causes: this will be represented by a number of rules r with the same head E and different causes ϕ. If each atom h_i appearing in the event E is assigned a probability α_i, such that $\sum_n \alpha_i \leq 1$, we get a probabilistic logic disjunction $(h_1 : \alpha_1) \vee \cdots \vee (h_n : \alpha_n)$ read as: "At most one of the h_i will become true as a result of this event with probability α_i". An atom h_i does not represent an outcome of one particular event, but rather the effect of this outcome on the domain, i.e., if different events can have the same effect on the domain, they might share the same atom.

If an event has a deterministic effect, i.e., it always causes some atom h with probability 1, we write h instead of $(h : 1)$. A normal logic program P is a set of rules $h \leftarrow \phi$, with h an atom and ϕ a conjunction. This kind of program can be viewed as a description of causal information about a *deterministic* process: we can read the rule as "ϕ causes a deterministic event, that causes h." Its semantics assigns a probability of 1 to a single interpretation and 0 to all other interpretations.

Syntax

A *Logic Program with Annotated Disjunctions* consists of a finite set of annotated disjunctive clauses. An annotated disjunctive clause C_i is of the form

$$h_{i1} : \Pi_{i1}; \ldots ; h_{in_i} : \Pi_{in_i} : -b_{i1}, \ldots , b_{im_i}.$$

$h_{i1}, \ldots h_{in_i}$ are logical atoms and $b_{i1}, \ldots , b_{im_i}$ are logical literals, $\Pi_{i1}, \ldots , \Pi_{in_i}$ are real numbers in the interval $[0, 1]$ such that $\sum_{k=1}^{n_i} \Pi_{ik} \leq 1$. $h_{i1} : \Pi_{i1}, \ldots , h_{in_i} : \Pi_{in_i}$ is called the *head* and is indicated with $head(C_i)$; $b_{i1}, \ldots , b_{im_i}$ is called the *body* and is indicated with $body(C_i)$. Note that if $n_i = 1$ and $\Pi_{i1} = 1$ the clause corresponds to a non-disjunctive clause. If $\sum_{k=1}^{n_i} \Pi_{ik} < 1$ the head of the annotated disjunctive clause implicitly contains an extra atom $null$ that does not appear in the body of any clause and whose annotation is $1 - \sum_{k=1}^{n_i} \Pi_{ik}$.

Example 18 *The following LPAD encodes the result of tossing a coin, on the base of the fact that it is biased or not:*

$$C_1 = heads(C) : 0.5; tails(C) : 0.5 : -toss(C), \neg biased(C).$$
$$C_2 = heads(C) : 0.6; tails(C) : 0.4 : -toss(C), biased(C).$$
$$C_3 = fair(coin) : 0.9; biased(coin) : 0.1.$$
$$C_4 = toss(coin) : 1.$$

This program models the fact that a fair coin lands on heads or on tails with probability 0.5, while a biased coin with probabilities 0.6 and 0.4 respectively. The third clause says that a certain coin $coin$ *has a probability of 0.9 of being fair and of 0.1 of being biased, the fourth one that* $coin$ *in certainly tossed.*

C_1, for instance, expresses the fact that for each coin c, precisely one of the following clauses will hold: $heads(c) : -toss(c), \neg biased(c)$ or $tails(c) : -toss(c), \neg biased(c)$, both with a probability of 0.5.

Semantics

An LPAD rule containing variables represents a number of simple experiments, one for each ground instantiation of this rule. The semantics of a LPAD program P will be defined using its grounding and restricting to its Herbrand base $H_B(P)$ and to the set of all its Herbrand interpretations $\mathcal{I}_P$. We denote the set of all ground LPADs as $\mathcal{P}_\mathcal{G}$ and by $ground(P)$ the grounding of one LPAD P. The semantics is defined by a *probability distribution* π on $\mathcal{I}_P$: π is a mapping from $\mathcal{I}_P$ to real numbers in [0,1] such that $\sum_{I \in \mathcal{I}_P} \pi(I) = 1$.

Each *ground instantiation of a clause* represents a probabilistic choice between a number of non-disjunctive clauses, equal to the number of the atoms in its head. This choice is made according to a *selection function*; some preliminary concepts have to be introduced now. An *atomic choice* is a triple (C_i, θ_j, k) where $C_i \in P$, θ_j is a substitution that grounds C_i and $k \in \{1, \ldots, n_i\}$. (C_i, θ_j, k) means that, for ground clause $C_i\theta_j$, the head h_{ik} was chosen. A set of atomic choices κ is *consistent* if $(C, \theta, i) \in \kappa, (C, \theta, j) \in \kappa \Rightarrow i = j$, i.e., only one head is selected for a ground clause. A *composite choice* κ is a consistent set of atomic choices. The *probability* $P(\kappa)$ *of a composite choice* κ is the product of the probabilities of the individual atomic choices, i.e. $P(\kappa) = \prod_{(C_i, \theta_j, k) \in \kappa} \Pi_{ik}$.

A *selection* σ is *a composite choice* that, for each clause $C_i\theta_j$ in $ground(P)$, contains an atomic choice (C_i, θ_j, k). We denote the set of all selections σ of a program P by $\mathcal{S}_P$ and we let $g(i)$ be the set of indexes of substitutions grounding C_i, i.e., $g(i) = \{j | \theta_j$ is a substitution grounding $C_i\}$. Each selection σ defines an *instance* of the LPAD, that is a normal logic program w_σ defined as $w_\sigma = \{(h_{ik} \leftarrow body(C_i))\theta_j | (C_i, \theta_j, k) \in \sigma\}$. w_σ is also called a *world* of P. This semantics means that a probabilistic rule in an LPAD expresses the fact that **exactly one atom in the head holds with a certain probability as a consequence of the body of the rule being true**.

Each selection σ in $\mathcal{S}_P$ is assigned a probability, which induces a probability on the corresponding program w_σ. We assume independence between the selections made for each rule. The probability $P(\sigma)$ of a selection σ is the probability of a composite choice κ, thus is given by the product of the probabilities of its individual atomic choices:

$$P(\sigma) = \prod_{(C_i,\theta_j,k)\in\sigma} \Pi_{ik}.$$

Moreover $P(\sigma)$ is equal to the probability of the world $P(w_\sigma)$, since selections define worlds.

Example 19 *If we consider the grounding of the LPAD in Example 18 with the variable C assuming value* coin*, 8 different* instances *(2 · 2 · 2) can be generated by choosing one of the possibilities for each clause, for example one is:*

$C_1 = heads(coin) : -toss(coin), \neg biased(coin).$
$C_2 = heads(coin) : -toss(coin), biased(coin).$
$C_3 = fair(coin).$
$C_4 = toss(coin).$

Each rule is independent of the other, since dependence is modeled within a rule, and a probability can be assigned to each instance: $0.5 \cdot 0.6 \cdot 0.9 \cdot 1 = 0.27.$

The meaning of the above instance of the coin program is given by the interpretation $\{toss(coin), fair(coin), heads(coin)\}$. The instances of an LPAD therefore define a probability distribution on the set of interpretations of the program: the probability of a certain interpretation I is the sum of the probability of all instances for which I is a model.

Example 20 *Returning to the example, there is one other instance of this LPAD which has* $\{toss(coin), fair(coin), heads(coin)\}$ *as its model, namely*

$C_1 = heads(coin) : -toss(coin), \neg biased(coin).$
$C_2 = tails(coin) : -toss(coin), biased(coin).$
$C_3 = fair(coin).$
$C_4 = toss(coin).$

The probability of this instance is 0.5 · 0.4 · 0.9 · 1 = 0.18. Therefore the probability of the interpretation is 0.27+0.18=0.45.

We consider only *sound* LPADs, where the meaning of an instance w_σ is given by its well founded model $WFM(w_\sigma)$ and require that all these models are two-valued.

Given a sound LPAD P, for each of its interpretations I in $\mathcal{I}_P$, the probability $\pi^*_P(I)$ assigned by P to I is the sum of the probabilities of all selections which lead to I, with $S(I)$

being the set of all selections σ for which $WFM(w_\sigma) = I$:

$$\pi_P^*(I) = \sum_{\sigma \in S(I)} P(\sigma).$$

There is a strong connection between the interpretations for which $\pi_P^*(I) > 0$ and the well established non-probabilistic semantics of logic programming, since each interpretation I for a program P is a traditional logic model for P (when ignoring the probabilities); moreover each logic program is also an LPAD and its semantics will assign probability 1 to its well founded model (and zero to all other interpretations).

Inference

Besides probabilities of interpretations, the basic inference task of probabilistic logic programs under the semantics π_P^* is calculating probabilities of queries, i.e., of existentially quantified conjunctions, according to a LPAD and possibly some evidence.

The set of all instances of a LPAD P is denoted as $\mathcal{W}_P$. A composite choice κ identifies a set of instances $\omega_\kappa = \{w_\sigma | \sigma \in \mathcal{S}_P, \sigma \supseteq \kappa\}$. A set of composite choices K identifies a set of instances $\omega_K = \bigcup_{\kappa \in K} \omega_\kappa$. A composite choice κ is an *explanation* for a query Q if Q is entailed by every instance (world) of ω_κ. A set of composite choices K is *covering* with respect to Q if every world w_σ in which Q is true is in ω_K.

The probability of a query Q given an instance w is the conditional probability $P(Q \mid w) = 1$ if $w \models Q$ and 0 otherwise.

The probability of a query Q is thus given by:

$$P(Q) = \sum_{w \in W_P} P(Q, w) = \sum_{w \in W_P} P(Q|w)P(w) = \sum_{w \in W_P : w \models Q} P(w). \tag{9.1}$$

The probability distribution over normal logic programs (instances) $P(w)$ is extended to queries and the probability of a query is obtained by marginalizing the joint distribution of the query and the programs $P(Q, w)$. The trivial way of computing $P(Q)$ proceeds by enumerating all possible ground instances of a LPAD P, that is often unfeasible for large programs. Instead, the number of proofs for a query is much more limited, as shown in Example 21.

Example 21 *Consider the following LPAD P inspired by the morphological characteristics of the Stromboli Italian island, on which we want to compute the probability of the query* eruption*:*

$$\begin{aligned}
C_1 &= eruption : 0.6\ ;\ earthquake : 0.3 :- sudden\_energy\_release, \\
&\quad fault\_rupture(X). \\
C_2 &= sudden\_energy\_release : 0.7. \\
C_3 &= fault\_rupture(southwest\_northeast). \\
C_4 &= fault\_rupture(east\_west).
\end{aligned}$$

The Stromboli island is located at the intersection of two geological faults, one in the southwest-northeast direction, the other in the east-west direction, and contains one of the three volcanoes that are active in Italy. This program models the possibility that an eruption or an earthquake occurs at Stromboli. If there is a sudden energy release under the island and there is a fault rupture (C_1), then there can be an eruption of the volcano on the island with probability 0.6, an earthquake in the area with probability 0.3 or no event (the implicit null *atom) with probability 0.1. The energy release occurs with probability 0.7 while we are sure that ruptures occur in both faults.*

P *defines 18 (3 · 3 · 2) possible instances: the first rule with three head atoms has two possible groundings* $X = southwest\_northeast$ *and* $X = east\_west$ *(3 · 3) and the second rule has two head atoms. The query* eruption *is true only in 5 of them. Its probability, according to Equation 9.1, is* $P(eruption) = 0.6 \cdot 0.6 \cdot 0.7 + 0.6 \cdot 0.3 \cdot 0.7 + 0.6 \cdot 0.1 \cdot 0.7 + 0.3 \cdot 0.6 \cdot 0.7 + 0.1 \cdot 0.6 \cdot 0.7 = 0.588$.

For instance, the first term $0.6 \cdot 0.6 \cdot 0.7$ *is obtained from the instance:*

$eruption : 0.6\ :- sudden\_energy\_release, fault\_rupture(southwest\_northeast).$
$eruption : 0.6\ :- sudden\_energy\_release, fault\_rupture(east\_west).$
$sudden\_energy\_release : 0.7.$
$fault\_rupture(southwest\_northeast).$
$fault\_rupture(east\_west).$

while the last term $0.1 \cdot 0.6 \cdot 0.7$ *from the instance:*

$null : 0.1\ :- sudden\_energy\_release, fault\_rupture(southwest\_northeast).$
$eruption : 0.6\ :- sudden\_energy\_release, fault\_rupture(east\_west).$
$sudden\_energy\_release : 0.7.$
$fault\_rupture(southwest\_northeast).$
$fault\_rupture(east\_west).$

Since it is often unfeasible to find all the instances where the query is true, *inference algorithms* search for *covering set of explanations* for the query instead. If we establish the following correspondences:

$$\begin{array}{ll}
C_i\theta_j & \rightarrow multivalued\ random\ variable\ X_{ij} \\
atomic\ choice\ (C_i, \theta_j, k) & \rightarrow assignment\ X_{ij} = k, k\ \in \{1, \ldots, n_i\}
\end{array}$$

the problem of computing the probability of a query Q can be reduced to computing the probability of the Boolean function defined over the vector of variables $\mathbf{X}$:

$$f_Q(\mathbf{X}) = \bigvee_{\kappa \in E(Q)} \bigwedge_{(C_i,\theta_j,k)\in\kappa} X_{ij} = k \tag{9.2}$$

It is a Disjunctive Normal Form (DNF) formula (a disjunction of conjunctive clauses), where $E(Q)$ is a covering set of explanations for Q and $X_{ij} = k$ indicates that the k_{th} atom has been chosen in the head of clause C_i grounded with substitution θ_j. Equations for a single explanation κ are conjoined and the conjunctions for the different explanations are disjointed. The probability that goal Q succeeds equals to the probability that the disjunction of these conjunctions is true (takes value 1), and this happens if the values of the variables correspond to an explanation for the query.

Example 22 (Example 21 cont.) *Clause C_1 has two groundings, $C_1\theta_1$ with $\theta_1 = \{X/southwest\_northeast\}$ and $C_1\theta_2$ with $\theta_2 = \{X/east\_west\}$, corresponding to the random variables X_{11} and X_{12} respectively. Clause C_2 has only one grounding $C_2\emptyset$ instead and it corresponds to the single random variable X_{21}. X_{11} and X_{12} can take three values since C_1 has three head atoms; similarly X_{21} can take two values since C_2 has two head atoms.*

The query $eruption$ has the covering set of explanations $E(eruption) = \{\kappa_1, \kappa_2\}$ where:

$$\begin{aligned}\kappa_1 &= \{(C_1, \{X/southwest\_northeast\}, 1), (C_2, \{\}, 1)\}\\ \kappa_2 &= \{(C_1, \{X/east\_west\}, 1), (C_2, \{\}, 1)\}\end{aligned}$$

Each atomic choice $(C_i, \theta_j, k) \in \kappa_i$ is represented by the propositional equation $X_{ij} = k$:

$$\begin{aligned}(C_1, \{X/southwest\_northeast\}, 1) &\rightarrow X_{11} = 1\\ (C_2, \{\}, 1) &\rightarrow X_{21} = 1\\ (C_1, \{X/east\_west\}, 1) &\rightarrow X_{12} = 1\end{aligned}$$

The set of explanations $E(eruption)$ can be encoded, according to the formula 9.2, by the function:

$$f_{eruption}(\mathbf{X}) = (X_{11} = 1 \wedge X_{21} = 1) \vee (X_{12} = 1 \wedge X_{21} = 1)$$

While each of these explanations can be assigned a probability, it is incorrect to sum them up in order to compute P(Q), since they are not statistically independent, differently from instances. In fact, the probability of the DNF formula

$$P(f_{eruption}(\mathbf{X})) = P((X_{11} = 1 \wedge X_{21} = 1) \vee (X_{12} = 1 \wedge X_{21} = 1))$$

is

$$P(f_{eruption}(\mathbf{X})) = P(X_{11} = 1 \wedge X_{21} = 1) + P(X_{12} = 1 \wedge X_{21} = 1) - P(X_{11} = 1 \wedge X_{21} = 1)P(X_{12} = 1 \wedge X_{21} = 1). \tag{9.3}$$

If we simply summed up $P(X_{11} = 1 \wedge X_{21} = 1)$ and $P(X_{12} = 1 \wedge X_{21} = 1)$ we would get $0.6 \cdot 0.7 + 0.6 \cdot 0.7 = 0.84 \neq 0.588$, while according to Equation 9.3 we correctly compute $0.6 \cdot 0.7 + 0.6 \cdot 0.7 - 0.6 \cdot 0.6 \cdot 0.7 = 0.588$, cf Example 21. The third product term in Equation 9.3 represents a *joint* event, indicating that explanations have first to be made disjoint (mutually exclusive) so that a summation can be computed. In the literature, the problem of computing the probability of DNF formulae is an NP-hard problem even if all variables are independent, and this is the problem of transforming sum-of-products into sum-of-disjoint-products. Some algorithms have been developed, however they seem to be limited to a few dozens of variables and a few hundreds of sums.

The most efficient technique up to now is represented by Multivalued Decision Diagrams (MDD). The advantage of MDDs is that they represent the Boolean function $f(\mathbf{X})$ by means of a generalization of the Shannon's expansion

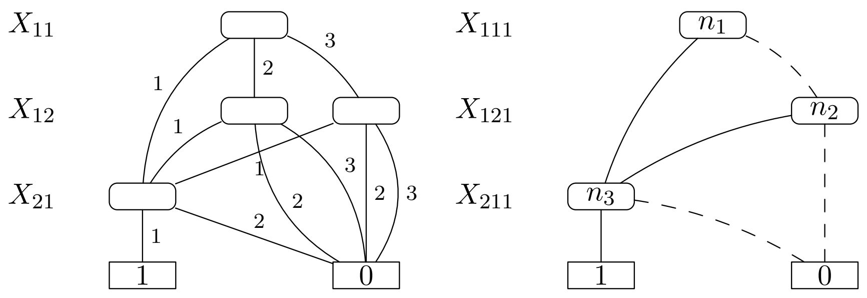
$$f(\mathbf{X}) = (X_1 = 1) \wedge f_{X_1=1}(\mathbf{X}) \vee \cdots \vee (X_1 = n) \wedge f_{X_1=n}(\mathbf{X})$$

where X_1 is the variable associated with the root node of the diagram and $f_{X_1=i}(\mathbf{X})$ is the function associated to the $i{-}th$ child of the root node. The expansion can be applied recursively to the functions $f_{X_1=i}(\mathbf{X})$. This expansion allows the probability of $f(\mathbf{X})$ to be expressed by means of the following recursive formula

$$P(f(\mathbf{X})) = P(X_1 = 1) \cdot P(f_{X_1=1}(\mathbf{X})) + ... + P(X_1 = n) \cdot P(f_{X_1=n}(\mathbf{X}))$$

because the disjuncts are mutually exclusive due to the presence of the $X_1 = i$ equations. In this way the MDD split paths on the basis of the values of a multi-valued variable and the branches are mutually disjoint, thus the probability of $f(\mathbf{X})$ can be computed by means of a dynamic programming algorithm that traverses the MDD and sums up probabilities. The reduced MDD corresponding to the query $eruption$ from Example 21 is shown in Figure 9.1a. The labels on the edges represent the values of the variable associated with the source node.

Since most packages for the manipulation of decision diagrams are restricted to work on Binary Decision Diagrams, multivalued variables have to be represented by means of binary variables (De Raedt et al., 2008a; Sang et al., 2005). For a multi-valued variable X_{ij},



(a) MDD. **(b)** BDD.

Figure 9.1: Decision diagrams for Example 21.

corresponding to ground clause $C_i\theta_j$, having n_i values, we use $n_i - 1$ Boolean variables $X_{ij1}, \ldots, X_{ijn_i-1}$ and we represent the equation $X_{ij} = k$ for $k = 1, \ldots n_i - 1$ by means of the conjunction $\overline{X_{ij1}} \wedge \ldots \wedge \overline{X_{ijk-1}} \wedge X_{ijk}$, and the equation $X_{ij} = n_i$ by means of the conjunction $\overline{X_{ij1}} \wedge \ldots \wedge \overline{X_{ijn_i-1}}$. The high and low child of each node of the BDD are disjoint, that is, following the edge to the high child corresponds to assigning the value true to the Boolean variable, while following the edge to the low child corresponds to the value false. Each Boolean variable X_{ijk} is associated a parameter π_{ik} that represents $P(X_{ijk} = 1)$. The parameters are obtained from those of multivalued variables in this way:

$$\begin{aligned}
\pi_{i1} &= \Pi_{i1} \\
\ldots & \\
\pi_{ik} &= \frac{P(X_{ij} = k)}{\prod_{j=1}^{k-1}(1 - \pi_{ij})} = \frac{\Pi_{ik}}{\prod_{j=1}^{k-1}(1 - \pi_{ij})} \\
\ldots &
\end{aligned}$$

up to $k = n_i - 1$.

Example 23 (Example 21 cont.) *According to the above transformation, X_{11} and X_{12} are 3-valued variables and are converted into two Boolean variables each one (X_{111} and X_{112} for the former, X_{121} and X_{122} for the latter); X_{21} is a 2-valued variable and is converted into the Boolean variable X_{211}. The set of explanations $E(eruption) = \{\kappa_1, \kappa_2\}$ can be now encoded by the equivalent function*

$$f'_{eruption}(\mathbf{X}) = (X_{111} \wedge X_{211}) \vee (X_{121} \wedge X_{211}) \tag{9.4}$$

with the first disjunct representing κ_1 and the second disjunct κ_2. The BDD encoding of $f'_{eruption}(\mathbf{X})$, corresponding to the MDD of Figure 9.1a, is shown in Figure 9.1b. A value *of 1 for the Boolean variables X_{111} and X_{121} means that, for the ground clauses $C_1\theta_1$ and $C_1\theta_2$, the head $h_{11} = eruption$ is chosen and the 1-branch from nodes n_1 and n_2 must be followed, regardless of the other variables for C_1 (X_{112}, X_{122}) that are in fact omitted from the diagram.*

Having built the BDD representing the Boolean function $f'_Q(\mathbf{X})$, in order to compute the probability a dynamic programming algorithm traverses the diagram from the root node to all leaves (De Raedt et al., 2007). At each inner node, probabilities from both children are calculated recursively and combined afterwards as it is done in Algorithm 1.

Algorithm 1 Probability of a query computed by traversing a BDD.

```
 1: function BDD_PROBABILITY($node\ n$)
 2:     if $n$ is 1-terminal then
 3:         return 1
 4:     end if
 5:     if $n$ is 0-terminal then
 6:         return 0
 7:     end if
 8:     let $h$ and $l$ be the high and low children of $n$
 9:     $prob(h)$ = BDD_PROBABILITY($h$)
10:     $prob(l)$ = BDD_PROBABILITY($l$)
11:     return $p_n \cdot prob(h) + (1 - p_n) \cdot prob(l)$
12: end function
```

For each node, the probability that the sub-BDD starting at that node is true is computed by summing the probability of the high and low child, weighted by the probability of the node's variable being assigned true and false respectively. Intermediate results are cached, and the algorithm has a time and space complexity linear in the size of the BDD. The probability of the root node corresponds to the probability of the query $P(Q)$, i.e., the probability of $f'_Q(\mathbf{X})$ taking value 1. The application of the Algorithm 1 to the BDD of Example 23 is illustrated in Figure 9.2. The probabilities computed by Algorithm 1 on the two sub-BDDs can be summed up as the corresponding events are statistically independent.

Even if BDDs allow to compactly represent explanations for queries, they might have an exponential growth in large programs characterized by many random variables. In order to contain the number of variables and thus simplify inference, we may consider grounding only some of the variables of clauses, at the expenses of the accuracy in modeling the domain. A typical compromise between accuracy and complexity is to consider the grounding of variables in the head only: in this way, a ground atom entailed by two separate ground instances of a clause is assigned the same probability, all other things being equal, of a ground atom entailed

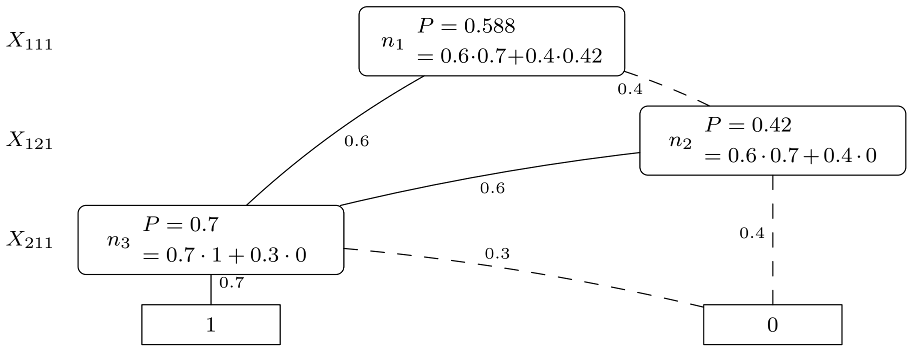

X_{111}
X_{121}
X_{211}
n_1
$P = 0.588$
$= 0.6{\cdot}0.7{+}0.4{\cdot}0.42$
n_2
$P = 0.42$
$= 0.6 \cdot 0.7 + 0.4 \cdot 0$
n_3
$P = 0.7$
$= 0.7 \cdot 1 + 0.3 \cdot 0$
0.4
0.6
0.6
0.4
0.3
0.7
1
0

Figure 9.2: BDD built to compute the probability of the query $Q = eruption$ for Example 21. The probabilities P of each node represent the intermediate values computed by Algorithm 1 when traversing the BDD. The probability of the query (0.588) is returned at the root node.

by a single ground clause, while in the full semantics the first would have a larger probability, as more evidence is available for its entailment. This simplified semantics can be interpreted as stating that a ground atom is entailed by a clause with the probability given by its annotation if there is a substitution for the variables appearing in the body only such that the body is true.

Example 24 (Example 21 cont.) *In the simplified semantics, C_1 is associated with a single random variable X_{11}. In this case T has 6 ($3 \cdot 2$) instances, the query* eruption *is true in 1 of them and its probability is $P(eruption) = 0.6 \cdot 0.7 = 0.42$. So* eruption *is assigned a lower probability with respect to the full semantics because the two independent groundings of clause C_1, differing in the fault name, are not considered separately anymore.*

Reducing the size of the BDD allows to apply parameter learning for LPADs on large-scale real world datasets.

One of the algorithms developed in this thesis is a variant of the BDD traversal algorithm for computing the probability of a query. In Section 10.2 we extend the computation on the BDD to optimize the parameters of an LPAD program with respect to a training set, by adding a “forward” traversal of the diagram to the current recursive “backward” traversal.

Chapter 10

Parameter Learning of LPADs

One typically distinguishes two problems within the statistical learning field. First, there is the problem of *parameter estimation*, where the goal is to estimate appropriate values for the parameters of a model, whose structure is fixed, and second, there is the problem of *structure learning*, where the learner must infer both the structure and the parameters of the model from data (Raedt, 2008). The first problem is tackled is this chapter, the second one in the next Chapter.

This chapter presents, after a general introduction about the parameter estimation problem in probabilistic models (Section 10.1), the parameter learning algorithm `EMBLEM` for LPADs based on the Expectation Maximization approach, where the expectations are computed directly using BDDs (Section 10.2). The chapter also features related works (Section 10.3) and experimental results on real world datasets (Section 10.4). Conclusive considerations can be found in Section 10.5.

10.1 Parameter Learning of Probabilistic Models

The problem of parameter estimation can be formalized as follows:

Given

- a set of examples E,
- a probabilistic model $M = (S, \lambda)$ with structure S and parameters λ,
- a probabilistic coverage relation $P(e|M)$ that computes the probability of observing the example e given the model M,

- a scoring function $score(E, M)$ that employs the probabilistic coverage relation $P(e|M)$

Find the parameters λ^* that maximize $score(E, M)$, that is,

$$\lambda^* = arg\ max_\lambda\ score(E, (S, \lambda))$$

This problem specification abstracts the specific class of models considered, and actually can be instantiated w.r.t. the different representation languages. The problem specification shows that parameter estimation is essentially an optimization problem that depends on the scoring function and type of model employed.

The standard scoring function is the probability of the model or hypothesis given the data. This yields the *maximum a posteriori hypothesis* H_{MAP}

$$H_{MAP} = arg\ max_H P(H|E) = arg\ max_H \frac{P(E|H)P(H)}{P(E)}$$

It can be simplified into the *maximum likelihood* hypothesis H_{ML} by applying Bayes' law and assuming that all hypotheses H are, a priori, equally likely, yielding:

$$H_{ML} = arg\ max_H P(E|H) \tag{10.1}$$

which is called the *likelihood function*.

It is typically assumed that the examples are independently and identically distributed (i.i.d.), which allows one to rewrite the expression in the following form (where the e_i correspond to the different examples):

$$H_{ML} = arg\ max_H \prod_{e_i \in E} P(e_i|H)$$

The probabilistic coverage relation $P(e|H)$ is employed, and it indicates the likelihood of observing e given the hypothesis (model) H. Typically, the goal is to learn a **generative** model, that is, a model that could have generated the data.

This contrasts with the traditional inductive logic programming setting, which is **discriminative**: positive examples have a strictly positive probabilistic coverage ($P(e|H) > 0$), the negative ones have a 0 probabilistic coverage. Within the above problem specification discriminative learning can be modeled by choosing an alternative scoring function, that maximizes the *conditional likelihood* function

$$H_{CL} = arg\ max_H \prod_{e_i \in E} P(class(e_i)|des(e_i), H) \tag{10.2}$$

where the examples e_i are split up into the class of interest (also called *target*) $class(e_i)$ and the description of the example $des(e_i)$. This function can be maximized by maximizing its logarithm instead, which is easier because the logarithm is a monotonic function. In literature it is thus referred as the *conditional log likelihood (LL) function*.

10.2 The EMBLEM Algorithm

The parameter estimation algorithm for LPADs, which is presented in the following, tackles a problem of *discriminative* learning defined as follows.

Given

- a set of training examples Q_i, corresponding to ground atoms for a set of *target* or *output* predicates,
- a background knowledge with ground facts for other non-target or *input* predicates, organized as a set of logical interpretations or "mega-examples",
- a probabilistic logical model M corresponding to a LPAD program P, composed of annotated disjunctive clauses C_i with unknown parameters (probabilities) $\lambda = \mathbf{\Pi} = \langle \Pi_{i1}, ..., \Pi_{in_i} \rangle$ in the heads,

Find the maximum likelihood probabilities $\mathbf{\Pi}^*$, i.e. those that maximize the conditional probability of the examples given the model and the input predicates.

EMBLEM algorithm learns maximum likelihood parameters of a LPAD by applying the Expectation Maximization algorithm where the expectations are computed directly on BDDs. It is based on the algorithms proposed in (Inoue et al., 2009; Ishihata et al., 2008a,b; Thon et al., 2008).

The application of the EM algorithm has the following justifications. Each training example Q_i corresponds to a query to the LPAD and the background data. In order to determine the probabilities Π_{ik}, the number of times a head h_{ik} has been chosen in an application of a rule C_i to find an explanation for the query is required. This frequency is indicated as c_{ik} and is not directly observable. Given the set of clauses involved in the SLD-derivation of the query, there are many possible selections σ which allows one to find a proof for the query: the information about which selection has been used is unknown. The Expectation Maximization (EM) algorithm deals with the case where the data are not fully observable, but only partially observable; if values for some variables are occasionally unobserved, there is *missing data*, while if values for some variables are always unobserved, the variables are called *latent*. In our case, the mega-examples record the truth value of all ground facts, but not the selections (that is, the atomic choices) which represent the latent variables, and the random variables c_{ik} represent a sufficient statistics, whose value contains all the information needed to compute any estimate of the unknown parameters. As introduced in Chapter 8, we would like to maximize the (log-)likelihood L of the data, which is a function of the parameters Π of the model $L(\Pi)$. This function depends on the unobserved values and a way of dealing with these values is to compute the *expected* likelihood function $Q(\Pi)$, where the expectation is taken over the *hidden* variables. The algorithm assumes that there is a current model $M(\Pi)$ and uses it to compute the expected values of the variables c_{ik}, that is $E[c_{ik}|M, \Pi]$. After randomly initializing the model parameters, the EM algorithm repeatedly performs the following two operations until the parameters have converged:

- E Step: Uses the current model and the observed data to determine the conditional distribution of the unobserved random variables c_{ik};
- M Step: Uses the observed random variables together with the distribution of the unobserved random variables to estimate the model parameters using frequency counting;

In the following the two steps of the algorithm are described in detail.

Construction of the BDDs

Among all predicates describing the domain, some of them have to be specified as *target* by the user, while the remainder are referred as *background*. The ground atoms in the mega-examples for the target predicates correspond to as many queries Q_i for which the BDDs are built, encoding the disjunction of their explanations; these atoms will be referred afterwards as (target) *examples*. The mega-examples must contain also negative atoms for target predicates, expressed as $neg(atom)$. These predicates are called *target or output* since EM tries to maximize the conditional log-likelihood only for the positive and negative facts of those predicates.

The predicates can be treated as closed-world or open-world. In the first case, the body of clauses is resolved only with facts in the mega-example. In the second case, the body of clauses is resolved both with facts and with clauses in the theory. If the latter option is set and the program is cyclic (see Def. 20), `EMBLEM` uses a depth bound on SLD-derivations to avoid going into infinite loops, as proposed by (Gutmann et al., 2010a), with D the value of the bound: derivations exceeding the limit D are cut.

Definition 20 (Acyclic programs) *A* level mapping *for a program T is a function* $| \; |: H_B(T) \rightarrow N$ *of ground atoms to natural numbers. For* $A \in H_B(T)$ $\; | A |$ *is the* level *of A. Given a level mapping* $| \; |$*, we extend it to ground negative literals by defining* $| \neg A | = | A |$*.*

- *A clause of T is called* acyclic *with respect to a level mapping* | |*, if for every ground instance* $A \leftarrow B$ *of it, the level of A is greater then the level of each literal in the body* B*.*
- *A program T is called* acyclic with respect to a level mapping | |*, if all its clauses are. T is called* acyclic *if it is acyclic with respect to some level mapping.*

We extend this definition to LPADs by requiring that the level of each atom in the head is greater than the level of each literal in the body. This ensures that each instance of the LPAD is an acyclic logic program.

Example 25 *Consider the program T that defines the predicate* $path/2$ *such that* $path(x, y)$ *is true if there is a path from* x *to* y *in a directed graph. Such a program contains the clauses*

$$path(X, Y) \leftarrow edge(X, Y).$$

$$path(X, Y) \leftarrow edge(X, Z), path(Z, Y).$$

plus a set E *of ground facts for the* $edge/2$ *relation that represent the edges between nodes of the graph.* $path/2$ *defines the transitive closure of* $edge/2$*.*
Suppose E *contains the only fact* $edge(a, b)$*. This program is not acyclic because it contains the ground rule*

$$path(a, a) \leftarrow edge(a, a), path(a, a).$$

that imposes the contradictory constraint $|path(a, a)| > |path(a, a)|$*.*

The search for proofs of a query Q is performed in practice by employing SLD-resolution in Prolog, against a database composed of the mega-examples. The paths from the root to individual leaves of the SLD-tree represent either a successful or a failed proof. Each successful proof in the SLD-tree has a set of clauses (and head atoms) employed in that proof, represented by a covering set of explanations, that is independent of other clauses in the LPAD. The set of composite choices leading to successful proofs is graphically represented as the set of paths from the root the the 1-leaf of a BDD.

Program transformation into a BDD For generating the BDD for a query (example) Q the algorithm "Probabilistic Inference with Tabling and Answer subsumption" (PITA) (Riguzzi and Swift, 2010) is applied, which builds explanations for every subgoal encountered during a derivation of the query. The input LPAD is transformed into a normal logic program in which the subgoals have an extra argument storing a BDD that represents their explanations.

The first step of the algorithm is to apply a program transformation to a LPAD to create a normal program that contains calls for manipulating BDDs. In the implementation, these calls provide a Prolog interface to the CUDD[1] C library, where BDDs are represented as pointers to their root node, and use the following predicates:

- *init, end*: for allocation and deallocation of a BDD manager, a data structure used to keep track of the memory for storing BDD nodes;
- *zero(-BDD), one(-BDD), and(+BDD1,+BDD2,-BDDO), or(+BDD1,+BDD2, -BDDO), not(+BDDI,-BDDO)*: Boolean operations between BDDs;
- *add_var(+NVal,+Probs,-Var)*: addition of a new multi-valued variable with *NVal* values and parameters *Probs*;
- *equality(+Var,+Value,-BDD)*: BDD represents $Var = Value$, i.e., the random variable Var is assigned $Value$ in the BDD;
- *ret_prob(+BDD,-P)*: returns the probability of the formula encoded by *BDD*.

add_var(+NVal,+Probs,-Var) adds a new random variable associated with a new instantiation of a rule with $NVal$ head atoms and parameters list $Probs$. The auxiliary predicate *get_var_n/4* is used to wrap *add_var/3* and avoid adding a new variable when one already exists for an instantiation. As shown below, a new fact *var(R,S,Var)* is asserted each time a new random variable is created, where R is an identifier for the LPAD rule, S is a list of constants, one for each variable of the clause, and Var is a integer that identifies the random variable associated with clause R under a specific grounding. The auxiliary predicate has the following definition:
$get\_var\_n(R, S, Probs, Var) \leftarrow (var(R, S, Var) \rightarrow true;$
$length(Probs, L), add\_var(L, Probs, Var), assert(var(R, S, Var)))$.

[1]`http://vlsi.colorado.edu/~fabio/`

where $Probs$ is a list of real numbers that stores the parameters in the head of rule R. R, S and $Probs$ are input arguments while Var is an output argument.

The transformation applies to clauses, literals and atoms:

- If h is an atom, $PITA_h(h)$ is h with the variable BDD added as the last argument;

- If b_j is an atom, $PITA_b(b_j)$ is b_j with the variable B_j added as the last argument.

- If b_j is negative literal $\neg a_j$, $PITA_b(b_j)$ is the conditional $(PITA'_b(a_j) \rightarrow not(BN_j, B_j); one(B_j))$, where $PITA'_b(a_j)$ is a_j with the variable BN_j added as the last argument; the BDD BN_j for a is negated if it exists (i.e. $PITA'_b(a_j)$ succeeds); otherwise the BDD for the constant function 1 is returned.

- A non-disjunctive fact $C_r = h$ is transformed into the clause $PITA(C_r) = PITA_h(h) \leftarrow one(BDD).$

- A disjunctive fact $C_r = h_1 : \Pi_1; \ldots; h_n : \Pi_n.$ where the parameters sum to 1, is transformed into the set of clauses $PITA(C_r)$
$$\begin{array}{lcll} PITA(C_r, 1) & = & PITA_h(h_1) \leftarrow & get\_var\_n(r, [], [\Pi_1, \ldots, \Pi_n], Var), \\ & & & equality(Var, 1, BDD). \\ \ldots & & & \\ PITA(C_r, n) & = & PITA_h(h_n) \leftarrow & get\_var\_n(r, [], [\Pi_1, \ldots, \Pi_n], Var), \\ & & & equality(Var, n, BDD). \end{array}$$
When the parameters do not sum to one, the clause is first transformed into $h_1 : \Pi_1 \vee \ldots \vee h_n : \Pi_n \vee null : 1 - \sum_1^n \Pi_i$ and then into the clauses above, where the list of parameters is $[\Pi_1, \ldots, \Pi_n, 1 - \sum_1^n \Pi_i]$ but the (n + 1)-th clause (for *null*) is not generated.

- The definite clause $C_r = h \leftarrow b_1, b_2, \ldots, b_m.$ is transformed into the clause
$$\begin{array}{lcll} PITA(C_r) & = & PITA_h(h) \leftarrow & PITA_b(b_1), PITA_b(b_2), and(B_1, B_2, BB_2), \\ & & & ..., PITA_b(b_m), and(BB_{m-1}, B_m, BDD). \end{array}$$

- The disjunctive clause $C_r = h_1 : \Pi_1; \ldots; h_n : \Pi_n \leftarrow b_1, b_2, \ldots, b_m.$
where the parameters sum to 1, is transformed into the set of clauses $PITA(C_r)$

$$\begin{array}{lcll} PITA(C_r,1) & = & PITA_h(h_1) \leftarrow & PITA_b(b_1), PITA_b(b_2), \mathit{and}(B_1,B_2,BB_2), \\ & & & ..., \\ & & & PITA_b(b_m), \mathit{and}(BB_{m-1},B_m,BB_m), \\ & & & \mathit{get\_var\_n}(r,VC,[\Pi_1,...,\Pi_n],Var), \\ & & & \mathit{equality}(Var,1,B), \mathit{and}(BB_m,B,BDD). \\ \ldots & & & \\ PITA(C_r,n) & = & PITA_h(h_n) \leftarrow & PITA_b(b_1), PITA_b(b_2), \mathit{and}(B_1,B_2,BB_2), \\ & & & ..., \\ & & & PITA_b(b_m), \mathit{and}(BB_{m-1},B_m,BB_m), \\ & & & \mathit{get\_var\_n}(r,VC,[\Pi_1,...,\Pi_n],Var), \\ & & & \mathit{equality}(Var,n,B), \mathit{and}(BB_m,B,BDD). \end{array}$$

where VC is a list containing each variable appearing in C_r. If the parameters do not sum to 1, the same technique used for disjunctive facts is used.

In order to answer queries, the goal $solve(Goal, P)$ is used, which is defined for the cases a depth D is used or not to derive the goal:

$$\begin{array}{ll} solve(Goal,P) \leftarrow & init, retractall(v(\_,\_,\_)), \\ & add\_bdd\_arg(Goal,BDD0,GoalOut), \\ & (bagof(BDD0,GoalOut,L) \rightarrow or\_list(L,BDD); zero(BDD)), \\ & ret\_prob(BDD,P), \\ & end. \end{array}$$

$$\begin{array}{ll} solve(Goal,P) \leftarrow & init, setting(depth\_bound,true), !, \\ & setting(depth,DB), retractall(v(\_,\_,\_)), \\ & add\_bdd\_arg\_db(Goal,BDD0,DB,GoalOut), \\ & (bagof(BDD0,GoalOut,L) \rightarrow or\_list(L,BDD); zero(BDD)), \\ & ret\_prob(BDD,P), \\ & end. \end{array}$$

Example 26 *Clause C_1 from the LPAD of Example 21 is translated into*

$$\begin{array}{lll} eruption(BDD) & \leftarrow & sudden\_energy\_release(B1), fault\_rupture(X,B2), \\ & & and(B1,B2,BB2), \\ & & get\_var\_n(1,[X],[0.6,0.3,0.1],Var), \\ & & equality(Var,0,B), and(BB2,B,BDD). \\ earthquake(BDD) & \leftarrow & sudden\_energy\_release(B1), fault\_rupture(X,B2), \\ & & and(B1,B2,BB2), \\ & & get\_var\_n(1,[X],[0.6,0.3,0.1],Var), \\ & & equality(Var,1,B), and(BB2,B,BDD). \end{array}$$

Clause C_2 is translated into

$$\begin{array}{lll} sudden\_energy\_release(BDD) & \leftarrow & get\_var\_n(2,[],[0.7,0.3],Var), \\ & & equality(Var,0,BDD). \end{array}$$

Clause C_3 is translated into

$fault\_rupture(southwest\_northeast, BDD) \quad \leftarrow \quad one(BDD).$

EM Cycle

After building the BDDs for each target example Q, EMBLEM starts the EM cycle, in which the steps of Expectation and Maximization are repeated until the LL of the examples reaches a local maximum or a maximum number of steps (NEM) is reached. EMBLEM is shown in Algorithm 2, where with $Theory$ we mean the LPAD program: it consists of a cycle where the procedures EXPECTATION and MAXIMIZATION are repeatedly called; procedure EXPECTATION returns the LL of the data that is used in the stopping criterion. EMBLEM stops when the difference between the LL of the current and the previous iteration drops below a threshold ϵ or when this difference is below a fraction δ of the current LL.

Algorithm 2 Function EMBLEM

```
1: function EMBLEM($Theory, D, NEM, \epsilon, \delta$)
2:     Build $BDDs$ by SLD derivations with depth bound $D$
3:     $LL = -inf$
4:     $N = 0$
5:     repeat                                              ▷ Start of EM cycle
6:         $LL_0 = LL$
7:         $LL =$ EXPECTATION($BDDs$)
8:         MAXIMIZATION
9:         $N = N + 1$
10:    until $LL - LL_0 < \epsilon \vee LL - LL_0 < -LL \cdot \delta \vee N > NEM$
11:    Update parameters of $Theory$
12:    return $LL, Theory$
13: end function
```

Expectation Step

The Expectation phase (see Algorithm 3) takes as input a list of BDDs, one for each target fact Q, and computes the probabilities $P(X_{ijk} = x|Q)$ for all C_is, $k = 1, \ldots, n_i - 1$, $j \in g(i) := \{j|\theta_j$ is a substitution grounding $C_i\}$ and $x \in \{0, 1\}$. From $P(X_{ijk} = x|Q)$ one can compute the expectations $\mathbf{E}[c_{ik0}|Q]$ and $\mathbf{E}[c_{ik1}|Q]$ where c_{ikx} is the number of times a Boolean variable X_{ijk} takes value x for $x \in \{0, 1\}$ and for all $j \in g(i)$. i.e, the ground head h_{ik} has been used (1) or not (0) in a proof. $\mathbf{E}[c_{ikx}|Q]$ is given by

$$\mathbf{E}[c_{ikx}|Q] = \sum_{j \in g(i)} P(X_{ijk} = x|Q)$$

Finally, the expectations $\mathbf{E}[c_{ik0}]$ and $\mathbf{E}[c_{ik1}]$ of the counts over all queries are computed as

$$\mathbf{E}[c_{ikx}] = \sum_{Q} \mathbf{E}[c_{ikx}|Q]$$

Algorithm 3 Function Expectation

```
1:  function EXPECTATION($BDDs$)
2:      $LL = 0$
3:      for all $BDD \in BDDs$ do
4:          for all $i \in Rules$ do
5:              for $k = 1$ to $n_i - 1$ do
6:                  $\eta^0(i,k) = 0;\ \eta^1(i,k) = 0$
7:              end for
8:          end for
9:          for all variables X do
10:             $\varsigma(X) = 0$
11:         end for
12:         GETFORWARD($root(BDD)$)
13:         $Prob$=GETBACKWARD($root(BDD)$)
14:         $T = 0$
15:         for $l = 1$ to $levels(BDD)$ do
16:             Let $X_{ijk}$ be the variable associated with level $l$
17:             $T = T + \varsigma(l)$
18:             $\eta^0(i,k) = \eta^0(i,k) + T \times (1 - \pi_{ik})$
19:             $\eta^1(i,k) = \eta^1(i,k) + T \times \pi_{ik}$
20:         end for
21:         for all $i \in Rules$ do
22:             for $k = 1$ to $n_i - 1$ do
23:                 $\mathbf{E}[c_{ik0}] = \mathbf{E}[c_{ik0}] + \eta^0(i,k)/Prob$
24:                 $\mathbf{E}[c_{ik1}] = \mathbf{E}[c_{ik1}] + \eta^1(i,k)/Prob$
25:             end for
26:         end for
27:         $LL = LL + \log(Prob)$
28:     end for
29:     return $LL$
30: end function
```

The conditional probability $P(X_{ijk} = x|Q)$ is given by $\frac{P(X_{ijk}=x,Q)}{P(Q)}$ (cf. Section 6.4), where

$$\begin{aligned} P(X_{ijk} = x, Q) &= \sum_{w_\sigma \in \mathcal{W}_P : w_\sigma \models Q} P(Q, X_{ijk} = x, \sigma) \\ &= \sum_{w_\sigma \in \mathcal{W}_P : w_\sigma \models Q} P(Q|\sigma) P(X_{ijk} = x|\sigma) P(\sigma) \\ &= \sum_{w_\sigma \in \mathcal{W}_P : w_\sigma \models Q} P(X_{ijk} = x|\sigma) P(\sigma) \end{aligned}$$

Now suppose only the merge rule is applied when building the BDD, fusing together identical sub-diagrams. The resulting diagram, that we call Complete Binary Decision Diagram (CBDD), is such that every path contains a node for every level.

Since there is a one to one correspondence between the instances where Q is true ($w_\sigma \models Q$) and the paths to a 1 leaf in a CBDD,

$$P(X_{ijk} = x, Q) = \sum_{\rho \in R(Q)} P(X_{ijk} = x|\rho) \prod_{d \in \rho} \pi(d)$$

where ρ is a path, $R(Q)$ is the set of paths in the CBDD for query Q that lead to a 1 leaf and, if the selection σ corresponds to ρ, then $P(X_{ijk} = x|\sigma) = P(X_{ijk} = x|\rho)$. d is an edge of ρ and $\pi(d)$ is the probability associated with the edge: if d is the 1-branch outgoing of a node associated with a variable X_{ijk}, then $\pi(d) = \pi_{ik}$, if d is the 0-branch, then $\pi(d) = 1 - \pi_{ik}$. See subsection 9.2 for the definition of π_{ik}.

Given a path $\rho \in R(Q)$, $P(X_{ijk} = x|\rho) = 1$ if ρ contains an x-branch from a node associated with variable X_{ijk} and 0 otherwise, so $P(X_{ijk} = x, Q)$ can be further expanded as

$$P(X_{ijk} = x, Q) \quad = \sum_{\rho \in R(Q) \wedge (X_{ijk}=x) \in \rho} \prod_{d \in \rho} \pi(d)$$

where $(X_{ijk} = x) \in \rho$ means that ρ contains an x-branch from the node associated with X_{ijk}. We can then write

$$P(X_{ijk} = x, Q) \quad = \sum_{n \in N(Q) \wedge v(n)=X_{ijk} \wedge \rho_n \in R_n(Q) \wedge \rho^n \in R^n(Q,x)} \prod_{d \in \rho^n} \pi(d) \prod_{d \in \rho_n} \pi(d)$$

where $N(Q)$ is the set of BDD nodes for query Q, $v(n)$ is the variable associated with node n, $R_n(Q)$ is the set containing the paths from the root to n and $R^n(Q, x)$ is the set of paths from n to the 1 leaf through its x-child. So

$$\begin{aligned} P(X_{ijk} = x, Q) &= \sum_{n \in N(Q) \wedge v(n)=X_{ijk}} \sum_{\rho_n \in R_n(Q)} \sum_{\rho^n \in R^n(Q,x)} \prod_{d \in \rho^n} \pi(d) \prod_{d \in \rho_n} \pi(d) \\ &= \sum_{n \in N(Q) \wedge v(n)=X_{ijk}} \sum_{\rho_n \in R_n(Q)} \prod_{d \in \rho_n} \pi(d) \sum_{\rho^n \in R^n(Q,x)} \prod_{d \in \rho^n} \pi(d) \\ &= \sum_{n \in N(Q) \wedge v(n)=X_{ijk}} F(n) B(child_x(n)) \pi_{ikx} \qquad (10.3) \end{aligned}$$

where π_{ikx} is π_{ik} if $x = 1$ and $(1 - \pi_{ik})$ if $x = 0$,

$$F(n) = \sum_{\rho_n \in R_n(Q)} \prod_{d \in \rho_n} \pi(d)$$

is the *forward probability* (Ishihata et al., 2008b), the probability mass (i.e., sum of the probabilities) of the paths from the root to n, and

$$B(n) = \sum_{\rho^n \in R^n(Q)} \prod_{d \in \rho^n} \pi(d)$$

is the *backward probability* (Ishihata et al., 2008b), the probability mass of paths from n to the 1 leaf.

The intuitive meaning of equation (10.3) is the following. Each path from the root of the BDD to the 1 leaf corresponds to an assignment of values to the variables that satisfies the Boolean formula represented by the BDD. The expression $F(n)B(child_x(n))\pi_{ikx}$ represents the sum of the probabilities of all the paths passing through the x-edge of node n. In every node n, the backward probability is the probability that starting from n one will reach the 1 leaf and represents the probability that the logical formula encoded by the sub-BDD rooted at n is true; the forward probability is the probability that starting at the root one will reach n. Hence in equation (10.3) we compute the probability that a person starting at the root reaches n, and ends up in the 1 leaf when leaving n through the x child.

By indicating with $e^x(n)$ the product in equation (10.3) we get

$$P(X_{ijk} = x, Q) = \sum_{n \in N(Q), v(n) = X_{ijk}} e^x(n) \tag{10.4}$$

The counts of equation (10.4) are stored in the variables $\eta^x(i,k)$ for $x \in \{0,1\}$ in Algorithm 5, i.e., in the end $\eta^x(i,k)$ contains

$$\sum_{j \in g(i)} P(X_{ijk} = x, Q).$$

Formula (10.4) is correct only for CBDDs, while for BDDs - generated by applying also the *deletion* rule - it is no longer valid since also paths where there is no node associated to X_{ijk} can contribute to $P(X_{ijk} = x, Q)$: the contribution of deleted paths must be taken into account. Suppose that levels are numbered in increasing order from top to bottom and that a node n is associated with variable Y, that has a level lower than variable X_{ijk}, and $child_1(n)$ is associated with variable W, that has a level higher than variable X_{ijk}. The nodes associated with variable X_{ijk} have been deleted from the paths from n to $child_1(n)$. In Figure 9.1b this happens with $n = n_1$, $Y = X_{111}$, $X_{ijk} = X_{121}$, $child_1(n) = n_3$, $W = X_{211}$: the path connecting n_1 to n_3 does not contain a node at the level of X_{121}. One can imagine that the current BDD has been obtained from a BDD having a node m associated with variable X_{ijk} that is a descendant of n along the 1-branch and whose outgoing edges both point to $child_1(n)$. The original BDD can be reobtained by applying a deletion operation that merges the two paths passing through m. The probability mass of the two paths that were merged was $e^0(n)(1-\pi_{ik})$ and $e^0(n)\pi_{ik}$ for the paths passing through the 0-child and 1-child of m respectively.

Formally, let $Del^x(X)$ be the set of nodes n such that the level of X is higher than that of n and is lower that of $child_x(n)$, i.e., X is deleted between n and $child_x(n)$. For the BDD in Figure 9.1b, for example, $Del^1(X_{121}) = \{n_1\}$, $Del^0(X_{121}) = \{\}$, $Del^1(X_{221}) = \{\}$, $Del^0(X_{221}) = \{n_2\}$. Then

$$\begin{aligned}
P(X_{ijk}=0,Q) &= \sum_{n\in N(Q),v(n)=X_{ijk}} e^x(n) + \\
&\quad (1-\pi_{ik})\left(\sum_{n\in Del^0(X_{ijk})} e^0(n) + \sum_{n\in Del^1(X_{ijk})} e^1(n)\right)\\
P(X_{ijk}=1,Q) &= \sum_{n\in N(Q),v(n)=X_{ijk}} e^x(n) + \\
&\quad \pi_{ik}\left(\sum_{n\in Del^0(X_{ijk})} e^0(n) + \sum_{n\in Del^1(X_{ijk})} e^1(n)\right)
\end{aligned}$$

EXPECTATION Function (Algorithm 3) This function first calls GETFORWARD and GETBACKWARD and computes $\eta^x(i,k)$ for non-deleted paths only. Then it updates $\eta^x(i,k)$ to take into account deleted paths.

Procedure GETFORWARD, shown in Algorithm 4, computes the value of the forward probabilities. It traverses the diagram one level at a time starting from the root level and propagating the values downwards. For each level it considers each node n and computes its contribution to the forward probabilities of its children. Then the forward probabilities of its children, stored in table F, are updated.

Forward probabilities express the likelihood of reaching a node n when starting from the root node and following edges according to their probability. It is defined as $F(root) = 1$ for the root node of the BDD. For any other node it is defined as:

$$F(n) = \sum_{\substack{p \in Nodes \\ n=child_1(p), var(p)=X_{ijk}}} F(p) \cdot \pi_{ik} + \sum_{\substack{p \in Nodes \\ n=child_0(p), var(p)=X_{ijk}}} F(p) \cdot (1 - \pi_{ik}).$$

The first sum considers all possible parent nodes p of n connected by a 1-branch. When being in p one will choose this edge to reach n with probability π_{ik}; the second sum considers all possible parent nodes that are linked to n by a 0-branch, which will be chosen with probability $1 - \pi_{ik}$. At the beginning $F(n)$ is 0 for all nodes n except the root.

Function GETBACKWARD, shown in Algorithm 5, computes the backward probability of nodes by traversing recursively the tree from the root to the leaves. When the calls of GETBACKWARD for both children of a node n return, values are propagated upwards from the leaves,and we have all the information that is needed to compute the $e^x(n)$ values and update the values of $\eta^x(i, k)$ for non-deleted paths.

The backward probabilities express the likelihood of reaching the 1 leaf when starting from a particular node n and proceeding to the high child $child_1(n)$ with probability π_{ik} and to the low child $child_0(n)$ with probability $1 - \pi_{ik}$. For the terminal nodes they are defined as

$$B(0) = 0 \qquad\qquad B(1) = 1,$$

and for inner nodes, as

$$B(n) = B(child_1(n)) \cdot \pi_{ik} + B(child_0(n)) \cdot (1 - \pi_{ik}).$$

Computing the forward and the backward probabilities of BDD nodes requires two traversals of the graph, so the cost is linear in the number of nodes. If $root$ is the root of a tree for a query Q then $B(root) = P(Q)$, i.e., the backward probability at the root node corresponds to the probability of the query, as was computed by Algorithm 1 in subsection 9.2. $P(Q)$ is needed to compute $P(X_{ijk} = x|Q)$. Moreover, $P(Q) = F(1)$ and $1 - P(Q) = F(0)$.

Finally the problem of deleted paths is solved, as in (Ishihata et al., 2008a), by keeping an array ς with an entry for every level l, that stores an algebraic sum of $e^x(n)$: those for nodes in lower levels that do not have a descendant in level l minus those for nodes in lower levels that have a descendant in level l. In this way it is possible to add the contributions of the deleted paths by starting from the root level and accumulating $\varsigma(l)$ for the various levels in a variable T: an $e^x(n)$ value which is added to the accumulator T for level l means that n is an ancestor for nodes in this level. When the x-branch from n reaches a node in a level l' such that $l' \geq l$,

$e^x(n)$ is subtracted from the accumulator, as it is not relative to a deleted node on the path anymore. This is implemented in a post processing phase in Algorithm 3.

Algorithm 4 Computation of the forward probability $F(n)$ in all BDD nodes n.

```
1: procedure GETFORWARD($root$)
2:     $F(root) = 1$
3:     $F(n) = 0$ for all nodes
4:     for $l = 1$ to $levels$ do        ▷ $levels$ is the number of levels of the BDD rooted at $root$
5:         $Nodes(l) = \emptyset$
6:     end for
7:     $Nodes(1) = \{root\}$
8:     for $l = 1$ to $levels$ do
9:         for all $node \in Nodes(l)$ do
10:            Let $X_{ijk}$ be $v(node)$, the variable associated with $node$
11:            if $child_0(node)$ is not terminal then
12:                $F(child_0(node)) = F(child_0(node)) + F(node) \cdot (1 - \pi_{ik})$
13:                Add $child_0(node)$ to $Nodes(level(child_0(node)))$        ▷ $level(node)$ returns the level of $node$
14:            end if
15:            if $child_1(node)$ is not terminal then
16:                $F(child_1(node)) = F(child_1(node)) + F(node) \cdot \pi_{ik}$
17:                Add $child_1(node)$ to $Nodes(level(child_1(node)))$
18:            end if
19:        end for
20:    end for
21: end procedure
```

Execution Example

Suppose you have the program of Example 21 and you have the single example $Q = eruption$. The BDD of Figure 9.1b is built and passed to EXPECTATION in the form of a pointer to its root node n_1. F and B values computed by this function are shown in Figure 10.1.

After initializing the η counters to 0, GETFORWARD is called with argument n_1. The F table for n_1 is set to 1 since this is the root. F is computed for the 0-child, n_2, as $0+1 \cdot 0.4 = 0.4$ and n_2 is added to $Nodes(2)$, the set of nodes for the second level. Then F is computed for the 1-child, n_3, as $0 + 1 \cdot 0.6 = 0.6$, and n_3 is added to $Nodes(3)$. At the next iteration of the cycle, level 2 is considered and node n_2 is fetched from $Nodes(2)$. The 0-child is a terminal so it is skipped, while the 1-child is n_3 and its F value is updated as $0.6 + 0.4 \cdot 0.6 = 0.84$. In the third iteration, node n_3 is fetched but, since its children are leaves, F is not updated.

Then GETBACKWARD is called on n_1. The function calls GETBACKWARD(n_2) that in turn calls GETBACKWARD(0). The latter call returns 0 because it is a terminal node. Then GETBACKWARD(n_2) calls GETBACKWARD(n_3) that in turn calls GETBACKWARD(1) and

Algorithm 5 Computation of the backward probability $B(n)$ in all BDD nodes n, updating of η and ς.

```
 1: function GETBACKWARD($node$)
 2:     if $node$ is a terminal then
 3:         return $value(node)$
 4:     else
 5:         Let $X_{ijk}$ be $v(node)$
 6:         $B(child_0(node))$ =GETBACKWARD($child_0(node)$)
 7:         $B(child_1(node))$ =GETBACKWARD($child_1(node)$)
 8:         $e^0(node) = F(node) \cdot B(child_0(node)) \cdot (1 - \pi_{ik})$
 9:         $e^1(node) = F(node) \cdot B(child_1(node)) \cdot \pi_{ik}$
10:         $\eta^0(i,k) = \eta^0_t(i,k) + e^0(node)$
11:         $\eta^1(i,k) = \eta^1_t(i,k) + e^1(node)$
12:         $l = l(node))$                                    ▷ $l(node)$ returns the level of $node$
13:         $\varsigma(l+1) = \varsigma(l+1) + e^0(node) + e^1(node)$
14:         $\varsigma(l(child_0(node))) = \varsigma(l(child_0(node))) - e^0(node)$
15:         $\varsigma(l(child_1(node))) = \varsigma(l(child_1(node))) - e^1(node)$
16:         return $B(child_0(node)) \cdot (1 - \pi_{ik}) + B(child_1(node)) \cdot \pi_{ik}$
17:     end if
18: end function
```

GETBACKWARD(0), returning respectively 1 and 0. Then GETBACKWARD(n_3) computes $e^0(n_3)$ and $e^1(n_3)$ in the following way:

$$e^0(n_3) = F(n_3) \cdot B(0) \cdot (1 - \pi_{21}) = 0.84 \cdot 0 \cdot 0.3 = 0$$

$$e^1(n_3) = F(n_3) \cdot B(1) \cdot (\pi_{21}) = 0.84 \cdot 1 \cdot 0.7 = 0.588$$

where $B(n)$ and $F(n)$ are respectively the backward and forward probabilities of node n. Now the counters for clause C_2 are updated:

$$\eta^0(2,1) = 0$$

$$\eta^1(2,1) = 0.588$$

while we do not show the update of ς since its value for the level of the leaves is not used afterwards. GETBACKWARD(n_3) now returns the backward probability of n_3:
$B(n_3) = 1 \cdot 0.7 + 0 \cdot 0.3 = 0.7$. GETBACKWARD$(n_2)$ can proceed to compute

$$e^0(n_2) = F(n_2) \cdot B(0) \cdot (1 - \pi_{11}) = 0.4 \cdot 0.0 \cdot 0.4 = 0$$

$$e^1(n_2) = F(n_2) \cdot B(n_3) \cdot (\pi_{11}) = 0.4 \cdot 0.7 \cdot 0.6 = 0.168$$

and $\eta^0(1,1) = 0$, $\eta^1(1,1) = 0.168$. The level following the one of X_{121} is 3 so $\varsigma(3) = e^0(n_2) + e^1(n_2) = 0 + 0.168 = 0.168$. Since X_{121} is also associated with the 1-child n_3, $\varsigma(3) = \varsigma(3) - e^1(n_2) = 0$. The 0-child is a leaf so we do not show the update of ς.

GETBACKWARD(n_2) then returns $B(n_2) = 0.7 \cdot 0.6 + 0 \cdot 0.4 = 0.42$ to GETBACKWARD(n_1), that computes $e^0(n_1)$ and $e^1(n_1)$ as

$e^0(n_1) = F(n_1) \cdot B(n_2) \cdot (1 - \pi_{11}) = 1 \cdot 0.42 \cdot 0.4 = 0.168$

$e^1(n_1) = F(n_1) \cdot B(n_3) \cdot (\pi_{11}) = 1 \cdot 0.7 \cdot 0.6 = 0.42$

and updates the η counters as $\eta^0(1,1) = 0.168$, $\eta^1(1,1) = 0.168 + 0.42 = 0.588$.

Finally ς is updated:

$\varsigma(2) = e^0(n_1) + e^1(n_1) = 0.168 + 0.42 = 0.588$

$\varsigma(2) = \varsigma(2) - e^0(n_1) = 0.42$

$\varsigma(3) = \varsigma(3) - e^1(n_1) = -0.42.$

GETBACKWARD(n_1) returns $B(n_1) = 0.7 \cdot 0.6 + 0.42 \cdot 0.4 = 0.588$ to EXPECTATION, that adds the contribution of deleted nodes by cycling over the BDD levels and updating T. Initially T is set to 0, then for level 1/variable X_{111} it is updated to $T = \varsigma(1) = 0$ which implies no modification of $\eta^0(1,1)$ and $\eta^1(1,1)$. For level 2/variable X_{121} T is updated to $T = 0 + \varsigma(2) = 0.42$ and the η table is modified as

$\eta^0(1,1) = 0.168 + 0.42 \cdot 0.4 = 0.336$

$\eta^1(1,1) = 0.588 + 0.42 \cdot 0.6 = 0.84.$

For level 3/variable X_{211} T becomes $0.42 + \varsigma(3) = 0$ so $\eta^0(2,1)$ and $\eta^0(2,1)$ are not updated. At this point the expected counts for the two rules can be computed:

$\mathbf{E}[c_{110}] = 0 + 0.336/0.588 = 0.5714285714$

$\mathbf{E}[c_{111}] = 0 + 0.84/0.588 = 1.4285714286$

$\mathbf{E}[c_{120}] = 0$

$\mathbf{E}[c_{121}] = 0$

$\mathbf{E}[c_{210}] = 0 + 0/0.588 = 0$

$\mathbf{E}[c_{211}] = 0 + 0.588/0.588 = 1.$

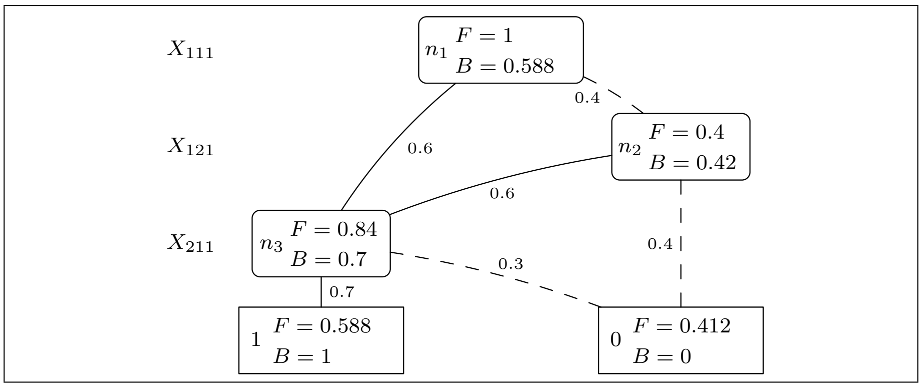


Figure 10.1: Forward and Backward probabilities for Example 3. F indicates the Forward probability and B the Backward probability of each node n.

Maximization Step

In the Maximization phase (see Algorithm 6), the π_{ik} parameters are computed for all rules C_i and $k = 1, \ldots, n_i - 1$ as

$$\pi_{ik} = \frac{\mathbf{E}[c_{ik1}]}{\mathbf{E}[c_{ik0}] + \mathbf{E}[c_{ik1}]}$$

for the next EM iteration.

Algorithm 6 Procedure Maximization

```
1: procedure MAXIMIZATION
2:     for all $i \in Rules$ do
3:         for $k = 1$ to $n_i - 1$ do
4:             $\pi_{ik} = \frac{\mathbf{E}[c_{ik1}]}{\mathbf{E}[c_{ik0}]+\mathbf{E}[c_{ik1}]}$
5:         end for
6:     end for
7: end procedure
```

10.3 Related Work

Binary Decision Diagrams

The use of Binary Decision Diagrams for probabilistic logic programming inference is related to their use for performing inference in Bayesian Networks. (Minato et al., 2007) presented a method for compiling BNs into exponentially-sized Multi-Linear Functions using a compact Zero-suppressed BDD representation. (Ishihata et al., 2011) compiled a BN with multiple evidence sets into a single Shared BDD, which shares common sub-graphs in multiple BDDs. (Darwiche, 2004) described an algorithm for compiling propositional formulas in conjunctive normal form into Deterministic Decomposable Negation Normal Form (d-DNNF) - a tractable logical form for model counting in polynomial time - with techniques from the Ordered BDD literature.

(Ishihata et al., 2008a,b) proposed an EM algorithm for learning the parameters of Boolean random variables given observations of a Boolean function over them, represented by a BDD. `EMBLEM` is an application of that algorithm to probabilistic logic programs. (Inoue et al., 2009) applies the algorithm of (Ishihata et al., 2008a,b) to the problem of computing the probabilistic parameters of abductive explanations.

Parameter Learning in Probabilistic Logic Languages

The approaches for learning probabilistic logic programs can be classified into three categories: those that employ *constraint techniques*, those that use *EM* and those that adopt *gradient descent*.

In the first class, (Riguzzi, 2004, 2007a, 2008) learn a subclass of ground programs by first finding a large set of clauses satisfying certain constraints and then applying mixed integer linear programming to identify a subset of the clauses that form a solution.

The following works fall into the second category.
(Thon et al., 2008) proposed an EM algorithm which computes expectations over decision diagrams; it learns parameters for the CPT-L language, a simple probabilistic logic language for describing sequences of relational states, that is less expressive than LPADs.

In (Koller and Pfeffer, 1997) the authors start out with a knowledge base consisting of partially specified first-order probabilistic logic rules with probabilistic parameters unknown; given a set of data cases they use a standard KBMC (Knowledge-Based Model Construction) algorithm to generate the network structure for each case. The conditional probability tables in the resulting networks are related to the parameters corresponding to the rules in the knowledge base. They use an extension to the standard EM algorithm for learning the parameters of these belief networks with fixed structure and hidden variables.

PRISM is a probabilistic logic (Sato, 1995; Sato and Kameya, 2001) introduced to improve the efficiency of the inference procedure under the distribution semantics, by imposing restrictions on the language. The same philosophy was followed by Probabilistic Horn Abduction (PHA) (Poole, 1993) and the Independent Choice Logic (ICL) (Poole, 1997). The key assumption is that the explanations for a goal are mutually exclusive, which overcomes the disjoint-sum problem. If the different explanations of a fact do not overlap, then its probability is simply the sum of the probabilities of its explanations.
In addition, PHA, ICL and PRISM employ disjoint statements of the form
$disjoint(p_1 : a_1; \ldots ; p_n : a_n)$, where the a_i are atoms for a particular predicate, and the p_i probability values that sum up to 1. For instance, the statement

$$disjoint(0.3 : gene(P, a); 0.15 : gene(P, b); 0.55 : gene(P, o)) \leftarrow$$

states that 1) the probabilities that (an instance) of the corresponding fact for $gene$ is true, and 2) an atom of the form $gene(P, X)$ instantiates to exactly one of these options.

The `PRISM` system is one of the first learning algorithms based on EM: it exploits logic programming techniques for computing expectations.

Causal Probabilistic Logic ($\mathbf{CP-logic}$) (Vennekens et al., 2009) is a probabilistic modeling language that is especially designed for representing causal relations. A CP-theory is a set of CP-events or rules of the same form of LPADs, hence these two languages are syntactically equivalent but define their semantics quite differently. (Blockeel and Meert, 2007; Meert et al., 2007, 2008) proposed to use the EM algorithm to induce parameters of ground CP-Logic theories, which works on the underlying Bayesian network.

Relational Information Bottleneck ($\mathbf{RIB}$) (Riguzzi and Di Mauro, 2012) is an algorithm that learns the parameters of SRL languages reducible to Bayesian Networks. In particular, it is presented by the authors the specialization of `RIB` to LPADs, so this system will be compared to `EMBLEM` in the next Section relative to experiments. Since the resulting network involve hidden variables, the use of techniques for learning from incomplete data such as the Expectation Maximization algorithm is required. RIB has shown good performances especially when some logical atoms are unobserved and is particularly suitable when learning from interpretations that share the same Herbrand base.

$\mathbf{CEM}$ is an implementation of EM based on the `cplint` inference library (Riguzzi, 2007b, 2009); this library allows to compute the probability of LPADs and CP-logic queries by using BDDs, when the program in one of these languages is acyclic. This system will be compared to `EMBLEM` in the next experimental Section.

$\mathbf{ProbLog}$ is a probabilistic extension of Prolog where some probabilistic facts f are labeled with a probability value. This value indicates the degree of belief, that is the probability that any ground instance $f\theta$ of f is true. It is also assumed that the $f\theta$ are marginally independent. The probabilistic facts are then augmented with a set of definite clauses defining further predicates (which should be disjoint from the probabilistic ones). An example is the program:

$0.9 : edge(a, c).$
$0.6 : edge(d, c).$
$0.9 : edge(d, b).$
$0.7 : edge(c, b).$
$path(X, Y) \leftarrow edge(X, Y).$
$path(X, Y) \leftarrow edge(X, Z), path(Z, Y).$

which specifies, with the first probabilistic fact, that with probability 0.9 there is an edge from a to c.

(Gutmann et al., 2011) presented the `LFI-ProbLog` algorithm that performs EM for learning the parameters of a ProbLog program. `EMBLEM` differs from this work in the construction of BDDs: while they build a BDD for an interpretation we focus on a target predicate, the one for which we want to obtain good predictions, and we build BDDs starting from atoms for the target predicate. Moreover, while we compute the contributions of deleted paths with the ς table, `LFI-ProbLog` treats missing nodes as if they were there and updates the counts accordingly. This system will be compared with `EMBLEM` in the next experimental Section.

Among the works that use a gradient descent technique, **LeProbLog** (Gutmann et al., 2010a, 2008) is a system developed again for ProbLog language. It starts from a set of queries annotated with a probability and from a ProbLog program. It tries to find the values of the parameters of the program that minimize the mean squared error of the probabilities of the queries. `LeProbLog` uses the Binary Decision Diagrams that represent the queries to compute the gradient.

Markov Logic Networks A different approach is taken by **Markov Logic** (Richardson and Domingos, 2006), that combines first-order logic with Markov networks. The idea is to view logical formulae as soft constraints on the possible worlds. The more formulae a world satisfies, the more likely it becomes. In a Markov logic network (MLN), this is realized by associating a weight with each formula that reflects how strong the constraint is, for example:

$1.5 : cancer(P) \leftarrow smoking(P)$
$1.1 : smoking(X) \leftarrow friends(X, Y), smoking(Y)$
$1.1 : smoking(Y) \leftarrow friends(X, Y), smoking(X)$

The first clause states the soft constraint that smoking causes cancer. So, interpretations in which persons that smoke have cancer are more likely than those where they do not (under the assumptions that other properties remain constant). Note that, with respect to all previous probabilistic languages, Markov Logic attaches to formulae *weights*, which are not probabilities but reflect how a world is probable depending on the number of formulae that it violates. For MLNs, `Alchemy` is a state-of-the-art system that offers various tools for inference, weight learning and structure learning of MLNs. (Lowd and Domingos, 2007) discusses how to perform weight learning by applying gradient descent of the conditional likelihood of queries for target predicates. This system will be compared with `EMBLEM` in the next experimental Section.

10.4 Experiments

The experiments are directed at verifying:

- the quality of the estimated parameters
- the algorithm performance in comparison with other state of the art SRL systems.

In the following a description of the datasets and performance evaluation metrics used is provided.

Datasets

The Internet Movie DataBase (Mihalkova and Mooney, 2007)[1] contains five mega-examples, each of which describes four movies, their directors, and the first-billed actors who appear in them. Each director is ascribed genres based on the genres of the movies he or she directed. The ‘gender’ predicate is used to state the genders of actors.

Cora (McCallum et al., 2000) is a collection of 1295 different citations to 112 computer science research papers from the Cora Computer Science Research Paper Engine. We used the version of the dataset of (Singla and Domingos, 2005)[2]. For each citation we know the title, authors, venue and the words that appear in it. The dataset encodes a problem of information integration from multiple sources and in particular an entity resolution problem: citations of the same paper often appear differently and the task is to determine which citations are referring to the same paper. The database is composed of five mega-examples and contains facts for the predicates `samebib(Citation1, Citation2)`, `sameauthor(Author1, Author2)`, `sametitle(Title1, Title2)`, `samevenue(Venue1, Venue2)` and `haswordauthor(Author, Word)`, `haswordtitle(Title, Word)`, `haswordvenue(Venue, Word)`.

UW-CSE (Richardson and Domingos, 2006)[3] records information about the Department of Computer Science and Engineering at the University of Washington; the domain is described through 10 types, that include: publication, person, course, project, academic quarter, etc. Instead, predicates include: `professor(Person)`, `student(Person)`, `area(X, Area)` (with `X` ranging over publications, persons, courses and projects), `publication(Title, Person)`,

[1]Available at `http://alchemy.cs.washington.edu/data/imdb`.
[2]Available at `http://alchemy.cs.washington.edu/data/cora`.
[3]Available at `http://alchemy.cs.washington.edu/data/uw-cse`.

`advisedBy(Person, Person)`, `yearsInProgram(Person, Years)`, `courseLevel(Course, Level)`, `taughtBy(Course, Person, Quarter)`, etc. Additionally, there are some equality predicates: `samePerson(Person, Person)`, `sameCourse(Course, Course)`, etc. which always have known, fixed values that are true iff the two arguments are the same constant. Here the problem is one of link prediction, as we wish to infer the truth of `advisedBy(Person, Person)`. The database is split into five mega--examples, each with data for a particular departmental area (AI, graphics, programming languages, systems and theory).

WebKB (Craven and Slattery, 2001)[1] consists of labeled web pages from the Computer Science departments of four universities, along with the words on the web pages and the links among them. We used the same set of training examples of (Craven and Slattery, 2001) which differs from the one used in (Gutmann et al., 2011; Lowd and Domingos, 2007). The dataset is split into four mega-examples, one for each university. Each web page is labeled with some subset of the following categories: student, faculty, research project and course. This dataset may be seen as a text classification problem, since we wish to infer the page's class given the information about words and links.

MovieLens (Herlocker et al., 1999) contains information about movies, users and ratings that users expressed about movies. We used the version of the dataset of (Khosravi et al., 2010)[2]. For each movie the dataset records the genres to which it belongs, by means of predicates of the form `<genre>(Movie, <gen_value>)`, where < `genre` > can be either `drama`, `action` or `horror` and `gen_value` is either `<genre>_0`, if the movie does not belong to the genre, or `<genre>_1`, if the movie belongs to the genre. Users' age, gender and occupation are recorded. Ratings from users on the movies range from 1 to 5. This dataset can be used to build a recommender system, i.e. a system that suggests items of interest to users based on their previous preferences, the preferences of other users, and attributes of users and items. We split the dataset into five mega-examples.

Mutagenesis (Srinivasan et al., 1996) contains information about a number of aromatic and heteroaromatic nitro drugs, including their chemical structures in terms of atoms, bonds and a number of molecular substructures such as six and five membered rings, benzenes, phenantrenes and others. The problem here is to predict the mutagenicity of the drugs. The

[1]Available at `http://alchemy.cs.washington.edu/data/webkb`.

[2]Available at `http://www.cs.sfu.ca/~oschulte/jbn/dataset.html`.

prediction of mutagenesis is important as it is relevant to the understanding and prediction of carcinogenesis, and not all compounds can be empirically tested for mutagenesis, e.g. antibiotics. Of the compounds, those having positive levels of log mutagenicity are labeled "active" and constitute the positive examples, the remaining ones are "inactive" and constitute the negative examples. The data is split into two subsets (188+42 examples). We considered the first one, composed of 125 positive and 63 negative compounds. We split the dataset into ten mega-examples.

Estimating Classifier Performance

The recommended procedure for evaluating a Machine Learning algorithm considers:

1. Use of *k-fold* cross-validation (k=5 or 10) for computing performance estimates;
2. Report of mean values of performance estimates with their standard deviations and 95% confidence intervals.

1. Use of k-fold cross-validation for computing performance estimates Given a model with unknown parameters and a data set which the model has to fit (the training data set), the fitting process optimizes the model parameters to make the model fit the training data as well as possible. If we then take an independent sample of validation data from the same population as the training data, it will generally turn out that the model does not fit the validation data as well as it fits the training data. This is called *overfitting*, and is particularly likely to happen when the size of the training data set is small, or when the number of parameters in the model is large. *Cross-validation* is a way to predict the fitting of a model to a hypothetical validation set when an explicit validation set is not available. One round of cross-validation involves partitioning the data set into complementary subsets, performing the analysis on one subset (called the training set), and validating the analysis on the other subset (called the validation set or testing set). To reduce variability, multiple rounds of cross-validation are performed using different partitions, and the validation results are averaged over the rounds to produce a single estimation. K-fold cross-validation needs to get *k* training/validation set pairs as follows: the dataset is randomly divided into k parts. To get each pair, k-1 parts are combined to form the training set and the remaining part is the validation set. This is done k times where for each pair, another of the k parts is left out as the validation set. The advantage of this method over repeated random sub-sampling is that all observations are used for both training and validation, and each observation is used for validation exactly once. 10-fold cross-validation is commonly used.

2. Report mean values of performance estimates with their standard deviations and 95% confidence intervals

- *Performance estimates.* In recent years *Receiver Operating Characteristics (ROC)* graphs and *Precision Recall (PR)* graphs have been increasingly adopted in the machine learning and data mining research communities, to visualize classifiers performance. In particular, the *Area Under the Curve* (AUC) for both the PR curve (AUCPR) and the ROC curve (AUCROC) are computed to numerically compare performances.

  The use of these graphs is widespread when evaluating algorithms that output probabilities of binary *class membership* values. In our case, the class is given by the target predicate(s) chosen for each dataset: for instance, for the Cora dataset, the predicate `samebib(citation1,citation2)` discriminates ground examples among those representing the same citation (positive instances) and those representing different ones.

  ROC graphs are two-dimensional graphs in which *True Positive (TP) rate* (also called *recall*) is plotted on the Y axis and *False Positive (FP) rate* is plotted on the X axis. These rates of a classifier are estimated as:

$$tp\, rate = \frac{Positives\ correctly\ classified}{Total\ positives}$$
$$fp\, rate = \frac{Negatives\ incorrectly\ classified}{Total\ negatives}$$

  A ROC graph depicts relative trade-offs between benefits (true positives) and costs (false positives). The AUCROC is equal to the probability that a classifier will rank a randomly chosen positive instance higher than a randomly chosen negative one. *Given two classifiers and their AUCROC, the one with the greater area has better average performance.*

  The parameter learning algorithms are probabilistic classifiers that output a probability that each *test set example is positive*: we can next sort this list in ascending order to rank the examples from the least positive ones (which are more likely to belong to the negative class) to the most positive ones (which are more likely to belong to the positive class). These probabilities give an indication of how likely it is that the positive class label applies. Such probability estimators are used with a threshold on the output probabilities to produce a discrete binary classifier: if their output is above the threshold a Yes is returned, else a No is returned, and each threshold value produces a different point in ROC space. One may imagine varying a threshold from 0 to 1 and tracing a curve through ROC space. Each point in the space represents a specific classifier, with a threshold for calling an example positive: this means that we have obtained a set of discrete classifiers.

When dealing with highly skewed datasets, Precision-Recall (**PR**) **curves** have been found to give a more informative picture of an algorithm's performance: when the number of negative examples greatly exceeds the number of positives examples, a large change in the number of false positives can lead to a small change in the false positive rate used in ROC analysis. In PR space one plots Recall on the X axis and Precision on the Y axis. *Precision* - defined as $\frac{Positives\ correctly\ classified}{True\ and\ false\ positives}$ - by comparing false positives to true positives rather than true negatives, mitigates the effect of the large number of negative examples on the algorithm's performance. Given two algorithms with comparable area in ROC space, in PR space one of them can show a clear advantage over the other by having a larger area.

- *95% Confidence Intervals*. They are a common way to describe the uncertainy associated with an estimate. In this context it is utilized in relation to a *paired two-tailed t-test*.

  A paired **t-test** is used to compare two population means, where there are two samples in which observations in one sample can be *paired* with observations in the other sample. Examples of where this might occur are: (1) before-and-after observations on the same subjects; (2) a comparison of two different methods of measurement or two different treatments where the measurements are applied to the same subjects. The experiments belong to case (2), where a comparison of different SRL algorithms over the same data sets is performed: the variations in AUCROC and AUCPR of `EMBLEM` compared to the other systems are computed and differences are reported as significant if a *two-tailed*, paired t-test produces a *p-value* less than 0.05.

  The *null hypothesis is the statement that we want to test*, stating, in general, that things are the same as each other, i.e., the two evaluated methods are equivalent. One has to take into account that almost certainly some difference in the means, *just due to chance*, may appear. So we need to consider "what's the probability of getting a difference in the means of a certain value, just by chance, if the null hypothesis is really true". Only when that probability is low we can reject the null hypothesis that the two methods (algorithms) are equivalent. The goal of statistical hypothesis testing is to estimate the probability of getting the observed results under the null hypothesis.

Given the pairs $i = 1, ..., k$ from k-fold validation, two classifiers are trained on the training set and are tested on the validation set, and their errors are recorded as x_i, y_i, where x, y indicate the two classifiers. The difference is $d_i = y_i - x_i$; when this is done *k* times we have a distribution of d_i containing *k* points. For large samples the corresponding error estimates follow the Normal distribution, and their difference d_i is also Normal. The null hypothesis is equivalent to say that this distribution has zero mean: $H_0 : \mu = 0$, while the alternative hypothesis is $H_1 : \mu \neq 0$.

To test the null hypothesis that the mean difference is zero (i.e. the two classifiers have the same error rate and so are equivalent), the complete procedure is as follows:

- Compute the difference (d_i) between the two observations in each pair;
- Compute the mean difference, $\bar{d}$;
- Compute the standard deviation of the differences, s_d, and use this to calculate the standard error of the mean difference, $SE(\bar{d}) = \frac{s_d}{\sqrt{k}}$;
- Compute the t-statistic $T = \bar{d}/SE(\bar{d})$; under the null hypothesis that $\mu = 0$, this statistic follows a t-distribution with $k - 1$ degrees of freedom;
- Use tables of the t-distribution to compare the value of T to the $t_{\alpha,k-1}$ distribution and rejects the null hypothesis if $|T| > t_{\alpha,k-1}$, with α significance level (see below). The value of α such that $|T| = t_{\alpha,k-1}$ is the *p-value* for the paired t-test, defined as the probability of accepting that the null hypothesis is true. The t-test has been applied in the experiments to the differences in AUCROC and AUCPR, i.e, the x_i/y_i values correspond to the area values computed for each fold i and for each algorithm.

So for example $p = 0.03$ is a shorthand way of saying "The probability of accepting the null hypothesis that the two methods are equivalent, is 0.03; the probability that a method, not by chance, performs better than the other one, is $1 - p$". A convention in most research is used which sets a significance level α of 0.05. This means that if the probability value p is less than α, the null hypothesis is rejected and an algorithm is better than another one; such results are referred to as 'statistically significant'. If p is greater than or equal to α, the null hypothesis is accepted. In some situations it is convenient to express the statistical significance as $1 - \alpha$:

this value is called the test confidence, since statistical significance can be considered to be the confidence one has in a given result. A *95% confidence interval* for the true mean difference is an interval of values that is expected with probability 95% to contain the true difference (where the true mean difference is likely to lie). Smaller levels of α increase confidence in the determination of significance, but run an increased risk of failing to reject a false null hypothesis (false negative determination), and so have less statistical power. Statistical significance is a statistical assessment of whether the observations reflect a pattern rather than just chance, since any given hypothesis is subject to *random* error. A result is deemed statistically significant if it is so extreme (without external variables which would influence the correlation results of the test) that such a result would be expected to arise simply by chance only in rare circumstances. Hence the result provides enough evidence to reject the hypothesis of 'no effect'.

Finally, the test is named after the *tail* of data under the far left and far right of a bell-shaped Normal data distribution, or bell curve. However, the terminology is extended to tests relating to distributions other than Normal. In general a test is called two-tailed if the null hypothesis is rejected for values of the test statistic falling into either tail of its sampling distribution, and it is called one-sided or one-tailed if the null hypothesis is rejected only for values of the test statistic falling into one specified tail of its sampling distribution. For example, if the alternative hypothesis is $\mu \neq \mu_0$, the null hypothesis of $\mu = \mu_0$ is rejected for small or for large values of the sample mean, the test is called two-tailed or two-sided. If the alternative hypothesis is $\mu > \mu_0$, the null hypothesis of $\mu \leq \mu_0$ is rejected only for large values of the sample mean and the test is called one-tailed or one-sided. If a 5% significance level is used, both tests have a region of rejection, 0.05, however, in the two-tailed case the rejection region must be split between both tails of the distribution - 0.025 in the upper tail and 0.025 in the lower tail - because the hypothesis specifies only a difference, not a direction.

Methodology

EMBLEM is implemented in Yap Prolog[1] and is compared with

- a few systems for parameter learning of Probabilistic Logic Programs:
  - RIB (Riguzzi and Di Mauro, 2012)
  - CEM (Riguzzi, 2007b, 2009)

[1]http://www.dcc.fc.up.pt/~vsc/Yap/

- `LeProbLog` (Gutmann et al., 2010a, 2008)
- `LFI-ProbLog` (Gutmann et al., 2010b, 2011)

- one system for parameter learning of Markov Logic Networks (MLNs):
  - `Alchemy` (Richardson and Domingos, 2006)

All experiments were performed on Linux machines with an Intel Core 2 Duo E6550 (2333 MHz) processor and 4 GB of RAM.

To compare the results with `LeProblog`, the translation of LPADs into ProbLog proposed in (De Raedt et al., 2008a) is exploited, in which a disjunctive clause with k head atoms and vector of variables $\vec{X}$ is modeled with k ProbLog clauses and $k-1$ probabilistic facts with variables $\vec{X}$.

To compare the results with `Alchemy`, the translation between LPADs and MLN of (Riguzzi and Di Mauro, 2012) is exploited, inspired by the translation between ProbLog and MLNs proposed in (Gutmann et al., 2010a). An MLN clause is translated into an LPAD clause in which the head atoms of the LPAD clause are the *null* atom plus the positive literals of the MLN clause while the body atoms are the negative literals.

For the Probabilistic Logic Programming systems we consider various *options*:

1. The first consists in choosing between associating a distinct random variable to each grounding of a probabilistic clause or a single random variable to a non-ground probabilistic clause expressing whether the clause is used or not. The latter case makes the problem easier. All experiments have been run first with the most difficult setting (a single random variable for each grounding) and have been re-run with the second easy setting only if `EMBLEM` failed to terminate under the first one.

2. The second option allows to set a limit on the depth of derivations as done in (Gutmann et al., 2010a), thus eliminating explanations associated to derivations exceeding the depth limit. This is necessary for problems that contain cyclic clauses, such as transitive closure clauses.

3. The third option allows to set the number of restarts for EM based algorithms. `EMBLEM` has been run with a number of restarts chosen to match its execution time with that of the fastest other algorithm.

All experiments except one (see below) for the Probabilistic Logic Programming systems have been performed using open-world predicates, meaning that, when resolving a literal for a target predicate, both facts in the database and rules are used to prove it. All experiments use the same value of the thresholds ϵ and δ for stopping the EM cycle.

The parameter settings for the PLP systems on the domains can be found in Table 10.2.

The datasets are divided into four, five or ten mega-examples, where each mega-example contains a connected group of facts and individual mega-examples are independent of each other. A *k-fold* ($k = 4, 5, 10$) cross-validation approach is adopted. The terms "fold" and "mega-example" will be used interchangeably in the following. Statistics on the domains are reported in Table 10.1. The number of negative testing examples is sometimes different from that of negative training examples because, while in training we explicitly provide negative examples, in testing we consider as negatives all the ground instantiations of the target predicates that are not positive.

As part of the test, Precision-Recall and Receiver Operating Characteristics curves are drawn using the methods reported in (Fawcett, 2006) and (Davis and Goadrich, 2006), the Area Under the Curve (AUCPR and AUCROC) is computed and, finally, average values on the k folds are reported in Tables 10.3 and 10.4. Table 10.5 shows the learning times in hours.

Tables 10.6 and 10.7 show the p-value of a paired two-tailed t-test at the 5% significance level of the difference in AUCPR and AUCROC between EMBLEM and the other systems on all datasets (significant differences in favor of EMBLEM in bold).

IMDB Four different LPADs are used, two for predicting the target predicate sameperson(Person1, Person2), and two for predicting samemovie(Movie1, Movie2), on the basis of the relations among actors, their movies and their directors. There is one positive example for each fact that is true in the data, while we sampled from the complete set of false facts three times the number of true facts in order to generate negative examples.

1. For predicting sameperson/2 this LPAD is used:

```
sameperson(X,Y):p:- movie(M,X),movie(M,Y).
sameperson(X,Y):p:- actor(X),actor(Y),workedunder(X,Z),
                    workedunder(Y,Z).
sameperson(X,Y):p:- gender(X,Z),gender(Y,Z).
sameperson(X,Y):p:- director(X),director(Y),genre(X,Z),genre(Y,Z).
```

Table 10.1: Characteristics of the datasets used with `EMBLEM`: target predicates, number of constants, of predicates, of tuples (ground atoms), of positive and negative training and testing examples for target predicate(s), of folds. The number of tuples includes the target positive examples.

Dataset	Target Predicate(s)	Const	Preds	Tuples	Pos.Ex.	Training Neg.Ex.	Testing Neg.Ex.	Folds
IMDB	sameperson(X,Y)(SP) samemovie(X,Y)(SM)	316	10	1540	SP:268 SM:20	SP:804 SM:60	SP:14350 SM:60	5
Cora	samebib(X,Y) sameauthor(X,Y) samevenue(X,Y) sametitle(X,Y)	3079	10	378589	63262	27764	304748	5
UW-CSE	advisedBy(X,Y)	1323	15	2673	113	4079	16601	5
WebKB	<course,faculty, researchProject, student>Page(P)	4942	8	290973	1039	15629	16249	4
Movielens	rating(U,M,R)	2627	7	169124	129779	50000	50000	5
Mutagenesis	active(D)	7045	20	15249	125	63	63	10

where p is a placeholder indicating a tunable parameter to be learned by `EMBLEM`. These rules state that two persons are the same if they appear in the same movie, or they worked under the same director, or they have the same gender, or they direct movies of the same genre.

For `LeProblog`, the queries given as input are obtained by annotating with 1.0 each positive example and with 0.0 each negative example, those given as input to `LFI-ProbLog` by annotating with *true* each positive example and with *false* each negative example. *The same procedure has been adopted in all experiments*. `LeProblog` and `LFI-ProbLog` have been run for a maximum of 100 iterations or until the difference in Mean Squared Error (MSE) (for `LeProblog`) or log likelihood (for `LFI-ProbLog`) between two iterations got smaller than 10^{-5}. Except where otherwise noted, these parameters are used in all experiments.

For `Alchemy`, it is applied the preconditioned rescaled conjugate gradient discriminative algorithm (Lowd and Domingos, 2007) *on every dataset*. Here `sameperson/2` is the only *non-evidence* predicate.

A second LPAD, taken from (Riguzzi and Di Mauro, 2012), has been created to evaluate

Table 10.2: Parameter settings for the experiments with `EMBLEM`, `RIB`, `CEM`, `LeProbLog` `LFI-ProbLog`. NR indicates the number of restarts only for `EMBLEM`, NI indicates the maximum number of iterations only for `LFI-ProbLog`.

.

Dataset	NI(LFI-ProbLog)	NR(EMBLEM)	LPAD cyclicity	depth D	semantics
IMDB-SP	100	500	no	no	standard
IMDBu-SP	100	40	no	no	standard
IMDB-SM	100	1	no	no	standard
IMDBu-SM	100	1	no	no	standard
CORA	10	120	no	no	standard
CORAT	10	1	yes	2	simplified
UW-CSE	100	1	yes	2	simplified
WebKB	10	1	yes	no(close-world)	standard
Movielens	100	1	yes	2	simplified
Mutagenesis	100	1	no	no	standard

the algorithms' performance when some atoms are *unseen*:

```
sameperson_pos(X,Y):p:- movie(M,X),movie(M,Y).
sameperson_pos(X,Y):p:- actor(X),actor(Y),workedunder(X,Z),
                        workedunder(Y,Z).
sameperson_pos(X,Y):p:- director(X),director(Y),genre(X,Z),genre(Y,Z).
sameperson_neg(X,Y):p:- movie(M,X),movie(M,Y).
sameperson_neg(X,Y):p:- actor(X),actor(Y),workedunder(X,Z),
                        workedunder(Y,Z).
sameperson_neg(X,Y):p:- director(X),director(Y),genre(X,Z),genre(Y,Z).
sameperson(X,Y):p:- \+sameperson_pos(X,Y),sameperson_neg(X,Y).
sameperson(X,Y):p:- \+sameperson_pos(X,Y),\+sameperson_neg(X,Y).
sameperson(X,Y):p:- sameperson_pos(X,Y),sameperson_neg(X,Y).
sameperson(X,Y):p:- sameperson_pos(X,Y),\+sameperson_neg(X,Y).
```

The `sameperson_pos`/2 and `sameperson_neg`/2 predicates are unseen in the data.

`Alchemy` has been run with the `−withEM` option that turns on EM learning. The other parameters for all systems are set as before.

Results are shown respectively in the *IMDB-SP* and *IMDBu-SP* rows of tables 10.3, 10.4, 10.5. Learning time matches `CEM` time, the fastest system among the others.

2. For predicting `samemovie`/2 this LPAD is used:

```
samemovie(X,Y):p:- movie(X,M),movie(Y,M),actor(M).
samemovie(X,Y):p:- movie(X,M),movie(Y,M),director(M).
samemovie(X,Y):p:- movie(X,A),movie(Y,B),actor(A),director(B),
                   workedunder(A,B).
samemovie(X,Y):p:- movie(X,A),movie(Y,B),director(A),director(B),
                   genre(A,G),genre(B,G).
```

To test the behavior when unseen predicates are present, the program for `samemovie/2` is transformed as for `sameperson/2`, thus introducing the unseen predicates `samemovie_pos/2` and `samemovie_neg/2`. The systems have been run with the same settings as IMDB-SP and IMDBu-SP, replacing `sameperson/2` with `samemovie/2`. Results are shown respectively in the *IMDB-SM* and *IMDBu-SM* rows of tables 10.3, 10.4, 10.5. `RIB` and `LFI-Problog` in this case give a memory error (indicated with “me”), due to the exhaustion of the available stack space during the execution of the algorithm.

Cora The Cora database contains citations to computer science research papers, and the task is to determine which citations are referring to the same paper, by predicting the predicate `samebib(Citation1, Citation2)`.

From the MLN proposed in (Singla and Domingos, 2006)[1] two LPADs have been obtained. The MLN contains 26 clauses stating regularities like: if two citations are the same, their authors, venues, etc., are the same, and vice-versa; if two fields of the same type have many words in common, they are the same.

The first LPAD contains 559 rules and differs from the direct translation of the MLN because rules involving words are instantiated with the different constants, only positive literals for the `hasword` predicates are used and transitive rules are not included:

```
samebib(B,C):p:- author(B,D),author(C,E),sameauthor(D,E).
samebib(B,C):p:- title(B,D),title(C,E),sametitle(D,E).
samebib(B,C):p:- venue(B,D),venue(C,E),samevenue(D,E).
samevenue(B,C):p:- haswordvenue(B,word_06), haswordvenue(C,word_06).
...
sametitle(B,C):p:- haswordtitle(B,word_10), haswordtitle(C,word_10).
....
sameauthor(B,C):p:- haswordauthor(B,word_a), haswordauthor(C,word_a).
.....
```

The dots stand for the rules for all the possible words. Positive and negative examples for the four target predicates are already available in the version of the dataset.

[1]Available at `http://alchemy.cs.washington.edu/mlns/er`.

In this case LFI-ProbLog has been run for a maximum of only 10 iterations (or until the difference in MSE between two iterations got smaller than 10^{-5}) due to its long learning time.

The second LPAD adds to the previous one the transitive rules for the predicates samebib/2, samevenue/2, sametitle/2 and sameauthor/2:

```
samebib(A,B):p:- samebib(A,C), samebib(C,B).
sameauthor(A,B):p:- sameauthor(A,C), sameauthor(C,B).
sametitle(A,B):p:- sametitle(A,C), sametitle(C,B).
samevenue(A,B):p:- samevenue(A,C), samevenue(C,B).
```

for a total of 563 rules. In this case stricter settings are imposed for EMBLEM, LeProbLog, CEM and LFI-ProbLog, since the theory is cyclic (cf. table 10.2).

For LeProbLog, the four predicates are separately learned because learning the whole theory at once gives a lack of memory error. This is equivalent to using a closed-world setting. For Alchemy, the four predicates are specified as non-evidence.

Results are shown respectively in the *Cora* and *CoraT* (Cora Transitive) rows of Tables 10.3, 10.4, 10.5. On CoraT Alchemy, CEM and LFI-ProbLog give a memory error, for a segmentation fault the first one (by the learnwts command) and for memory exhaustion the others, while RIB is not applicable because it is not possible to split the input examples into smaller independent interpretations as required by it.

UW-CSE The interest in this dataset has emerged in the context of social network analysis, where one seeks to reason about a group of people: in particular *link prediction* tackles the problem of predicting relationships from people's attributes, and UW-CSE represents a benchmark in that direction if we try to predict which professors advise which graduate students. Hence, the target predicate is advisedBy(Person1, Person2).

The theory used has been obtained from the MLN of (Singla and Domingos, 2005)[1] and contains 86 rules, such as (S stands for $student$ and P for $professor$):

```
advisedby(S,P):p:- courselevel(C,level_500), taughtby(C,P,Q), ta(C,S,Q).
advisedBy(S,P):p:- publication(Pub,S), publication(Pub,P), student(S).
student(S):p:- advisedBy(S,P).
```

[1]Available at http://alchemy.cs.washington.edu/mlns/uw-cse.

As one can see from this example, the theory is cyclic. The negative examples have been generated by considering all couple of persons `(a,b)` where `a` and `b` appear in an `advisedby/2` fact in the data and by adding a negative example `advisedBy(a,b)` if it is not in the data.

For `Alchemy`, `advisedBy/2` is the only non-evidence predicate. `RIB` and `LFI-ProbLog` in this case exhaust the available memory.

WebKB The goal is to predict the four predicates `coursePage(Page)`, `facultyPage(Page)`, `studentPage(Page)` and `researchProjectPage(Page)`, representing the various possible pages' classes, for which the dataset contains both positive and negative examples.

The theory is obtained by translating the MLN of (Lowd and Domingos, 2007)[1] into an LPAD with 3112 rules. It contains a rule of the form

```
<class1>Page(Page1):p:- linkTo(Page2,Page1), <class2>Page(Page2).
```

for each couple of classes `(<class1>,<class2>)`, and rules of the form

```
<class>Page(Page):p:- has(<word>,Page).
```

for each possible page class and word. The first type of rule states that $Page1$ of class $class1$ is linked to $Page2$ of class $class2$ with probability p; the second type states that the page $Page$ of class $class$ contains the word $word$ with probability p. Examples of rules are:

```
coursePage(Page1):p:- linkTo(Page2,Page1),coursePage(Page2).
coursePage(Page):p:- has('abstract',Page).
```

As one can see from this example, the theory is cyclic. Running `EMBLEM` with a depth bound equal to the lowest value (two) and an open-world setting gives a lack of memory error, so a closed-world setting is needed for the target predicates in the body of clauses (target predicates are resolved only with facts in the database). `LeProbLog` and `LFI-ProbLog` have been run on a sample containing respectively 5% and 1% of the training set since the complete set leads to exceedingly long learning times, and in addition `LFI-ProbLog` has been run for a maximum of 10 iterations; despite that, it spends anyway a considerable time. For `Alchemy`, the four target predicates are specified as non-evidence predicates; we also set the flag $-$`noAddUnitClauses` to 1 (unit predicates are not added to the MLN) since otherwise inference would give a lack of memory error. `RIB` and `CEM` in this case terminate for lack of memory.

[1] Available at `http://alchemy.cs.washington.edu/mlns/webkb`.

MovieLens The target predicate is rating(User, Movie, Rating): we wish to predict the rating on a movie by a user. The LPAD contains 4 rules:

```
rating(A,B,R):p:- rating(A,C,R),B\==C,drama(B,drama_1),drama(C,drama_1).
rating(A,B,R):p:- rating(A,C,R),B\==C,action(B,action_1),action(C,action_1).
rating(A,B,R):p:- rating(A,C,R),B\==C,horror(B,horror_1),horror(C,horror_1).
rating(A,B,R):p:- rating(C,B,R),A\==C.
```

The first three rules state that a user A assigns the same rating R to two different movies B and C, if they belong to the same genre, either drama or action or horror, with probability p; the last one states that two different users equally rate the same movie with probability p.
In this case stricter settings are imposed for EMBLEM, LeProbLog, CEM and LFI-ProbLog, since the theory is cyclic (cf. table 10.2). For Alchemy, rating/3 is specified as non-evidence predicate.

RIB, CEM, Alchemy and LFI-ProbLog give a memory error.

Mutagenesis To predict the mutagenicity of the drugs, we remind that the compounds having positive levels of log mutagenicity are labeled "active", so the goal is to predict if a drug is active, i.e. the target predicate active(Drug).

The fundamental Prolog facts are bond(compound,atom1,atom2,bondtype) - stating that in *compound* a bond of type *bondtype* can be found between the atoms *atom1* and *atom2* - and atm(compound,atom,element,atomtype,charge), stating that *compound*'s *atom* is of element *element*, is of type *atomtype* and has partial charge *charge*. From these facts many elementary molecular substructures can be defined, and we used the tabulation of these, available in the dataset, rather than the clause definitions based on bond/4 and atm/5. This greatly sped up learning.

The theory has been obtained by running Aleph[1] on the database with a ten-fold cross-validation and choosing randomly one of the ten theories for parameter learning. The selected theory contains 17 rules, such as:

```
active(A):p:-  bond(A,B,C,2), bond(A,C,D,1), ring_size_5(A,E).
```

relating the activity of drug A to its atoms' bonds and its structure. Predicates representing molecular substructures use function symbols to represent lists of atoms, for example, in ring_size_5(Drug, Ring), Ring is a list of atoms composing a 5-membered ring in the drug's

[1]http://www.cs.ox.ac.uk/activities/machlearn/Aleph/aleph.html

structure. `Alchemy` is not applicable to this dataset because it does not handle function symbols.

Table 10.3: Results of the experiments on all datasets in terms of *Area Under the ROC Curve* averaged over the folds. *me* means memory error during learning; *no* means that the algorithm was not applicable.

Dataset	`EMBLEM`	`LeProbLog`	`Alchemy`	`RIB`	`CEM`	`LFI-ProbLog`
IMDB-SP	0.93	0.87	0.91	0.93	0.93	0.89
IMDBu-SP	0.90	0.92	0.50	0.90	0.89	0.50
IMDB-SM	1.00	0.98	0.93	me	0.71	me
IMDBu-SM	1.00	0.98	0.54	me	0.44	me
Cora	1.00	0.99	0.70	0.99	0.99	0.99
CoraT	0.999	0.998	me	no	me	me
UW-CSE	0.99	0.94	0.96	me	0.87	me
WebKB	0.85	0.51	0.88	me	me	0.55
MovieLens	0.84	0.77	me	me	me	me
Mutagenesis	0.99	0.98	no	0.90	0.92	0.89

Table 10.4: Results of the experiments on all datasets in terms of *Area Under the PR Curve* averaged over the folds. *me* means memory error during learning; *no* means that the algorithm was not applicable.

Dataset	`EMBLEM`	`LeProbLog`	`Alchemy`	`RIB`	`CEM`	`LFI-ProbLog`
IMDB-SP	0.20	0.1	0.11	0.19	0.20	0.14
IMDBu-SP	0.18	0.13	0.02	0.17	0.12	0.02
IMDB-SM	1.00	0.93	0.82	me	0.54	me
IMDBu-SM	1.00	0.93	0.34	me	0.56	me
Cora	0.995	0.91	0.47	0.94	0.995	0.996
CoraT	0.99	0.98	me	no	me	me
UW-CSE	0.75	0.28	0.29	me	0.64	me
WebKB	0.34	0.07	0.50	me	me	0.07
MovieLens	0.87	0.82	me	me	me	me
Mutagenesis	0.992	0.991	no	0.95	0.96	0.93

Overall remarks From the results we can observe that:

- on IMDB-SP `EMBLEM` has better performance than the other systems in both AUCPR and AUCROC (except for `CEM`/AUCPR), with six differences out of ten statistically

Table 10.5: *Execution time* in hours of the experiments, averaged over the folds.

Dataset	EMBLEM	LeProbLog	Alchemy	RIB	CEM	LFI-ProbLog
IMDB-SP	0.010	0.350	1.540	0.016	0.010	0.037
IMDBu-SP	0.010	0.230	1.540	0.0098	0.012	0.057
IMDB-SM	3.6e-4	0.005	0.003	-	0.005	-
IMDBu-SM	3.220	0.012	0.011	-	0.047	-
Cora	2.480	13.25	1.300	2.490	11.95	44.07
CoraT	0.380	5.670	-	-	-	-
UW-CSE	2.810	2.920	1.950	-	0.530	-
WebKB	0.048	0.114	0.052	-	-	11.32
MovieLens	0.070	20.01	-	-	-	-
Mutagenesis	2.49e-5	0.130	-	0.040	0.040	0.019

significant. Moreover, it takes less time than all other systems except `CEM`. On IMDBu-SP `EMBLEM` has the best performance except for `LeProbLog`/AUCROC, again with six significant differences.

- On IMDB-SM, `EMBLEM` reaches value 1 for PR and ROC areas with only one restart, in less time than the other systems, so in this case we did not execute it to match the learning time of another algorithm. Two out of six differences are significant; on IMDBu-SM, it still reaches the highest area but with the longest execution time associated with one restart, so it was not possible to match its time with the one of another system. One out of six differences are significant. `RIB` and `LFI-ProbLog` are not able to terminate on this dataset.

- On Cora, `EMBLEM` shows the best performance along with `CEM` and `LFI-ProbLog`, but in much less time, with four significant differences out of ten. On CoraT, it has comparable performance, but with a much lower learning time, than `LeProbLog` - the only other system able to complete learning on this more complex theory.

- On UW-CSE, it has better performance with respect to all the algorithms for AUCPR and AUCROC with five out of six differences significant. Again `RIB` and `LFI-ProbLog` are not able to terminate.

- On WebKB, `EMBLEM` shows significantly better areas with respect to `LeProbLog` and `LFI-ProbLog`, and worse areas with respect to `Alchemy`, with the differences being

Table 10.6: Results of *t-test* on all datasets, relative to AUCROC. p is the p-value of a paired two-tailed t-test between `EMBLEM` and the other systems (significant differences in favor of `EMBLEM` at the 5% level in bold). `E` is `EMBLEM`, `LeP` is `LeProbLog`, `A` is `Alchemy`, `C` is `CEM`, `LFI` is `LFI-ProbLog`.

Dataset	`E-LeP`	`E-A`	`E-R`	`E-C`	`E-LFI`
IMDB-SP	**0.001**	**0.015**	0.344	0.351	**0.006**
IMDBu-SP	0.140	**1e-5**	0.217	**0.002**	**5.3e-7**
IMDB-SM	0.374	0.256	-	**0.018**	-
IMDBu-SM	0.374	0.256	-	0.055	-
Cora	0.069	**0.033**	**0.049**	0.457	0.766
CoraT	0.131	-	-	-	-
UW-CSE	**0.028**	**0.005**	-	0.291	-
WebKB	**0.002**	0.171	-	-	**0.005**
MovieLens	**7.6e-7**	-	-	-	-
Mutagenesis	0.199	-	0.109	0.196	**5.4e-4**

statistically significant except one case. We remind that this dataset is one of the most problematic: it is the only one where `EMBLEM` has been run with a closed-world setting for the target predicates (simpler than an open-world setting, which failed in this case) and the size of the training set for `LeProbLog` and `LFI-ProbLog` has been reduced in order to contain the computation time.

- On MovieLens, `EMBLEM` achieves higher areas with respect to `LeProbLog` in a significantly lower time, with the differences statistically significant, while all the others systems are not able to complete.

- On Mutagenesis, `EMBLEM` shows better performance than all other systems, with the differences being statistically significant in three out of eight cases. Moreover, it is the fastest.

Looking at the overall results, `LeProbLog` seems to be the closest system to `EMBLEM` from the point of view of performances, being able to always complete learning as `EMBLEM`, but with longer times (except for two cases). On the contrary, `RIB` and `LFI-ProbLog` incurred in many difficulties in treating the datasets. `EMBLEM`'s AUCPR and AUCROC are higher or equal than those of the other systems except on IMDBu-SP, where `LeProbLog` achieves a non-statistically significant higher AUCROC, WebKB, where `Alchemy` achieves a non-statistically significant higher AUCROC and a statistically significant higher AUCPR, and Cora, where

Table 10.7: Results of *t-test* on all datasets, relative to AUCPR. p is the p-value of a paired two-tailed t-test between EMBLEM and the other systems (significant differences in favor of EMBLEM at the 5% level in bold). E is EMBLEM, LeP is LeProbLog, A is Alchemy, C is CEM, LFI is LFI-ProbLog.

Dataset	E-LeP	E-A	E-R	E-C	E-LFI
IMDB-SP	**0.013**	**0.013**	0.217	0.374	**0.004**
IMDBu-SP	0.199	**4.5e-5**	0.127	**0.001**	**5.5e-5**
IMDB-SM	0.374	0.179	-	**0.024**	-
IMDBu-SM	0.374	**2.2e-4**	-	0.278	-
Cora	0.073	**0.007**	**0.011**	1.000	0.681
CoraT	0.104	-	-	-	-
UW-CSE	**2.6e-4**	**4.9e-4**	-	**0.009**	-
WebKB	**0.018**	**0.001**	-	-	**0.016**
MovieLens	**8e-7**	-	-	-	-
Mutagenesis	0.16	-	**0.046**	0.097	**0.001**

LFI-ProbLog achieves a non-statistically significant higher AUCPR. Differences between EMBLEM and the other systems are statistically significant in favor of it in 34 out of 64 cases at the 5% significance level and in 21 out of 64 cases at the 1% significance level.

10.5 Conclusions

We have proposed a technique which applies a EM algorithm to BDDs for learning the parameters of Logic Programs with Annotated Disjunctions. The problem is, given an LPAD, to efficiently learn parameters for the disjunctive heads of the program clauses. The resulting algorithm EMBLEM returns the parameters that best describe the data and can be applied to all probabilistic logic languages that are based on the Distribution Semantics. EMBLEM exploits the BDDs that are built during inference to efficiently compute the expectations for the hidden variables.

We tested the algorithm over the real world datasets IMDB, Cora, UW-CSE, WebKB, MovieLens, Mutagenesis, and evaluated its performance through the AUCPR, the AUCROC, the learning times and the t-test for the statistical significance. Then we compared EMBLEM in terms of these metrics with other five parameter learning systems.

These results show that EMBLEM achieves higher ROC areas on all datasets except two and higher PR areas on all datasets except two, and that the improvements are statistically significant in 34 out of 66 cases. Its speed allows to perform a large number of restarts making it escape local maxima and achieve higher AUCPR and AUCROC. Moreover it uses less memory than `RIB`, `CEM`, `LFI-ProbLog` and `Alchemy`, allowing it to solve larger problems, and often in lower time. Finally, all the other systems except `Le-ProbLog` are not able to terminate on some domains, differently from `EMBLEM`.

`EMBLEM` is available in the `cplint` package in the source tree of Yap Prolog and information on its use can be found at `http://sites.google.com/a/unife.it/ml/emblem`.

Chapter 11

Structure Learning of LPADs

So far, we have addressed only the parameter estimation problem, and have assumed that the structure of the probabilistic model is given and fixed.

This chapter presents, after a general introduction about the problem of learning the structure of probabilistic models (Section 11.1), two structure learning algorithms for LPADs called `SLIPCASE` and `SLIPCOVER` (Sections 11.2 and 11.3) - the second being an evolution of the first. The chapter also features related works (Section 11.4) and experimental results (Section 11.5).

The algorithms learn both the structure and the parameters of Logic Programs with Annotated Disjunctions, by exploiting the EM algorithm over Binary Decision Diagrams proposed in (Bellodi and Riguzzi, 2012a). They can be applied to all probabilistic logic languages that are based on the distribution semantics. We tested them over the real datasets HIV, UW-CSE, WebKB, Mutagenesis and Hepatitis and evaluated its performance - in comparison with `SEM-CP-Logic`, `LSM`, `Aleph` and `ALEPH++ExactL1` - through the AUCPR, the AUCROC and the AUCNPR on Mutagenesis and Hepatitis, the learning times and the t-test for the statistical significance.
`SLIPCOVER` achieves the largest values under all metrics in most cases; `SLIPCASE` often follows `SLIPCOVER`.

This shows that the application of well known ILP and PLP techniques to the SRL field gives results that are competitive or superior to the state of the art.

11.1 Structure Learning of Probabilistic Models

The structure learning problem can be defined as follows:

Given

- a set of examples E,
- a language $\mathcal{L}_M$ of possible models of the form $M = (S, \lambda)$ with structure S and parameters λ,
- a probabilistic coverage relation $P(e|M)$ that computes the probability of observing the example e given the model M,
- a scoring function $score(E, M)$ that employs the probabilistic coverage relation $P(e|M)$

Find the model $M^* = (S, \lambda)$ that maximizes $score(E, M)$, that is,

$$M^* = argmax_M \; score(E, M)$$

This problem is essentially a search problem. There is a space of possible models to be considered, defined by $\mathcal{L}_M$, and the goal is to find the best one according to the scoring function. So solution techniques traverse the space of possible models in $\mathcal{L}_M$, by using operators for traversing the space and determining extreme points in the search space. For instance, in the case of Bayesian networks, the extreme points could be fully connected Bayesian networks (where there is an edge between any random variable and those that precede it in a given order) and one that contains no links at all. One of the possible techniques to evaluate a candidate structure S is based first on estimating the parameters λ (using the methods developed earlier), and then using the scoring function to determine the overall score of the resulting model.

Structure Learning in Logic Programs with Annotated Disjunctions

The structure learning algorithms for LPADs, which are presented in the next Section, tackle a problem of *discriminative* learning defined as follows.

Given

- a set of training examples Q_i, corresponding to ground atoms for a set of *target* or *output* predicates,

- a background knowledge with ground facts for other non-target or *input* predicates, organized as a set of logical interpretations or “mega-examples”,
- a probabilistic logical model M corresponding to a *trivial LPAD* or an *empty LPAD* $\mathbf{P}$, with unknown parameters (probabilities) $\mathbf{\Pi}$,
- a language bias to guide the construction of the refinements of the models,

Find the maximum likelihood LPAD $\mathbf{P}^*$ and probabilities $\mathbf{\Pi}^*$ such that maximize the conditional probability of the atoms for the output predicates given the atoms of the input predicates.

11.2 The `SLIPCASE` Algorithm

`SLIPCASE` learns the structure and the parameters of an LPAD by starting from an initial user-defined one: a good starting point is a trivial theory composed of one probabilistic clause with empty body of the form $target\_predicate(\overline{V}) : 0.5$. for each target predicate, where $\overline{V}$ is a tuple of variables. The algorithm performs a beam search in the *space of refinements* of the theory guided by the log likelihood of the data.

First the parameters of the initial theory are optimized by `EMBLEM` and the theory is inserted in the beam (see Algorithm 7). Then an iterative phase begins, where at each step the theory with the highest log likelihood is drawn from the beam. Such a theory is the first since the theories are kept ordered in the beam according to decreasing LL.

Then `SLIPCASE` finds the set of refinements of the selected theory that are allowed by the *language bias*: `modeh` and `modeb` declarations in Progol style are used to this purpose (see below). Following (Ourston and Mooney, 1994; Richards and Mooney, 1995) the admitted refinements are: the addition of a literal to a clause, the removal of a literal from a clause and the addition of a clause with an empty body, in order to generalize the current theory; the removal of a clause to specialize the current theory. For each refinement, a log likelihood estimate is computed by running the procedure BOUNDEDEMBLEM (see Algorithm 8) that performs a limited number of Expectation-Maximization steps. BOUNDEDEMBLEM differs from `EMBLEM` only in line 10, where it imposes that iterations are at most $NMax$. The evaluated refinements are inserted in order of LL in the beam and if they exceed the maximum allowed beam size b, those with the lowest LL (at the bottom of the beam) are removed. The highest-LL refinement is recorded as the $Best\ Theory$ found so far.

Beam search ends when one of the following occurs first: the maximum number of steps is reached, the beam is empty, the difference between the LL of the current theory or the best previous LL drops below a threshold ϵ. At that stage the parameters of the $Best\ Theory$ found so far are re-computed with `EMBLEM` and the resulting theory is returned.

Algorithm 7 Function SLIPCASE

```
function SLIPCASE($Th, MaxSteps, \epsilon, \epsilon 1, \delta, b, NMax$)
    Build $BDDs$
    ($LL, Th$) =EMBLEM($Th, \epsilon, \delta$)                    ▷ $Th = initial\ theory$
    $Beam = [(Th, LL)]$
    $BestLL = LL$
    $BestTh = Th$
    $Steps = 1$
    repeat
        Remove the first couple $(Th, LL)$ from $Beam$
        Find all refinements $Ref$ of $Th$
        for all $Th'$ in $Ref$ do
            $(LL'', Th'')$ =BoundedEMBLEM($Th', \epsilon, \delta, NMax$)
            if $LL'' > BestLL$ then
                Update $BestLL, BestTh$
            end if
            Insert $(Th'', LL'')$ in $Beam$ in order of $LL''$
            if $size(Beam) > b$ then
                Remove the last element of $Beam$
            end if
        end for
        $Steps = Steps + 1$
    until $Steps > MaxSteps$ or $Beam$ is empty or $(BestLL - Previous\_BestLL) < \epsilon 1$
    $(LL, ThMax)$ =EMBLEM($BestTh, \epsilon, \delta$)
    return $ThMax$
end function
```

The Language Bias

The language bias is used to limit the search space of theories since the algorithm knows that certain restrictions must apply to the output theory. These are expressed by means of:

- `input/output` modes: they specify the output (target) and the input (non-target) predicates of the domain (with their arity), by means of the declarations `output/1`, `input/1`;
- `mode` declarations: following (Muggleton, 1995), a mode declaration m is either a head declaration
  `modeh(r, s)` or a body declaration `modeb(r, s)`, where s, the *schema*, is a ground literal and r is an integer called the *recall*. A schema is a template for literals in the head or body

Algorithm 8 Function BoundedEMBLEM

```
1: function BoundedEMBLEM($Theory, \epsilon, \delta, NMax$)
2:     Build $BDDs$
3:     $LL = -inf$
4:     $N = 0$
5:     repeat
6:         $LL_0 = LL$
7:         $LL =$ Expectation($BDDs$)
8:         Maximization
9:         $N = N + 1$
10:    until $LL - LL_0 < \epsilon \vee LL - LL_0 < -LL \cdot \delta \vee N > NMax$
11:    Update the parameters of $Theory$
12:    return $LL, Theory$
13: end function
```

of a clause and can contain constants of the domain or the placemarker terms of the form $\#$`type`, $+$`type` and $-$`type`, which stand, respectively, for ground terms, input variables and output variables of a type (cf. Section 5.4). An input variable in a body literal must be either an input variable in the head or an output variable in a preceding body literal of a clause in the language bias. If M is a set of `mode` declarations, $L(M)$ is the *language of* M, i.e. the set of clauses $C = h_1; \ldots ; h_n :- b_1, \ldots , b_m$ such that the head atoms h_i (resp. body literals b_i) are obtained from some head (resp. body) declaration in M by replacing all # placemarkers with ground terms and + (resp. -) placemarkers with input (resp. output) variables and by maintaining the constants.
An example of language bias for the UW-CSE domain is:

```
/* input/output modes */
output(advisedby/2).   (target predicate)
input(student/1).
input(professor/1).
input(inphase/2).
input(hasposition/2).
input(publication/2).
input(yearsinprogram/2).
input(taughtby/3).
input(ta/3).
input(courselevel/2).
input(tempadvisedby/2).
input(projectmember/2).
input(sameperson/2).
input(samecourse/2).
input(sameproject/2).
```

```
/* mode declarations */
modeh(*,advisedby(+person,+person)).     (allowed in the head)

modeb(*,professor(+person)).             (allowed in the body)
modeb(*,student(+person)).
modeb(*,courselevel(+course, -level)).
modeb(*,hasposition(+person, -position)).
modeb(*,inphase(+person, -phase)).
modeb(*,tempadvisedby(+person, -person)).
modeb(*,yearsinprogram(+person, -year)).
modeb(*,publication(-title, +person)).
modeb(*,hasposition(+person, faculty)).
modeb(*,hasposition(+person, faculty_affiliate)).
modeb(*,hasposition(+person, faculty_adjunct)).
modeb(*,hasposition(+person, faculty_visiting)).
modeb(*,hasposition(+person, faculty_emeritus)).
modeb(*,projectmember(-project, +person)).
modeb(*,taughtby(+course, -person, -quarter)).
modeb(*,ta(+course, -person, -quarter)).
modeb(*,taughtby(-course, +person, -quarter)).
modeb(*,ta(-course, +person, -quarter)).
...
```

11.3 The SLIPCOVER Algorithm

SLIPCOVER learns an LPAD by first identifying good candidate clauses and then searching for a theory guided by the LL of the data. As EMBLEM, it takes as input a set of mega-examples and an indication of which predicates are target. The mega-examples must contain positive and negative examples for all predicates that may appear in the head of clauses, either target or non-target (background predicates).

Search in the Space of Clauses

SLIPCOVER performs a cycle on the set of predicates that can appear in the head of clauses, either target or background, and, for each predicate, it performs a beam search in the space of clauses. The set of initial beams is returned by function INITIALBEAMS shown in Algorithm 9.

Function INITIALBEAMS The search over the space of clauses is performed according to a language bias expressed by means of *mode* declarations, as done for SLIPCASE, cf. Section

Algorithm 9 Function INITIALBEAMS

```
1: function INITIALBEAMS($NInt, NS, NA$)
2:     $IB \leftarrow \emptyset$
3:     for all predicates $P/Ar$ do
4:         $Beam \leftarrow []$
5:         for all modeh declarations $modeh(r, s)$ with $P/Ar$ predicate of $s$ do
6:             for $i = 1 \rightarrow NInt$ do
7:                 Select randomly a mega-example $I$
8:                 for $j = 1 \rightarrow NA$ do
9:                     Select randomly an atom $h$ from $I$ matching $schema(s)$
10:                    Bottom clause $BC$ ←SATURATION($h, r, NS$), let $BC$ be $Head :- Body$
11:                    $Beam \leftarrow [((Head, Body), -\infty)|Beam]$
12:                end for
13:            end for
14:        end for
15:        for all modeh declarations $modeh(r, [s_1, \ldots, s_n], [a_1, \ldots, a_n], PL)$ with $P/Ar$ in $PL$ appearing in $s_1, \ldots, s_n$ do
16:            for $i = 1 \rightarrow NInt$ do
17:                Select randomly a mega-example $I$
18:                for $j = 1 \rightarrow NA$ do
19:                    Select randomly a set of atoms $h_1, \ldots, h_n$ from $I$ matching $schema(s_1), \ldots, schema(s_n)$
20:                    Bottom clause $BC$ ←SATURATION($(h_1, \ldots, h_n), r, NS$), let $BC$ be $Head :- Body$
21:                    $Beam \leftarrow [((Head, Body), -\infty)|Beam]$
22:                end for
23:            end for
24:        end for
25:        $IB \leftarrow IB \cup \{(P/Ar, Beam)\}$
26:    end for
27:    return $IB$
28: end function
```

We extend this type of mode declaration with placemarker terms of the form "-#" which are treated as "#" when defining $L(M)$ but differ in the creation of the bottom clauses (see below).

The initial set of beams IBs, one for each predicate appearing in a head declaration, is generated by SLIPCOVER by building a set of *bottom clauses* as in Progol (Muggleton, 1995), see Algorithm 9. In order to generate a bottom clause for a mode declaration $m = modeh(r, s)$, an input mega-example is selected and an answer h for the goal $schema(s)$ is selected, where $schema(s)$ denotes the literal obtained from s by replacing all placemarkers with distinct variables $X_1, \ldots, X_n$. Then, h is saturated with body literals using Progol's saturation method (see Algorithm 10), a deductive procedure used to find atoms related to h. The terms in h are used to initialize a growing set of input terms $InTerms$: these are the terms corresponding to + placemarkers in s. Then, each body declaration m is considered in turn. The terms from t

Algorithm 10 Function SATURATION

```
 1: function SATURATION($Head, r, NS$)
 2:     $InTerms = \emptyset$,
 3:     $BC = \emptyset$                                                    ▷ $BC$: bottom clause
 4:     for all arguments $t$ of $Head$ do
 5:         if $t$ corresponds to a $+type$ then
 6:             add $t$ to $InTerms$
 7:         end if
 8:     end for
 9:     Let $BC$'s head be $Head$
10:     repeat
11:         $Steps \leftarrow 1$
12:         for all modeb declarations $modeb(r, s)$ do
13:             for all possible subs. $\sigma$ of variables corresponding to $+type$ in $schema(s)$ by terms from $InTerms$ do
14:                 for $j = 1 \to r$ do
15:                     if goal $b = schema(s)$ succeeds with answer substitution $\sigma'$ then
16:                         for all $v/t \in \sigma$ and $\sigma'$ do
17:                             if $v$ corresponds to a $-type$ or $-\#type$ then
18:                                 add $t$ to the set $InTerms$ if not already present
19:                             end if
20:                         end for
21:                         Add $b$ to $BC$'s body
22:                     end if
23:                 end for
24:             end for
25:         end for
26:         $Steps \leftarrow Steps + 1$
27:     until $Steps > NS$
28:     Replace constants with variables in $BC$, using the same variable for equal terms
29:     return $BC$
30: end function
```

are substituted into the + placemarkers of m to generate a set Q of goals. Each goal is then executed against the database and up to r (the recall) successful ground instances (or all if $r = \star$) are added to the body of the clause. Each term corresponding to a - or -# placemarker in m is inserted into $InTerms$ if it is not already present. This cycle is repeated for a user defined number NS of times.

The resulting ground clause $h :- b_1, \ldots, b_m$ is then processed to obtain a program clause by replacing each term in a + or - placemarker with a variable, using the same variable for identical terms. Terms corresponding to # or -# placemarker are instead kept in the clause. The initial beam associated with predicate P/Ar of h will contain the clause with the empty body $h : 0.5.$ for each bottom clause $h :- b_1, \ldots, b_m$ (cf. line 15 of Algorithm 9). This process is repeated for a number $NInt$ of input mega-examples and a number NA of answers, thus obtaining $NInt \cdot NA$ bottom clauses.

We extended the mode declaration by allowing head declarations of the form $modeh(r, [s_1, \ldots, s_n], [a_1, \ldots, a_n], [P_1/Ar_1, \ldots, P_k/Ar_k])$. These mode declarations are used to generate clauses with more than two head atoms. In them, $s_1, \ldots, s_n$ are schemas, $a_1, \ldots, a_n$ are atoms such that a_i is obtained from s_i by replacing placemarkers with variables, P_i/Ar_i are the predicates admitted in the body with their arity. $a_1, \ldots, a_n$ is used to indicate which variables should be shared by the atoms in the head: in order to generate the head, the goal $a_1, \ldots, a_n$ is called and NA answers that ground all a_is are kept. From these, the set of input terms t is built and body literals are computed as above. The resulting bottom clauses then have the form $a_1 \ ; \ \ldots \ ; \ a_n :- b_1, \ldots, b_m$ and the initial beam will contain clauses with an empty body of the form $a_1 : \frac{1}{n+1} \ ; \ \ldots \ ; \ a_n : \frac{1}{n+1}$.

Clause Beam Search After having built the initial bottom clauses, SLIPCOVER, shown in Algorithm 11, performs a cycle for each predicate that can appear in the head of clauses, either target or background. In each iteration, it performs a beam search in the space of clauses for the predicate (line 9).

For each clause Cl of the form $Head :- Body$, with $Literals$ admissible in the body, the CLAUSEREFINEMENTS function, shown in Algorithm 12, computes refinements by adding a literal from $Literals$ to the body. Furthermore, the refinements must respect the input-output modes of the bias declarations, must be connected (i.e., each body literal must share a variable with the head or a previous body literal) and their number of variables must not exceed a user defined number NV. The tuple (Cl', $Literals'$) indicates a refined clause Cl' together with the new set $Literals'$ of literals allowed in its body.

At line 13 of Algorithm 11, parameter learning is executed for a theory composed of the single refined clause. For each goal for the current predicate, EMBLEM builds the BDD encoding its explanations by deriving them from the single-clause theory (together with the facts in the mega-examples); derivations exceeding the depth limit D are cut. Then the parameters and the LL of the data are computed by the EM algorithm; LL is used as score of the updated clause $(Cl'', Literals')$. This clause is then inserted into a list of promising clauses.

Algorithm 11 Function SLIPCOVER

```
1: function SLIPCOVER($NInt, NS, NA, NI, NV, NB, NTC, NBC, D, NEM, \epsilon, \delta$)
2:     $IBs$ =INITIALBEAMS($NInt, NS, NA$)
3:     $TC \leftarrow []$
4:     $BC \leftarrow []$
5:     for all $(PredSpec, Beam) \in IBs$ do
6:         $Steps \leftarrow 1$
7:         $NewBeam \leftarrow []$
8:         repeat                                                          ▷ Clause search
9:             while $Beam$ is not empty do
10:                Remove the first couple $((Cl, Literals), LL)$ from $Beam$    ▷ Remove the first bottom clause
11:                $Refs \leftarrow$CLAUSEREFINEMENTS($(Cl, Literals), NV$)   ▷ Find all refinements $Refs$ of $(Cl, Literals)$
   with at most $NV$ variables
12:                for all $(Cl', Literals') \in Refs$ do
13:                    $(LL'', \{Cl''\}) \leftarrow$EMBLEM($\{Cl'\}, D, NEM, \epsilon, \delta$)
14:                    $NewBeam \leftarrow$INSERT($(Cl'', Literals'), LL'', NewBeam, NB$)
15:                    if $Cl''$ is range restricted then
16:                        if $Cl''$ has a target predicate in the head then
17:                            $TC \leftarrow$INSERT($(Cl'', Literals'), LL'', TC, NTC$)
18:                        else
19:                            $BC \leftarrow$INSERT($(Cl'', Literals'), LL'', BC, NBC$)
20:                        end if
21:                    end if
22:                end for
23:            end while
24:            $Beam \leftarrow NewBeam$
25:            $Steps \leftarrow Steps + 1$
26:        until $Steps > NI$
27:    end for
28:    $Th \leftarrow \emptyset, ThLL \leftarrow -\infty$                                   ▷ Theory search
29:    repeat
30:        Remove the first couple $(Cl, LL)$ from $TC$
31:        $(LL', Th') \leftarrow$EMBLEM($Th \cup \{Cl\}, D, NEM, \epsilon, \delta$)
32:        if $LL' > ThLL$ then
33:            $Th \leftarrow Th', ThLL \leftarrow LL'$
34:        end if
35:    until $TC$ is empty
36:    $Th \leftarrow Th \bigcup_{(Cl,LL) \in BC} \{Cl\}$
37:    $(LL, Th) \leftarrow$EMBLEM($Th, D, NEM, \epsilon, \delta$)
38:    return $Th$
39: end function
```

Two lists are used, TC for target predicates and BC for background predicates. The clause is inserted in TC if a target predicate appears in its head, otherwise in BC. The insertion is in order of LL. If the clause is not range restricted, i.e., if some of the variables in the head do not appear in a positive literal in the body, then it is inserted neither in TC nor in BC. These lists have a maximum size: if an insertion increases the size over the maximum, the last element is removed. In Algorithm 11, the function INSERT($I, Score, List, N$) is used to insert a clause

Algorithm 12 Function CLAUSEREFINEMENTS

```
1: function CLAUSEREFINEMENTS($(Cl, Literals), NV$)        ▷ $Cl = h : 0.5 :- true.$
2:     $Refs = \emptyset, Nvar = 0$;        ▷ Nvar: number of different variables in a clause
3:     for all $b \in Literals$ do
4:         $Literals' \leftarrow Literals \setminus \{b\}$
5:         Add $b$ to $Cl$ body obtaining $Cl'$
6:         $Nvar \leftarrow$ number of $Cl'$ variables
7:         if $Cl'$ is connected $\wedge$ $Nvar < NV$ then
8:             $Refs \leftarrow Refs \cup \{(Cl', Literals')\}$
9:         end if
10:    end for
11:    return $Refs$
12: end function
```

I with score $Score$ in a list $List$ with at most N elements. Beam search is repeated until the beam becomes empty or a maximum number NI of iterations is reached.

The separate search for clauses has similarity with the covering loop of ILP systems such as Aleph and Progol. Differently from the ILP case, however, the test of an example requires the computation of all its explanations, while in ILP the search stops at the first matching clause. The only interaction among clauses in probabilistic logic programming happens if the clauses are recursive. If not, then adding clauses to a theory only adds explanations for the example increasing its probability, so clauses can be added individually to the theory. If the clauses are recursive, the examples for the head predicates are used to resolve literals in the body, thus the test of examples on individual clauses approximates the case of the test on a complete theory. As will be shown by the experiments, this approximation is often sufficient for identifying good clauses.

Search in the Space of Theories

After the clause search phase, SLIPCOVER performs a greedy search in the space of theories: it starts with an empty theory and adds a target clause at a time from the list TC. After each addition, it runs EMBLEM and computes the LL of the data as the score of the resulting theory. If the score is better than the current best, the clause is kept in the theory, otherwise it is discarded. This is done for each clause in TC.

Finally, SLIPCOVER adds all the clauses in BC to the theory and performs parameter learning on the resulting theory. The clauses that are never used to derive the examples will get a value of 0 for the parameters of atoms in their head and are removed in a post processing phase.

Execution Example

We now show an example of execution on the UW-CSE dataset.

Language bias The language bias contains `modeh` declarations for one-head clauses such as

```
modeh(*,advisedby(+person,+person)).              (target p.)
modeh(*,taughtby(+course, +person, +quarter)).    (background p.)
```

and `modeh` declarations for disjunctive head clauses such as

```
modeh(*,[advisedby(+person,+person),tempadvisedby(+person,+person)],
  [advisedby(A,B),tempadvisedby(A,B)],
  [professor/1,student/1,hasposition/2,inphase/2,
  taughtby/3,ta/3,courselevel/2,yearsinprogram/2]).

modeh(*,[student(+person),professor(+person)],
  [student(P),professor(P)],
  [hasposition/2,inphase/2,taughtby/3,ta/3,courselevel/2,
  yearsinprogram/2,advisedby/2,tempadvisedby/2]).

modeh(*,[inphase(+person,pre_quals),inphase(+person,post_quals),
  inphase(+person,post_generals)],
  [inphase(P,pre_quals),inphase(P,post_quals),inphase(P,post_generals)],
  [professor/1,student/1,taughtby/3,ta/3,courselevel/2,
  yearsinprogram/2,advisedby/2,tempadvisedby/2,hasposition/2]).
```

Moreover, the bias contains `modeb` declarations such as

```
modeb(*,courselevel(+course, -level)).
modeb(*,courselevel(+course, #level)).
```

Bottom clauses An example of a bottom clause that is generated from the first `modeh` declaration and the example `advisedby(person155,person101)` is

```
advisedby(A,B):0.5 :- professor(B),student(A),hasposition(B,C),
  hasposition(B,faculty),inphase(A,D),inphase(A,pre_quals),
  yearsinprogram(A,E),taughtby(F,B,G),taughtby(F,B,H),taughtby(I,B,J),
  taughtby(I,B,J),taughtby(F,B,G),taughtby(F,B,H),
  ta(I,K,L),ta(F,M,H),ta(F,M,H),ta(I,K,L),ta(N,K,O),ta(N,A,P),
  ta(Q,A,P),ta(R,A,L),ta(S,A,T),ta(U,A,O),ta(U,A,O),ta(S,A,T),
  ta(R,A,L),ta(Q,A,P),ta(N,K,O),ta(N,A,P),ta(I,K,L),ta(F,M,H).
```

An example of a bottom clause generated from the second `modeh` declaration for disjunctive head clauses and the atoms `student(person218),professor(person218)` is

```
student(A):0.33; professor(A):0.33 :- inphase(A,B),inphase(A,post_generals),
                                      yearsinprogram(A,C).
```

Search in the space of clauses When searching in the space of clauses for the `advisedby/2` predicate, an example of a refinement generated from the first bottom clause is

```
advisedby(A,B):0.5 :- professor(B).
```

`EMBLEM` is then applied to the theory composed of this single clause, using the positive and negative facts for `advisedby/2` as queries for which to build BDDs. The only parameter is updated obtaining:

```
advisedby(A,B):0.108939 :- professor(B).
```

Successively, the clause is further refined in

```
advisedby(A,B):0.108939 :- professor(B),hasposition(B,C).
```

An example of a refinement that is generated from the second bottom clause is

```
student(A):0.33; professor(A):0.33 :- inphase(A,B).
```

The updated refinement after `EMBLEM` is

```
student(A):0.5869;professor(A):0.09832 :- inphase(A,B).
```

Search in the space of theories When searching the space of theories, `SLIPCOVER` generates the program

```
advisedby(A,B):0.1198 :-  professor(B),inphase(A,C).
advisedby(A,B):0.1198 :-  professor(B),student(A).
```

with a LL of -350.01. After `EMBLEM` we get

```
advisedby(A,B):0.05465 :-  professor(B),inphase(A,C).
advisedby(A,B):0.06893 :-  professor(B),student(A).
```

with a LL of -318.17. Since the LL increased, the last clause is retained and at the next iteration a new clause is added:

```
advisedby(A,B):0.12032 :- hasposition(B,C),inphase(A,D).
advisedby(A,B):0.05465 :- professor(B),inphase(A,C).
advisedby(A,B):0.06893 :- professor(B),student(A).
```

11.4 Related Work

SLIPCASE & SLIPCOVER

Our work on structure learning for Probabilistic Logic Programs makes extensive use of well known ILP techniques: the *Inverse Entailment* algorithm (Muggleton, 1995) for finding the most specific clauses allowed by the language bias and the strategy for the identification of good candidate clauses are exploited by the SLIPCOVER algorithm. This makes SLIPCOVER closely related to the ILP systems Progol (Muggleton, 1995) and **Aleph** (Srinivasan, 2012), that perform structure learning of a pure logical theory by building a set of clauses where specified background predicates can appear in the body. Aleph is compared with SLIPCOVER in the experimental Section.

The use of log likelihood as heuristics rather than a scoring function as proposed in (Friedman, 1998) for SEM depends on the fact that it was giving better results with a limited additional cost. We think that is due to the fact that, while in SEM the number of incomplete or unseen variables is fixed, in SLIPCASE/SLIPCOVER the revisions can introduce or remove unseen variables from the underlying Bayesian Network.

SLIPCOVER is based on SLIPCASE - of which it is an evolution - (Bellodi and Riguzzi, 2012b) and on EMBLEM (Bellodi and Riguzzi, 2012a) for performing parameter learning. The two algorithms for structure learning differ mainly in the search strategy: SLIPCASE performs a beam search in the space of theories, starting from a trivial LPAD and using the LL of the data as the guiding heuristics. At each step of the search, the theory with the highest LL is removed from the beam and a set of refinements is generated and evaluated by means of LL; then they are inserted in order of LL in the beam.

SLIPCOVER search strategy differs because is composed of two phases: (1) beam search in the space of clauses in order to find a set of promising clauses and (2) greedy search in the space of theories. The beam searches performed by the two algorithms differ because SLIPCOVER generates refinements of a *single* clause at a time, which are evaluated through LL. The search in the space of theories starts from an empty theory which is iteratively extended with one clause at a time from those generated in the previous beam search. Moreover, in SLIPCOVER background clauses, the ones with a non-target predicate in the head, are treated separately, by adding them en bloc to the best theory for target predicates. SLIPCOVER search strategy allows a more effective exploration of the search space, resulting both in time savings and in a higher quality of the final theories, as shown by the experiments.

Structure Learning in Probabilistic Logic Languages

Previous works on learning the structure of probabilistic logic programs include (Kersting and De Raedt, 2008) that proposed a scheme for learning both the probabilities and the structure of Bayesian Logic Programs, by combining techniques from the learning from interpretations setting of ILP with score-based techniques for learning Bayesian Networks. We share with this approach the scoring function, the LL of the data given a candidate structure and the greedy search in the space of structures.

(De Raedt et al., 2008b) presented an algorithm for performing theory compression on ProbLog programs. Theory compression means removing as many clauses as possible from the theory in order to maximize the likelihood w.r.t. a set of positive and negative examples. No new clause can be added to the theory.

$\mathbf{SEM-CP-Logic}$ (Meert et al., 2008) learns parameters and structure of ground CP-logic programs. It performs learning by considering the Bayesian networks equivalent to CP-logic programs and by applying techniques for learning Bayesian networks. In particular, it applies the Structural Expectation Maximization (SEM) algorithm (Friedman, 1998): it iteratively generates refinements of the equivalent Bayesian network and it greedily chooses the one that maximizes the BIC score (Schwarz, 1978). In SLIPCOVER, we use the LL as a score because experiments with BIC were giving inferior results. Moreover, SLIPCOVER differs from SEM-CP-Logic because it searches the clause space and it refines clauses with standard ILP refinement operators, which allow to learn non ground theories. This system will be compared with SLIPCASE and SLIPCOVER in the experimental Section.

(Getoor et al., 2007) described a comprehensive framework for learning statistical models called Probabilistic Relational Models (PRMs). These extend Bayesian networks with the concepts of objects, their properties, and relations between them, and specify a template for a probability distribution over a database. The template includes a relational component, that describes the relational schema for the domain, and a probabilistic component, that describes the probabilistic dependencies that hold in it. A method for the automatic construction of a PRM from an existing database is shown, together with parameter estimation, structure scoring criteria and a definition of the model search space.

(Costa et al., 2003) presented an extension of logic programs that makes it possible to specify a joint probability distribution over missing values in a database or logic program, in analogy to PRMs. This extension is based on constraint logic programming (CLP) and is called CLP(BN). Existing ILP systems like Aleph can be used to learn CLP(BN) programs with simple modifications.

(Paes et al., 2006) described the first theory revision system for SRL, PFORTE for "Probabilistic First-Order Revision of Theories from Examples", which starts from an approximate initial theory and applies modifications in places that performed badly in classification. PFORTE uses a two step-approach. The completeness component uses generalization operators to address failed proofs and the classification component addresses classification problems using generalization and specialization operators. It is presented as an alternative to algorithms that learn from scratch.

Markov Logic Networks Structure learning has been thoroughly investigated for Markov Logic Networks (MLN): in (Kok and Domingos, 2005) the authors proposed two approaches. The first is a beam search that adds a clause at a time to the theory using weighted pseudo-likelihood as a scoring function. The second is called shortest-first search and adds the k best clauses of length l before considering clauses with length $l + 1$.

(Mihalkova and Mooney, 2007) proposed a bottom-up algorithm for learning Markov Logic Networks (MLNs) called BUSL that is based on relational pathfinding: paths of true ground atoms that are linked via their arguments are found and generalized into First Order rules.

(Huynh and Mooney, 2008) introduced a two-step method for MLNs structure learning: (1) learning a large number of promising clauses through a specific configuration of Aleph (ALEPH++), followed by (2) the application of a new discriminative MLN parameter learning algorithm. This algorithm differs from the standard weight learning one (Lowd and Domingos, 2007) in the use of an exact probabilistic inference method and of a L1-regularization of the parameters, in order to encourage assigning low weights to clauses. The complete method is defined $\mathbf{ALEPH++ExactL1}$; it is compared with SLIPCOVER in the experimental Section.

In (Kok and Domingos, 2009), the structure of Markov Logic theories is learned by applying a generalization of relational pathfinding. A database is viewed as a hypergraph with constants as nodes and true ground atoms as hyperedges. Each hyperedge is labeled with a predicate symbol. First a hypergraph over clusters of constants is found, then pathfinding is applied on this "lifted" hypergraph. The resulting algorithm is called LHL.

(Kok and Domingos, 2010) presented the algorithm "Learning Markov Logic Networks using Structural Motifs" (**LSM**). It is based on the observation that relational data frequently contain recurring patterns of densely connected objects called *structural motifs*. `LSM` limits the search to these patterns. Like `LHL`, `LSM` views a database as a hypergraph and groups nodes that are densely connected by many paths and the hyperedges connecting the nodes into a motif. Then it evaluates whether the motif appears frequently enough in the data and finally it applies relational pathfinding to find rules. This process, called *createrules* step, is followed by weight learning with the `Alchemy` system. `LSM` was experimented on various datasets and found to be superior to other methods, thus representing the state of the art in Markov Logic Networks' structure learning and in Statistical Relational Learning in general. It is compared with `SLIPCOVER` in the experimental Section.

A different approach is taken in (Biba et al., 2008) where the algorithm "Discriminative Structure Learning" (`DSL`) is presented, that performs learning of MLNs by repeatedly adding a clause to the network through iterated local search, which performs a walk in the space of local optima. We share with this approach the discriminative nature of the algorithm and the scoring function.

11.5 Experiments

The experiments are directed to verify:

- the quality of the estimated LPAD structure and parameters;
- the algorithm performance in comparison with other state of the art SRL systems.

Datasets

HIV (Beerenwinkel et al., 2005) records mutations in HIV reverse transcriptase gene in patients that are treated with the drug zidovudine. It contains 364 examples, each of which specifies the presence or not of six classical zidovudine mutations, denoted by atoms of the form "`41L`". These atoms indicate the location where the mutation occurred (e.g., *41*) and the amino acid to which the position mutated (e.g., *L* for Leucine). The goal is to discover causal relations between the occurrences of mutations in the virus. The database is split into five mega-examples.

For *UW-CSE* (Richardson and Domingos, 2006)[1], *WebKB* (Craven and Slattery, 2001)[2] and *Mutagenesis*(Srinivasan et al., 1996) cf. Section 10.4.

Hepatitis[3] (Khosravi et al., 2012) is derived from the *PKDD02 Discovery Challenge database* (Berka et al., 2002) and contains information on the laboratory examinations of hepatitis B and C infected patients. Seven tables are used to store this information. The goal is to predict the type of hepatitis of a patient. The database is split into five mega-examples.

Estimating Performance

Similarly to the experiments for EMBLEM,

- A *k-fold* ($k = 4, 5, 10$) cross-validation approach is adopted;
- Precision-Recall and Receiver Operating Characteristics curves are drawn, and the Area Under the Curve (AUCPR and AUCROC respectively) is computed. Recently, (Boyd et al., 2012) showed that the AUCPR is not adequate to evaluate the performance of learning algorithms when the skew is larger than 0.5: skew is the ratio between the number of positive examples and the total number of examples. Since for Mutagenesis and Hepatitis domains the skew is close to 0.5, it has been computed for them the Normalized Area Under the PR Curve (AUCNPR) (Boyd et al., 2012);
- a paired two-tailed t-test at the 5% significance level is performed.

Methodology

SLIPCASE and SLIPCOVER exploit EMBLEM, that learns LPAD parameters and is described in detail in Section 10.2. They are implemented in Yap Prolog[4] and are compared with

- two systems for structure learning of Probabilistic Logic Programs:
  - SEM-CP-Logic (Meert et al., 2008)
  - Aleph (Srinivasan, 2012)
- two systems for structure learning of Markov Logic Networks:

[1]Available at http://alchemy.cs.washington.edu/data/uw-cse.
[2]Available at http://alchemy.cs.washington.edu/data/webkb.
[3]http://www.cs.sfu.ca/~oschulte/jbn/dataset.html
[4]http://www.dcc.fc.up.pt/~vsc/Yap/

- `LSM` (Kok and Domingos, 2010)
- `ALEPH++ExactL1` (Huynh and Mooney, 2008)

All experiments were performed on Linux machines with an Intel Core 2 Duo E6550 (2333 MHz) processor and 4 GB of RAM.

`SLIPCASE` offers the following *options*:

1. the options provided by `EMBLEM` for parameter learning, in particular we recall: the limit on the depth D of derivations, for structures that contain cyclic clauses, such as transitive closure clauses; ϵ and δ for stopping the EM cycle;
2. the number of theory refinement iterations, NIT;
3. the number of iterations for BOUNDEDEMBLEM, $NMax$;
4. the size of the beam, NB;
5. the maximum number of variables in a clause, NV;
6. the maximum number of rules in the learned theory, NR;
7. ϵ_s, δ_s, which are respectively the minimum difference and relative difference between the LL of a theory in two consecutive refinement iterations;
8. the semantics (standard or simplified).

All experiments with `SLIPCASE` have been performed using $\epsilon_s = 10^{-4}$ and $\delta_s = 10^{-5}$ (except Mutagenesis where we set $\epsilon_s = 10^{-20}$ and $\delta_s = 10^{-20}$) and $NMax = +\infty$ since `EMBLEM` usually converges quickly. `EMBLEM`'s parameters ϵ, δ for stopping the EM cycle are always set as $\epsilon = 10^{-4}$ and $\delta = 10^{-5}$.

`SLIPCOVER` offers the following *options*:

1. the options provided by `EMBLEM` for parameter learning, in particular we recall: the limit on the depth D of derivations, for structures that contain cyclic clauses, such as transitive closure clauses; ϵ and δ for stopping EM cycle; NEM, maximum number of steps of the EM cycle;
2. the number of mega-examples from which to build the bottom clauses, $NInt$;

3. the number of bottom clauses to be built for each mega-example, NA;
4. the number of saturation steps, NS; it is always set to 1 to limit the size of the bottom clauses;
5. the maximum number of clause search iterations, NI;
6. the maximum number of variables in a rule, NV;
7. the size of the beam, NB;
8. the maximum numbers NTC and NBC of target and background clauses, respectively;
9. the semantics (standard or simplified).

The parameters NV, NB and the semantics are shared with `SLIPCASE`.

For all experiments with `SLIPCOVER`, we set $\epsilon = 10^{-4}$, $\delta = 10^{-5}$ and $NEM = +\infty$, since we observed that `EMBLEM` usually converges quickly.

All the other parameters have been chosen to avoid lack of memory errors and to keep computation time within 24 hours. This is true also for the depth bound D used in domains where the language bias allows recursive clauses. The values for D are typically 2 or 3; when the theory is not cyclic this parameter is not relevant.

Statistics on the domains are reported in Table 11.1.

Table 11.1: Characteristics of the datasets used with `SLIPCASE` and `SLIPCOVER`: target predicates, number of constants, of predicates, of tuples (ground atoms), of positive and negative training and testing examples for target predicate(s), of folds. The number of tuples includes the target positive examples.

Dataset	Target Predicate(s)	Const	Preds	Tuples	Pos.Ex.	Training Neg.Ex.	Testing Neg.Ex.	Folds
HIV	41L,67N,70R, 210W,215FY, 219EQ	0	6	2184	590	1594	1594	5
UW-CSE	advisedby(X,Y)	1323	15	2673	113	4079	16601	5
WebKB	<course,faculty, researchProject, student>Page(P)	4942	8	290973	1039	15629	16249	4
Mutagenesis	active(D)	7045	20	15249	125	63	63	10
Hepatitis	type(X,T)	6491	19	71597	500	500	500	5

The parameter settings for for SLIPCASE and SLIPCOVER on the domains can be found in Tables 11.2 and 11.3.

Table 11.2: Parameter settings for the experiments with SLIPCASE. '-' means the parameter is not relevant.

Dataset	NIT	NV	NB	NR	D	semantics
HIV	10	-	5	10	3	standard
UW-CSE	10	5	20	10	-	standard
WebKB	10	5	20	10	-	simplified
Mutagenesis	10	5	20	10	-	standard
Hepatitis	10	5	20	10	-	standard

Table 11.3: Parameter settings for the experiments with SLIPCOVER. '-' means the parameter is not relevant.

Dataset	NInt	NS	NA	NI	NV	NB	NTC	NBC	D	semantics
HIV	1	1	1	10	-	10	50	-	3	standard
UW-CSE	1	1	1	10	5	100	10000	200	2	simplified
WebKB	1	1	1	5	4	15	50	-	2	standard
Mutagenesis	1	1	1	10	5	20	100	-	-	standard
Hepatitis	1	1	1	10	5	20	1000	-	-	simplified

For Aleph, we modified the standard settings as follows: the maximum number of literals in a clause is set to 7 (instead of the default 4) for UW-CSE and Mutagenesis, since here clause bodies are generally long. The minimum number of positive examples covered by an acceptable clause is set to 2. The search strategy is forced to continue until all remaining elements in the search space are definitely worse than the current best element (normally, search would stop when all remaining elements are no better than the current best), by setting the `explore` parameter to `true`. The `induce` command is used to learn the clauses.
We report results only for UW-CSE, WebKb and Mutagenesis since on HIV and Hepatitis Aleph returns the set of examples as the final theory, not being able to find good enough generalizations. In the tests, the head of each learned clause is annotated with probability 0.5 in order to turn the sharp logical classifier into a probabilistic one and to assign higher probability to those examples that have more successful derivations.

For SEM-CP-logic, we report the results only on HIV as the system learns only ground theories and the other datasets require theories with variables.

For LSM, the weight learning step can be generative or discriminative, according to whether the aim is to accurately predict all or a specific predicate respectively; for the discriminative case we use the preconditioned scaled conjugate gradient technique, because it was found to be the state of the art (Lowd and Domingos, 2007).

For ALEPH++ExactL1, we use the induce_cover command and the parameter settings for Aleph specified in (Huynh and Mooney, 2008), on the datasets on which Aleph can return a theory.

Tables 11.4 and 11.5 show respectively the AUCPR and AUCROC averaged over the folds for all algorithms and datasets. Table 11.6 shows the AUCNPR for all algorithms tested on the datasets Mutagenesis and Hepatitis. Table 11.7 shows the learning times in hours; times for SEM-CP-logic on HIV cannot be included since they are not mentioned in (Meert et al., 2008).

Tables 11.8 and 11.9 show the p-value of a paired two-tailed t-test at the 5% significance level of the difference in AUCPR and AUCROC between SLIPCOVER and SLIPCASE/LSM/SEM-CP-logic/Aleph/ALEPH++ExactL1 on all datasets (significant differences in favor of SLIPCOVER in bold).

Figures 11.1, 11.3, 11.5, 11.7 and 11.9 show the PR curves for all datasets, while Figures 11.2, 11.4, 11.6, 11.8 and 11.10 show ROC curves. These curves have been obtained by collecting the testing examples, together with the probabilities assigned to them in testing, in a single set and then building the curves with the methods of (Davis and Goadrich, 2006; Fawcett, 2006).

HIV The goal is to discover causal relations between the occurrences of mutations in the virus, so all the predicates 41L, 67N, 70R, 210W, 215FY and 219EQ corresponding to the mutations are set as target. We created each fold as the grouping of 72 or 73 examples.

The input trivial theory for SLIPCASE is composed of six probabilistic clauses of the form <mutation>:0.2. The language bias allows each of the six atoms to appear in the head and in the body, so the theory is recursive.

The language bias for SLIPCOVER allows each atom to appear in the head and in the body (cyclic theory). NBC is not relevant since all predicates are target.

For testing, we compute the probability of each mutation in each example given the value of the remaining mutations. The presence of a mutation in an example is considered as a positive example, while its absence as a negative example.

For SEM-CP-Logic, we test the learned theory reported in (Meert et al., 2008) over each of the five folds.

For LSM, we use the generative training algorithm to learn weights, because all the predicates are target, and the MC-SAT algorithm for inference over the test fold, by specifying all the six mutations as query atoms.

Results The medical literature states that 41L, 215FY and 210W tend to occur together, and that 70R and 219EQ tend to occur together as well. SLIPCASE and LSM find only one of these two connections and the simple MLN learned by LSM may explain its low AUCs. SLIPCOVER instead learns many more clauses where both connections are found, with higher probabilities than the other clauses. The longer learning time with respect to the other systems mainly depends on the theory search phase, since the TC list can contain up to 50 clauses and the final theories have on average 40, so many theory refinement steps are executed.

In the following we show examples of rules that are learned by the systems, focusing on those expressing the above connections.

SLIPCOVER learns the clauses

```
70R:0.950175 :- 219EQ.
41L:0.24228  :- 215FY,210W.
41L:0.660481 :- 210W.
41L:0.579041 :- 215FY.
219EQ:0.470453 :- 67N,70R.
219EQ:0.400532 :- 70R.
215FY:0.795429 :- 210W,219EQ.
215FY:0.486133 :- 41L,219EQ.
215FY:0.738664 :- 67N,210W.
215FY:0.492516 :- 67N,41L.
215FY:0.475875 :- 210W.
215FY:0.924251 :- 41L.
210W:0.425764  :- 41L.
```

SLIPCASE instead learns

```
41L:0.68 :- 215FY.
215FY:0.95 ; 41L:0.05 :- 41L.
210W:0.38 ; 41L:0.25  :- 41L, 215FY.
```

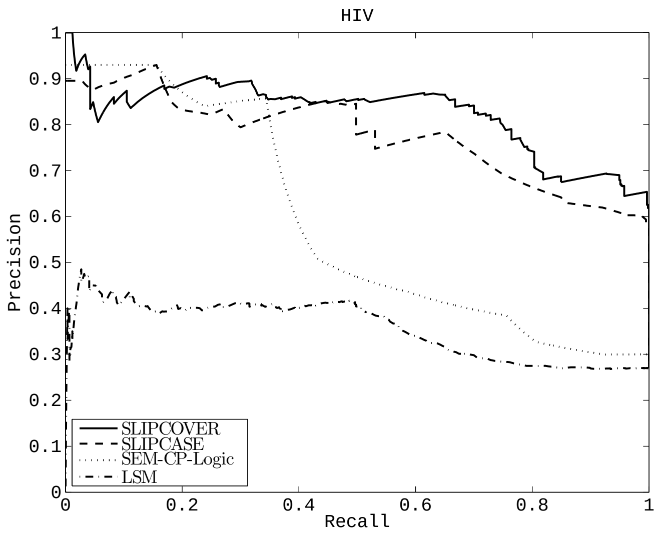


Figure 11.1: PR curves for HIV.

The clauses learned by SEM-CP-Logic that include the two connections are

```
70R:0.30   :-  219EQ.
215FY:0.90 :-  41L.
210W:0.01  :-  215FY.
```

LSM learns

```
1.19 !g41L(a1) v g215FY(a1)
0.28  g41L(a1) v !g215FY(a1)
```

UW-CSE The goal is to predict the `advisedby(X, Y)` predicate, namely the fact that a person `X` is advised by another person `Y`.

The input theory for SLIPCASE is composed of two clauses of the form `advisedby(X,Y):0.5`. The language bias allows `advisedby/2` to appear only in the head and all the other predicates only in the body, so the algorithm can be run with no depth bound.

The language bias for SLIPCOVER allows all predicates to appear in the head and in the body of clauses; all except `advisedby/2` are background predicates. Moreover, nine modeh facts declare disjunctive heads, as shown in Section 11.3. These modeh facts have been defined by looking at the hand crafted theory used for parameter learning in (Bellodi and Riguzzi, 2012a): for each disjunctive clause in the theory, a modeh fact is derived. The clauses of the

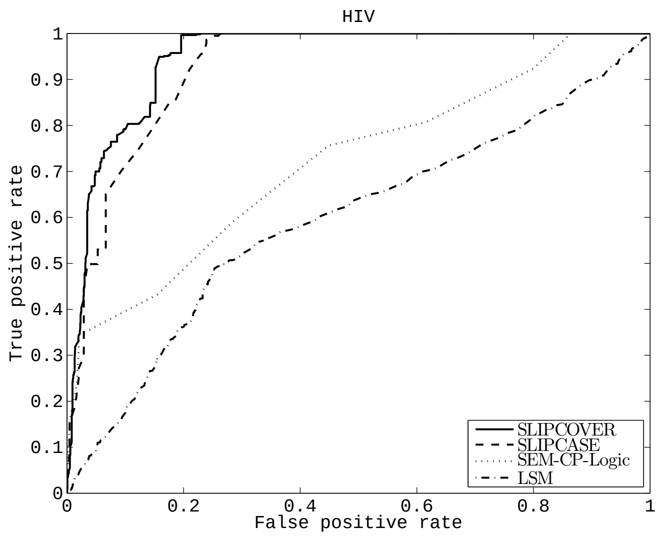


Figure 11.2: ROC curves for HIV.

final theories have one to five head atoms. The simplified semantics has been used to limit learning time.

For LSM, we use the discriminative training algorithm for learning the weights, by specifying advisedby/2 as the only non-evidence predicate, and the MC-SAT algorithm for inference over the test folds, by specifying advisedby/2 as the query predicate.

For Aleph and ALEPH++ExactL1 the language bias allows advisedby/2 to appear in the head only and all the other predicates in the body only.

Results SLIPCASE, due to the restrictive language bias (only advisedby/2 in the clauses' head), learns simple programs composed by a single clause per fold; this also explains the low learning time. In two folds out of five it learns the theory

```
advisedby(A,B):0.264403 :- professor(B), student(A).
```

An example of a theory learned by LSM is

```
3.77122  professor(a1) v !advisedBy(a2,a1)
0.03506  !professor(a1) v !advisedBy(a2,a1)
2.27866  student(a1) v !advisedBy(a1,a2)
1.25204  !student(a1) v !advisedBy(a1,a2)
0.64834  hasPosition(a1,a2) v !advisedBy(a3,a1)
1.23174  !advisedBy(a1,a2) v inPhase(a1,a3)
```

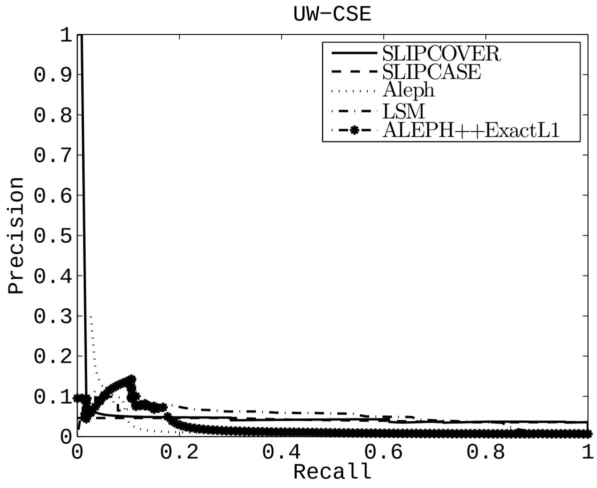


Figure 11.3: PR curves for UW-CSE.

SLIPCOVER learns theories able to better model the domain, at the expense of a longer learning time, which is however the lowest after SLIPCASE. Examples of clauses learned by SLIPCOVER are

```
advisedby(A,B):0.205829 ; tempadvisedby(A,B):0.20422 :- inphase(A,C),
                                                        professor(B).
advisedby(A,B):0.0750594 :- hasposition(B,C),inphase(A,D).
advisedby(A,B):0.118801 :- hasposition(B,C),student(A).
hasposition(A,faculty):0.3197;hasposition(A,fac_affiliate):0.2174;
  hasposition(A,fac_adjunct):0.1479;hasposition(A,fac_emeritus):0.1006;
  hasposition(A,fac_visiting):0.0684751 :- professor(A).
hasposition(A,faculty):0.5673;hasposition(A,fac_affiliate):0.2454;
  hasposition(A,fac_adjunct):0.1061;hasposition(A,fac_emeritus):0.0459;
  hasposition(A,fac_visiting):0.0198 :- taughtby(B,A,C),courselevel(B,D).
hasposition(A,faculty):0.5984 :- professor(A),taughtby(B,A,C).
professor(A):0.402283 :- hasposition(A,B).
professor(A):0.936545 :- taughtby(B,A,C),taughtby(D,A,E),
                         hasposition(A,faculty).
student(A):0.869182 :- ta(B,A,C).
student(A):0.737475 ; professor(A):0.193594 :- ta(B,A,C).
yearsinprogram(A,year_1):0.4151;yearsinprogram(A,year_2):0.2428:-student(A).
```

Aleph and ALEPH++ExactL1 mainly differ in the number of learned clauses, while body literals and their ground arguments are essentially the same. ALEPH++ExactL1 works on more complex MLNs than LSM, and performs slightly better.

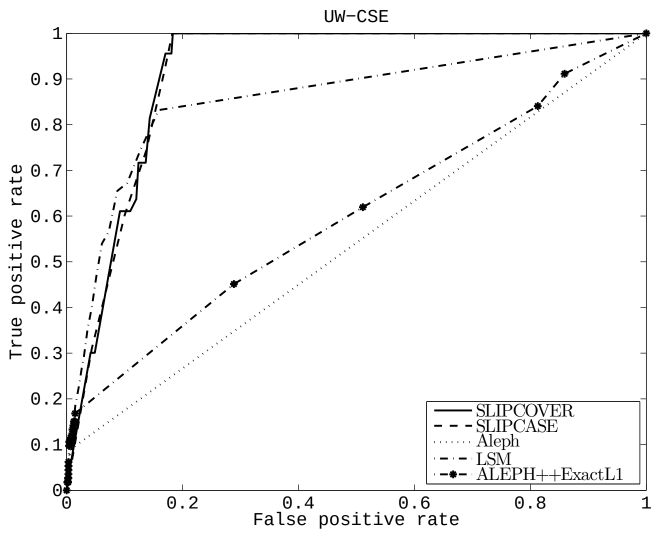


Figure 11.4: ROC curves for UW-CSE.

WebKB The goal is to predict the web pages four categories `coursePage`, `studentPage`, `facultyPage`, `researchProjectPage`.

The input theory for `SLIPCASE` is composed of four clauses of the form
$<$ `class` $>$ `Page(P)` : 0.5. with `class` $=$ {`course`, `faculty`, `researchProject`, `student`}.
The language bias allows predicates representing the four categories both in the head and in the body of clauses, so the theory is recursive. Moreover, the body can contain the atom `linkTo(Id, Page1, Page2)` (linking two pages) and the atom `has(word, Page)` with `word` a constant. The target predicates are treated as closed world, so their literals in clause bodies are resolved only with examples in the background and not with other clauses to limit execution time, therefore the depth D is not relevant. We use a single random variable for each clause instead of one for each grounding of each clause as on option for `EMBLEM` (simplified semantics) to limit the learning time.

The language bias for `SLIPCOVER` allows predicates representing the four categories both in the head and in the body of clauses.

`LSM` fails on this dataset because the weight learning phase quickly exhausts the available memory on our machines (4 GB). This dataset is in fact quite large, with 15 MB input files on average.

For `Aleph` and `ALEPH++ExactL1`, we overcame the limit of one target predicate per run by executing `Aleph` four times on each fold, once for each target predicate. In each run,

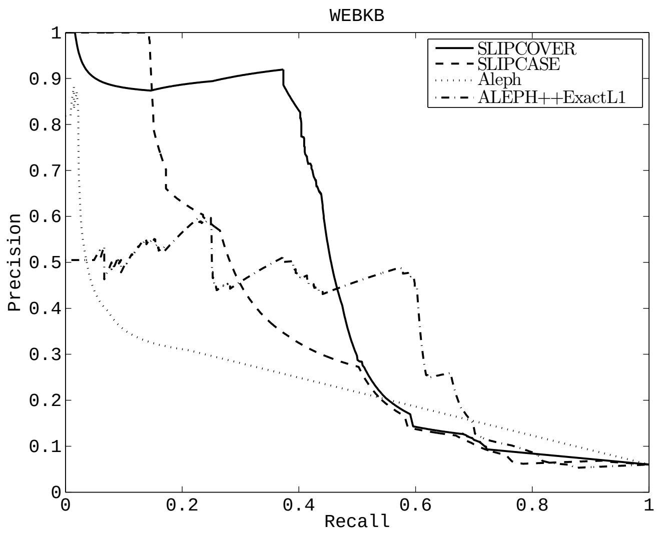


Figure 11.5: PR curves for WebKB.

we remove the target predicate from the `modeb` declarations to prevent `Aleph` from testing cyclic theories and going into a loop.

Results A fragment of a theory learned by `SLIPCOVER` is

```
studentPage(A):0.9398:- linkTo(B,C,A),has(paul,C),has(jame,C),has(link,C).
researchProjectPage(A):0.0321475:- linkTo(B,C,A),has(project,C),
                       has(depart,C), has(nov,A),has(research,C).
facultyPage(A):0.436275 :- has(professor,A),has(comput,A).
coursePage(A):0.0630934 :- has(date,A),has(gmt,A).
```

`Aleph` and `ALEPH++ExactL1` learn many more clauses for every target predicate than `SLIPCOVER`. For the `coursePage` predicate for example `ALEPH++ExactL1` learns

```
coursePage(A) :-   has(file,A), has(instructor,A), has(mime,A).
coursePage(A) :-   linkTo(B,C,A), has(digit,C), has(theorem,C).
coursePage(A) :-   has(instructor,A), has(thu,A).
coursePage(A) :-   linkTo(B,A,C), has(sourc,C), has(syllabu,A).
coursePage(A) :-   linkTo(B,A,C), has(homework,C), has(syllabu,A).
coursePage(A) :-   has(adapt,A), has(handout,A).
coursePage(A) :-   has(examin,A), has(instructor,A), has(order,A).
coursePage(A) :-   has(instructor,A), has(vector,A).
coursePage(A) :-   linkTo(B,C,A), has(theori,C), has(syllabu,A).
coursePage(A) :-   linkTo(B,C,A), has(zpl,C), has(topic,A).
coursePage(A) :-   linkTo(B,C,A), has(theori,C), has(homework,A).
coursePage(A) :-   has(decemb,A), has(instructor,A), has(structur,A).
```

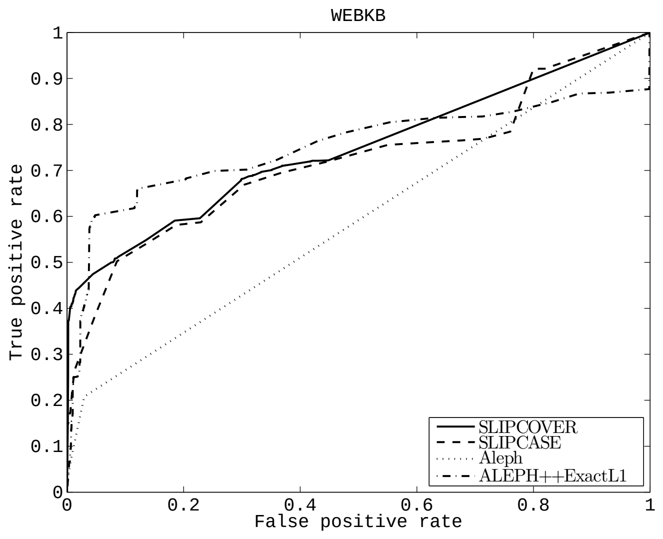


Figure 11.6: ROC curves for WebKB.

```
coursePage(A) :-   has(apr,A), has(client,A), has(cours,A).
   ...
```

In this domain SLIPCASE learns fewer clauses (many with an empty body) for each fold than SLIPCOVER. Moreover, SLIPCASE search strategy generates thousands of refinements for each theory extracted from the beam, while SLIPCOVER beam search generates less than a hundred refinements from four bottom clauses (one for each target predicate), thus achieving a lower learning time.

Mutagenesis The goal is to predict if a drug is active, i.e. the target predicate active(drug). For a more detailed description of the dataset see Section 10.4.
The input theory for SLIPCASE is composed of two clauses of the form active(A):0.5. The language bias for SLIPCASE and SLIPCOVER allows active/1 only in the head, so D is not relevant.

LSM failed on this dataset because the structure learning phase (*createrules* step) quickly gives a memory allocation error when generating bond/4 groundings.

Results On this dataset, SLIPCOVER learns more complex programs with respect to those learned by SLIPCASE, that contain only two or three clauses for each fold.

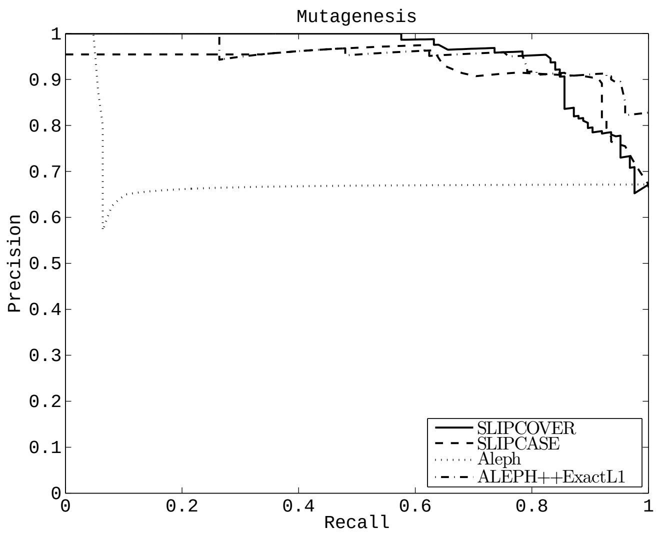


Figure 11.7: PR curves for Mutagenesis.

(Srinivasan et al., 1994) report the results of the application of `Progol` to this dataset. In the following we presents the clauses learned by `Progol` paired with the most similar clauses learned by `SLIPCOVER` and `ALEPH++ExactL1`.

`Progol` learned

```
active(A) :- atm(A,B,c,10,C),atm(A,D,c,22,E),bond(A,D,B,1).
```

where a carbon atom *c* of type 22 is known to be in an aromatic ring.

`SLIPCOVER` learns

```
active(A):9.41508e-06 :- bond(A,B,C,7), atm(A,D,c,22,E).
active(A):1.14234e-05 :- benzene(A,B), atm(A,C,c,22,D).
```

where a bond of type 7 is an aromatic bond and benzene is a 6-membered carbon aromatic ring.

`Progol` learned

```
active(A) :- atm(A,B,o,40,C), atm(A,D,n,32,C).
```

`SLIPCOVER` instead learn:

```
active(A):5.3723e-04 :-  bond(A,B,C,7), atm(A,D,n,32,E).
```

The clause learned by `Progol`

```
active(A):-  atm(A,B,c,27,C),bond(A,D,E,1),bond(A,B,E,7).
```

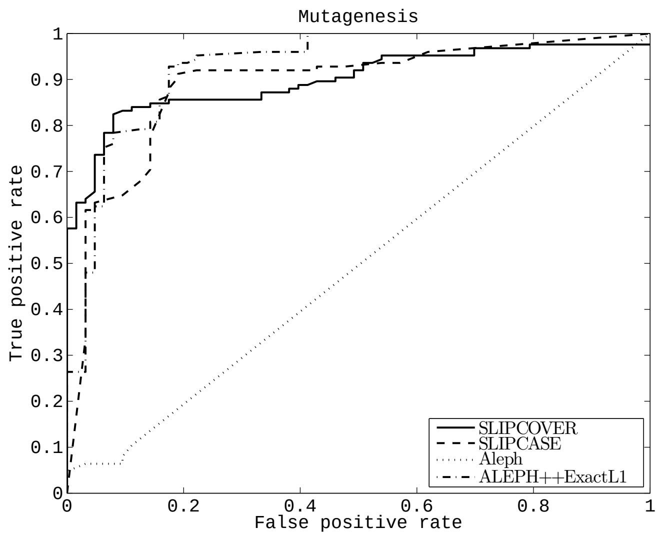


Figure 11.8: ROC curves for Mutagenesis.

where a carbon atom *c* of type 27 merges two 6-membered aromatic rings, is similar to SLIPCOVER's

```
active(A):0.135014 :- benzene(A,B), atm(A,C,c,27,D).
```

ALEPH++ExactL1 instead learns from all the folds

```
active(A) :- atm(A,B,c,27,C), lumo(A,D), lteq(D,-1.749).
```

The Progol clauses

```
active(A) :- atm(A,B,h,3,0.149).
active(A) :- atm(A,B,h,3,0.144).
```

mean that a compound with a hydrogen atom h of type 3 with partial charge 0.149 or 0.144 is active. Very similar charge values (0.145) are found by ALEPH++ExactL1.

SLIPCOVER learns

```
active(A):0.945784 :- atm(A,B,h,3,C),lumo(A,D),D=<-2.242.
active(A):0.01595  :- atm(A,B,h,3,C),logp(A,D),D>=3.26.
active(A):0.00178048 :- benzene(A,B),ring_size_6(A,C),atm(A,D,h,3,E).
```

SLIPCASE instead learned clauses that relate the activity mainly to benzene compounds and energy and charge values; for instance the theory learned from one fold is:

```
active(A):0.299495 :-  benzene(A,B),lumo(A,C),lteq(C,-1.102),benzene(A,D),
         logp(A,E),lteq(E,6.79),gteq(E,1.49),gteq(C,-2.14),gteq(E,-0.781).
active(A) :-  lumo(A,B),lteq(B,-2.142),lumo(A,C),gteq(B,-3.768),lumo(A,D),
              gteq(C,-3.768).
```

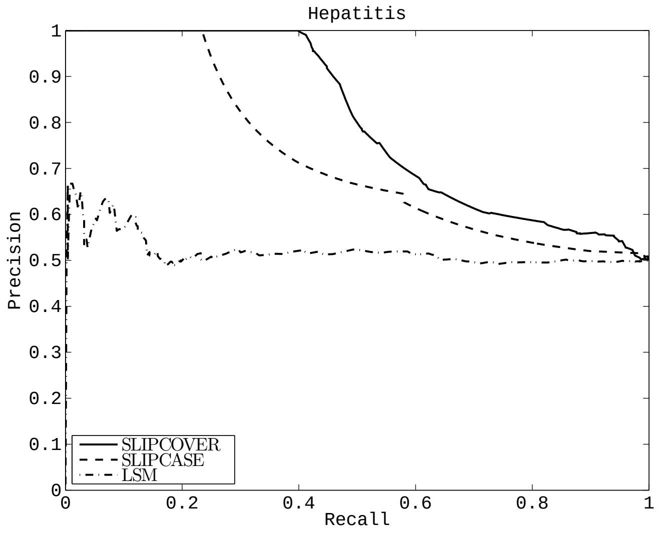


Figure 11.9: PR curves for Hepatitis.

Hepatitis The goal is to predict the type of hepatitis of a patient, so the target predicate is type(patient, type) where type can be type_b or type_c. We generated negative examples for type/2 by adding, for each fact type(patient, type_b), the fact neg(type(patient, type_c)) and for each fact type(patient, type_c), the fact neg(type(patient, type_b)).

The input theory for SLIPCASE contains the two clauses `type(A,type_b):0.5.` and `type(A,type_c):0.5.`

The language bias for SLIPCASE and texttttSLIPCOVER allows type/2 only in the head and all the other predicates in the body of clauses, hence the depth D is not relevant. NBC is not relevant as only `type/2` can appear in clause heads and the simplified semantics is necessary to limit learning time.

For LSM, we use the discriminative training algorithm for learning the weights, by specifying type/2 as the only non-evidence predicate, and the MC-SAT algorithm for inference over the test fold, by specifying type/2 as the query predicate.

Results Examples of clause learned by SLIPCOVER are

```
type(A,type_b):0.344348 :- age(A,age_1).
type(A,type_b):0.403183 :- b_rel11(B,A),fibros(B,C).
type(A,type_c):0.102693 :- b_rel11(B,A),fibros(B,C),b_rel11(D,A),
                           fibros(D,C),age(A,age_6).
type(A,type_c):0.0933488 :- age(A,age_6).
```

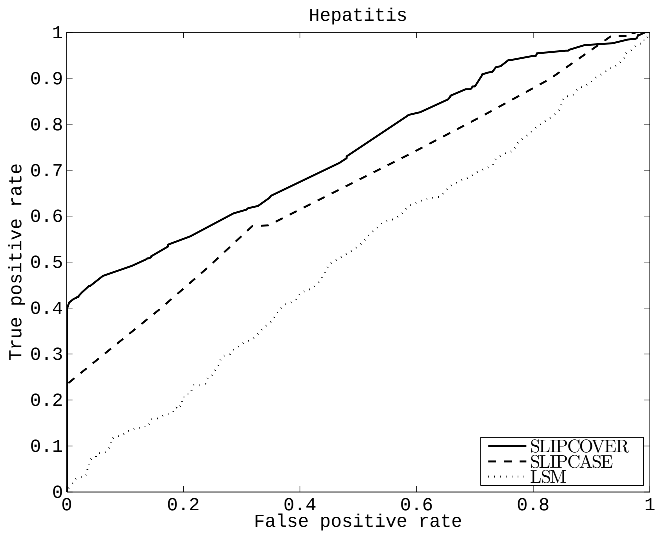


Figure 11.10: ROC curves for Hepatitis.

```
type(A,type_c):0.770442 :-  b_rel11(B,A),fibros(B,C),b_rel13(D,A).
```

Examples of clauses learned by `SLIPCASE` are

```
type(A,type_b):0.210837.
type(A,type_c):0.52192 :- b_rel11(B,A),fibros(B,C),b_rel11(D,A),fibros(B,E).
type(A,type_b):0.25556.
```

`LSM` long execution time is mainly affected by the *createrules* phase, where `LSM` counts the true groundings of all possible unit and binary clauses to find those that are always true in the data: it takes 17 hours on all folds; moreover this phase produces only one short clause in every fold.

Table 11.4: Results of the experiments in terms of the *Area Under the PR Curve* averaged over the folds. '-' means that the algorithm is not applicable. The standard deviations are also shown.

System	HIV	UW-CSE	WebKB	Mutagenesis	Hepatitis
`SLIPCOVER`	0.82 ± 0.05	0.11 ± 0.08	0.47 ± 0.05	0.95 ± 0.01	0.80 ± 0.01
`SLIPCASE`	0.78 ± 0.05	0.03 ± 0.01	0.31 ± 0.21	0.92 ± 0.08	0.71 ± 0.05
`LSM`	0.37 ± 0.03	0.07 ± 0.02	-	-	0.53 ± 0.04
`SEM-CP-L.`	0.58 ± 0.03	-	-	-	-
`Aleph`	-	0.07 ± 0.02	0.15 ± 0.05	0.73 ± 0.09	-
`ALEPH++`	-	0.05 ± 0.006	0.37 ± 0.16	0.95 ± 0.009	-

Table 11.5: Results of the experiments in terms of the *Area Under the ROC Curve* averaged over the folds. '-' means that the algorithm is not applicable. The standard deviations are also shown.

System	HIV	UW-CSE	WebKB	Mutagenesis	Hepatitis
SLIPCOVER	0.95 ± 0.01	0.95 ± 0.01	0.76 ± 0.01	0.89 ± 0.05	0.74 ± 0.01
SLIPCASE	0.93 ± 0.01	0.89 ± 0.03	0.70 ± 0.03	0.87 ± 0.05	0.66 ± 0.06
LSM	0.60 ± 0.003	0.85 ± 0.21	-	-	0.52 ± 0.06
SEM-CP-L.	0.72 ± 0.02	-	-	-	-
Aleph	-	0.55 ± 0.001	0.59 ± 0.04	0.53 ± 0.04	-
ALEPH++	-	0.58 ± 0.07	0.73 ± 0.27	0.90 ± 0.004	-

Table 11.6: *Normalized Area Under the PR Curve* for the high-skew datasets. The skew is the proportion of positive examples on the total testing examples.

System	Mutagenesis	Hepatitis
Skew	0.66	0.5
SLIPCOVER	0.91	0.71
SLIPCASE	0.86	0.58
LSM	-	0.32
Aleph	0.51	-
ALEPH++	0.91	-

Overall remarks From the results we can observe that:

- On HIV, SLIPCOVER achieves significantly higher areas with respect to SLIPCASE, SEM-CP-Logic and LSM; in turn, SLIPCASE is able to achieve higher AUCPR and AUCROC with respect to LSM and SEM-CP-logic;
- On UW-CSE, SLIPCOVER achieves higher AUCPR and significantly higher AUCROC than all other systems. SLIPCASE achieves higher AUCROC after SLIPCOVER, but the lowest AUCPR. This is a difficult dataset, as testified by the low values of areas achieved by all systems, and represents a challenge for structure learning algorithms;
- On WebKB, SLIPCOVER achieves higher AUCPR and AUCROC than the other systems but the differences are not statistically significant;
- On Mutagenesis, SLIPCOVER achieves higher AUCPR and AUCROC than the other systems, except ALEPH++ExactL1, which achieves the same AUCPR as SLIPCOVER

Table 11.7: *Execution time* in hours of the experiments on all datasets. '-' means that the algorithm is not applicable.

System	HIV	UW-CSE	WebKB	Mutagenesis	Hepatitis
SLIPCOVER	0.115	0.040	0.807	20.924	0.036
SLIPCASE	0.010	0.018	5.689	1.426	0.073
LSM	0.003	2.653	-	-	25
Aleph	-	0.079	0.200	0.002	-
ALEPH++	-	0.061	0.320	0.050	-

Table 11.8: Results of *t-test* on all datasets relative to AUCPR. p is the p-value of a paired two-tailed t-test between SLIPCOVER and the other systems (significant differences in favor of SLIPCOVER at the 5% level in bold). SC is SLIPCASE, SO is SLIPCOVER, L is LSM, SEM is SEM-CP-Logic, A is Aleph, A++ is ALEPH++ExactL1.

System Couple	HIV	UW-CSE	WebKB	Mutagenesis	Hepatitis
SO-SC	**0.02**	0.13	0.24	0.15	**0.04**
SO-L	**4.11e-5**	0.40	-	-	**3.18e-4**
SO-SEM	**4.82e-5**	-	-	-	-
SO-A	-	0.11	0.06	**2.84e-4**	-
SO-A++	-	0.18	0.57	0.90	-

Table 11.9: Results of *t-test* on all datasets relative to AUCROC. p is the p-value of a paired two-tailed t-test between SLIPCOVER and the other systems (significant differences in favor of SLIPCOVER at the 5% level in bold). SC is SLIPCASE, SO is SLIPCOVER, L is LSM, SEM is SEM-CP-Logic, A is Aleph, A++ is ALEPH++ExactL1.

System Couple	HIV	UW-CSE	WebKB	Mutagenesis	Hepatitis
SO-SC	**0.008**	**0.025**	0.14	0.49	**0.050**
SO-L	**2.52e-5**	0.29	-	-	**0.003**
SO-SEM	**6.16e-5**	-	-	-	-
SO-A	-	**4.26e-6**	0.11	**3.93e-5**	-
SO-A++	-	**3.15e-4**	0.88	0.66	-

and non statistically significant higher AUCROC. The differences between SLIPCOVER and Aleph are instead statistically significant. SLIPCASE has lower areas than SLIPCOVER and ALEPH++ExactL1.

- On Hepatitis, SLIPCOVER achieves significantly higher AUCPR and AUCROC than SLIPCASE and LSM. Our algorithms are both much faster than LSM, which takes several hours.

Thus SLIPCOVER achieves larger areas than all the other systems in both AUCPR and AUCROC, for all datasets except Mutagenesis, where ALEPH++ExactL1 behaves slightly better in terms of AUCROC. SLIPCOVER always outperforms SLIPCASE due to the more advanced language bias and search strategy. SLIPCASE outperforms the remaining systems on three datasets out of five for AUCROC and two datasets for AUCPR.

We experimented with various SLIPCASE parameters in order to obtain an execution time similar to SLIPCOVER's and the best match we could find is the one shown. Increasing the number of SLIPCASE iterations often gave a memory error when building BDDs so we could not find a closer match.

Both SLIPCOVER and SLIPCASE always outperform Aleph, showing that a probabilistic ILP system can better model the domain than a purely logical one.

SLIPCOVER's advantage over LSM lies in a smaller memory footprint, that allows it to be applied in larger domains, and in the effectiveness of the bottom clauses in guiding the search, in comparison with the more complex clause construction process in LSM.

SLIPCOVER improves on ALEPH++ExactL1 by being able to learn disjunctive clauses and by more tightly combining the structure and parameter searches.

The similarity in learning times between HIV and UW-CSE for SLIPCASE despite the difference in the number of predicates for the two domains is due to the different specifications in the language bias for the theory refinements' generation: every predicate in HIV can be used in the clauses' body and in the head, while in UW-CSE only one is allowed for the head.
The long learning time spent on WebKB is probably due to the knowledge base size and to the cyclicity of the LPAD.

The area differences between SLIPCOVER and the other systems are statistically significant in its favor in 15 out of 30 cases at the 5% significance level.

Part IV

Foundations of Description Logics

Chapter 12

The Present and the Future of the Web

Today the Web provides the simplest way to share information and literally everyone writes Web pages. The *Hypertext Markup Language* (HTML) is typically the language used to code information about renderization (font size, color, position on screen, etc.) and hyperlinks to other Web pages or resources (files, e-mail addresses, etc.) on the Web. The Web keeps growing very fast, however most pages are still designated for human consumption and cannot be processed by machines. Computers are used only to display the information, that is to decode the color schema, headers and links.

Web search engines, the most popular tools to help retrieve Web pages, do not offer support to interpret the results; this situation is progressively getting worse as the size of search results is becoming too large, since most users only browse through the top results, discarding the remaining ones. Finding relevant information on the Web is not as easy as we would desire.

In the next two Sections we discuss the characteristics of the current “syntactic” Web and of its (possible) future “semantic” Web. For a detailed coverage of these aspects see (Breitman et al., 2007).

12.1 The Syntactic Web

Today’s Web may be defined as the *Syntactic Web*, where information presentation is carried out by computers, and the interpretation and identification of relevant information is delegated to human beings. Because the volume of digital data is growing at an exponential rate, it is becoming impossible for human beings to manage its complexity. This phenomenon, called information overload, poses a question: why can’t computers do this job for us?

One of the reasons resides in the fact that Web pages do not contain information about themselves, i.e., about their contents and the subjects to which they refer.

Web search engines help identify relevant Web pages, but they suffer from the following limitations:

- Search results might contain a large number of entries, but they might have low precision (being of little interest);
- Search results are sensitive to the vocabulary used. Indeed, users frequently formulate their search in a vocabulary different from that which the relevant Web pages adopt;
- Search results are a list of references to individual Web pages but, among them, there are many entries that belong to the same Web site.

The semantic content, that is, the meaning of the information in a Web page, is coded in a way that is accessible to human beings alone. There is a need to add more semantics to the Web pages so that they can be processed by machines as well as by humans.

12.2 The Semantic Web

In 2001, Berners-Lee, Hendler and Lassila published a revolutionary article in *Scientific American*, entitled "The Semantic Web: a new form of Web Content That Is Meaningful to Computers Will Unleash a Revolution of New Possibilities", where they describe future scenarios in which the Semantic Web will have a fundamental role in the day life of individuals.

In one of these scenarios, Lucy needs to schedule a series of medical consultations for her mother. A series of restrictions applies to this scenario: Lucy's tight schedule, geographical location constraints, doctor's qualifications, adherence to their Social Security plan. To help Lucy find a solution, there is a software agent, capable of negotiating among different parties: the doctor, Lucy's agenda and medical services directory. Although each party codes its information in a different way, because of a semantic layer, they are able to interact and exchange data in a meaningful way. The enabling technology is what the authors called the Semantic Web. Most of the actions described in the scenario can be achieved in the Syntactic Web of today, but with many comes-and-goes between different Web sites.

In order to organize Web content, artificial intelligence researchers proposed a series of *conceptual models*. The central idea is to categorize information similarly to classify living beings: biologists use the Linnaean taxonomy, adopted by the scientific community worldwide. On the other hand, in the same environment we can find Web sites designed for specialists, personal Web pages, vendors' Web sites: in this anarchical scenario it is difficult to imagine that a single organization model could prevail. Hendler's prediction is that every business, enterprise, university and organization on the Web of the future will have its own organizational model.

The most important concepts of Semantic Web are discussed in the remainder of this section and are graphically represented in Figure 12.1.

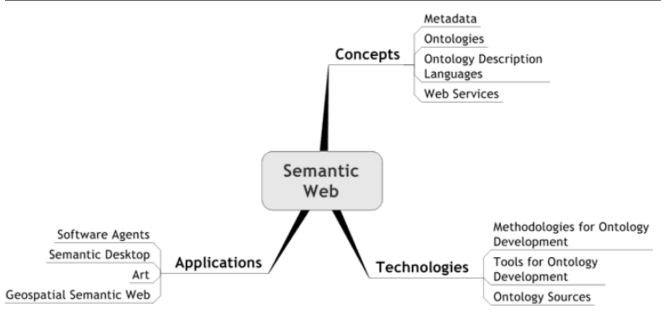


Figure 12.1: Themes related to the Semantic Web.

Metadata Metadata are data about data and serve to index Web pages in the Semantic Web, allowing other computers to acknowledge what the Web page is about. The number of institutions and objects - Web pages - to be catalogued are both enormous and distributed all over the world, coded in different languages, by different groups.

Ontologies The word *ontology* comes from the Greek *ontos* (being) + *logos* (word). It was introduced in philosophy in the XIX century by German philosophers:

The subject of Ontology is the study of the categories of things that exist in some domain. The product of such a study, called an ontology, is a catalogue of the types of things that are assumed to exist in a domain of interest D from the perspective of a person who uses a language L for the purpose of talking about D. The types in the ontology represent the predicates, word senses, or concept and relation types of L. (Sowa 1997)

In computer science, ontologies were adopted in AI to facilitate knowledge sharing and reuse. Today they are used in areas such as intelligent information integration, cooperative information systems, agent-based software engineering and electronic commerce. Ontologies are conceptual models that capture the vocabulary used in semantic applications, guaranteeing communication free of ambiguities. They will be the *language of the Semantic Web*. In Chapter 13 we discuss ontologies, their formalisms, types and basic elements.

Formal Systems Formal systems provide the ability to deduce new sentences from existing sentences using specific inference rules. Logical inference is an essential component of a Semantic Web ontology formalism. Because First Order Logic is intractable, the Semantic Web community has been exploring Description Logic as the paradigm formal system. In Chapter 14 we introduce Description Logic.

Ontology description languages Ontology description languages are designed to define ontologies. They are sometimes called lightweight or markup or Web-based ontology languages. The Resource Description Framework (RDF) is a general purpose language for representing information about resources in the Web and, to some extent, a lightweight ontology language. The lack of expressiveness of RDF was partly eased with the introduction of the RDF Vocabulary Description Language 1.0: RDF Schema, which offers primitives to model hierarchies of classes and properties. The Ontology Inference Layer (Oil) is the result of the On-To-Knowledge Project and is based on Description Logic. The Defense Advanced Research Projects Agency (DARPA) sponsored the DARPA Agent Markup Language (DAML) Program. These two languages were amalgamated into DAML+Oil. A reformatted version of it served as a starting point for the Web Ontology Language (OWL). In Section 13.4 we review OWL.

Methodologies and Tools for Ontology Development The number of tools for ontology editing, visualization and verification grows. The best examples are the Protégé and OilEd tools, which sprung from large cooperation projects involving many universities and countries. Crafting an ontology today is possibly no harder than creating a Web page. The number of lightweight ontologies, that is, developed by independent groups and organizations rather than by knowledge engineers, is rapidly growing as can be verified by visiting some of the public ontology repositories, such as the DAML one.

Applications of Semantic Web Technologies Applications are not limited to indexing Web pages. Other areas provide challenges, for example consider software agents, defined as autonomous software applications that act for the benefit of their users. A personal agent in the Semantic Web will be responsible for understanding the desired tasks and user preferences, searching for information on available resources, communicating with other agents, and comparing information to provide adequate answers. So the solution developed must allow information sharing and have efficient communication. In Section 13.5 examples of applications are provided.

Chapter 13

Ontologies in Computer Science

This chapter introduces the fundamental building blocks about ontologies. Section 13.1 summarizes the various uses of the term ontology in computer science. Section 13.2 reports different classifications of ontologies known in literature. Section 13.3 describes the main components of an ontology and Section 13.4 the background for a better understanding of ontology description languages and tools. Section 13.5 illustrates application fields of ontologies.

13.1 Defining the term Ontology

The word *ontology* can be used as an uncountable noun ("Ontology" with the uppercase initial) and as a countable noun (an "ontology" with lowercase initial).

In the first case it refers to a philosophical discipline, that deals with the nature and structure of things per se, even independently of their actual existence.

In the second case, used in Computer Science, it refers to a special kind of information object or computational artifact. The path followed by the Ontology concept from Philosophy to Computer Science was the result of different requirements in various fields:

- In the field of *Artificial Intelligence* (AI) the need for knowledge representation came from the goal to make an agent do tasks autonomously and systematically: the agent's decisions must be made based on knowledge. So it was necessary to find a method for representing knowledge in a computational environment.

- The object-oriented paradigm gave *Software Engineering* a new style of representing elements, by classifying the world into objects with attributes (properties) and methods (possible actions that they could do). Object-orientation is a hierarchical way of thinking about the world where an object inherits properties and methods from its parents. At a higher level, software engineers found that representing concepts - the meaning of things - may also help to simplify some problems like systems interoperability.

- The *Database* community needed conceptual high level models to give an abstract representation of a problem domain without considering implementation issues.

Therefore, three different areas have the same problem of *representation of concepts*. This representation is a starting point to generate knowledge. Differently from Philosophy, Computer Science assumes that everything that can be represented is real: concepts are primary principles and all the things that exist in the world are susceptible to being represented by a concept which captures its meaning (process of *conceptualization)*.

Currently, the most common definition of ontology in Computer Science is Gruber's: ontology is an "explicit specification of a conceptualization".

Example 27 *A computational ontology can be used to formally model the structure of a system, the relevant entities and relations: an example can be a company with all its employees and their interrelationships. The ontology engineer analyzes the relevant entities (subjects, objects, processes, etc.) and organizes them into concepts and relations. The backbone of an ontology consists of a generalization/specialization hierarchy of concepts, i.e., a taxonomy.*

Here Person, Manager *and* Researcher *might be relevant concepts, where the first is superconcept of the latter two.* Cooperates-with *can be a relevant relation. A concrete person working in a company would then be an* instance *of some concepts.*

For detailed references on ontologies see (Staab and Studer, 2009) and (Sharman et al., 2007).

13.2 Classification of Ontologies

There are several classifications of ontologies, based on different parameters. Guarino (1998) classifies them by their level of generality in:

- top-level ontologies, which describe domain-independent concepts such as space, time, etc., and which are independent of specific problems;

- domain and task ontologies which describe, respectively, the vocabulary related to a generic domain and a generic task;
- application ontologies, which describe concepts depending on a particular domain and task.

Van Heijst, Schreiber and Wielinga (1997) classify them according to their use in:

- terminological ontologies, which specify which terms are used to represent the knowledge;
- information ontologies, which specify storage structure data;
- knowledge modeling ontologies, which specify the conceptualization of the knowledge.

Fensel (2004) classifies ontologies in:

- domain ontologies, which capture the knowledge valid for a particular domain;
- metadata ontologies, which provide a vocabulary for describing the content of on-line information sources;
- generic ontologies, which capture general knowledge about the world providing basic notions for things like time, space, state, etc;
- representational ontologies, that define the basic concepts for the representation of knowledge;
- method and tasks ontologies, which provide terms specific for particular tasks and methods.

Gomez-Perez, Fernandez-Lopez and Corcho (2003) classify ontology based on the level of specification of relationships among the terms, in:

- lightweight ontologies, which include concepts, concept taxonomies, relationships between concepts and properties that describe concepts;
- heavyweight ontologies, which add axioms and constraints to lightweight ontologies. Those axioms and constraints clarify the intended meaning of the terms involved into the ontology.

13.3 Ontology Representation

Ontology comprises four main components: concepts, instances, relations and axioms. A general definition of these components is provided in the following.

- A *Concept* (also known as a *class* or a *term*) is an abstract group, set or collection of objects. It is the fundamental element of the domain and usually represents a group or class whose members share common properties. This component is represented in hierarchical graphs that look similar to object-oriented systems. A concept can be a "super-class", representing a parent class, or a "subclass" which represents a subordinate or child class. For instance, person could represent a class with many subclasses, such as students, employees, retirees.
- An *Instance* (also known as an *individual*) is the 'ground-level' component of an ontology which represents a specific object or element of a concept or class. For example, "Italy" could be an instance of the class "European countries" or simply "countries".
- A *Relation* (also known as a slot) is used to express relationships between instances of two concepts. More specifically, it describes the relationship between instances of a first concept, representing the domain, and instances of a second concept, representing the range. For example, "study" could be a relationship between individuals of the concept "person" (which is a domain concept) and individuals of "university" or "college" (which is a range concept).
- An *Axiom* is used to impose constraints on classes or instances, so axioms are generally expressed using logic-based languages; they are used to verify the consistency of the ontology.

13.4 Ontology Description Languages

Ontology description languages are specifically designed to define ontological knowledge systems. They recently received considerable attention, boosted by the emergence of the Semantic Web. Such languages should be easily understood by computers.

On 10 February, 2004, the World Wide Web Consortium (W3C) announced its support for two Semantic Web technology standards, RDF and OWL. A layered model for the Semantic

Web can be constructed to correlate ontology description languages, OWL, RDF and RDF Schema, XML, as depicted in Figure 13.1.

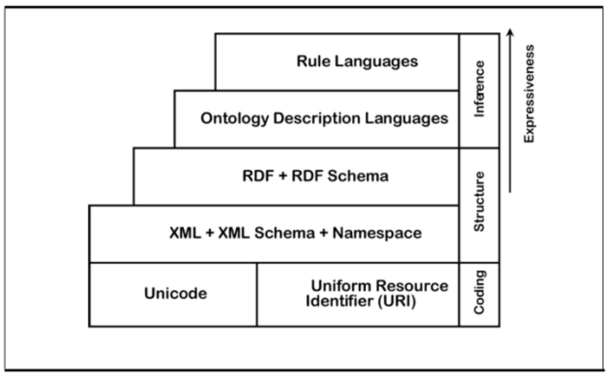

Rule Languages
Ontology Description Languages
RDF + RDF Schema
XML + XML Schema + Namespace
Unicode
Uniform Resource Identifier (URI)
Inference
Structure
Coding
Expressiveness

Figure 13.1: An architecture for the Semantic Web.

The bottom layer offers character encoding (Unicode) and referencing (URI) mechanisms. The second introduces XML as the document exchange standard. The third layer accommodates RDF and RDF Schema as mechanisms to describe the resources available on the Web. XML is designed for syntax, while RDF is intended for semantics. RDF can be used in several applications, one of the most important being resource discovery, used to enhance search engine capabilities. The RDF model is based on triples: a resource (the subject), the object and the predicate. It is possible to say that <subject> has a property <predicate> valued by <object>. RDFS is used to define RDF vocabularies.
Ontology description languages appear in the fourth layer to capture more semantics; they are also called ontology languages, Web ontology languages or markup ontology languages. Examples are:

- *Ontology Interchange Language (OIL)*, which provides modelling primitives used in frame-based and DL-oriented ontologies.

- DARPA Agent Markup Language (DAML) + Ontology Inference Layer (OIL), or *DAML+OIL*. DAML+OIL has many limitations: it lacks property constructors, it has no composition or transitive closure, its only property types are transitive and symmetrical, sets are the only collection type (there are no bags or lists), there is no comparison in data value, it allows only unary and binary relations, and there are neither default values nor variables.

- **Web Ontology Language (OWL)**: was built using RDF to remedy the weaknesses in DAML+OIL. It provides a richer integration and interoperability of data between communities and domains. OWL is an extension of RDF Schema; in other words, it builds on RDF and RDFS, using XML syntax and the RDF meaning of classes and properties. W3C classifies OWL into three sublanguages: OWL Lite, OWL DL and OWL Full.

  OWL Lite is the simplest version of OWL and provides a classification hierarchy and simple constraints; it permits only the expression of relationships with maximum cardinality equal to 0 or 1, thus being designed for easy implementation. The disadvantage of this sublanguage is restricted expressiveness.

  OWL DL is so called because it uses Description Logic to represent the relations between objects and their properties. Indeed, it provides maximum expressiveness while preserving the completeness of reasoning. OWL Lite is a sublanguage of OWL DL.

  The sublanguage *OWL Full* provides the highest expressiveness and the syntactic freedom of RDF but without preserving guarantees on computational complexity. OWL Lite and OWL DL are sublanguages of OWL Full.

  OWL is supported by tools and infrastructure:

  - APIs (e.g., OWL API, Thea, OWLink)
  - Development environments (e.g., Protégé, Swoop, TopBraid Composer, Neon)
  - Reasoners and Information Systems (e.g., Pellet, Racer, HermiT, Quonto, etc.)

The topmost layer introduces expressive rule languages, that provide knowledge representation structures. In practical applications, as well as in human communication, we need to use a *language* **L** to refer to the elements of a conceptualization: for instance, to express the fact that person a cooperates with b, we have to introduce a specific symbol (a predicate symbol), *cooperates-with*, which is intended to represent a certain conceptual relation.

Looking at Figure 13.2, at one extreme we have rather informal approaches for the language **L** that may allow the definitions of terms only, with little or no specification of the meaning of the term. At the other end, we have formal approaches, i.e., logical languages that allow specifying formal logical theories. As we move along the spectrum, the amount of meaning specified and the degree of formality increases (reducing ambiguity); there is also increasing support for automated reasoning.

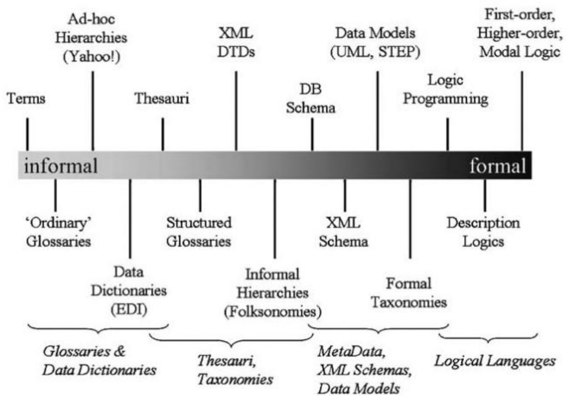


Figure 13.2: Different approaches to the language according to (Uschold and Gruninger, 2004). Typically, logical languages are eligible for the formal, explicit specification, and thus for ontologies.

In practice, **the rightmost category** of logical languages is usually considered as **formal**. Here one encounters the trade-off between expressiveness and efficiency:

- *higher-order logic, full First Order Logic or modal logic* are very expressive, but do often not allow for sound and complete reasoning and if they do, reasoning sometimes remains intractable. Gruber proposes using frames and First Order Logic. This schema uses classes, relations, functions, formal axioms and instances. Classes are the representation of relevant concepts in the domain; classes are organized in taxonomies. Relations represent different types of associations between individuals in a domain. Functions are a special case of relations. Formal axioms are sentences always true and are used to generate new knowledge and to verify the consistency of the ontology. Instances represent elements in the ontology.

- just before the above logics, there are less stringent *subsets of First Order Logic*, which feature decidable and more efficient reasoners. They can be split in two major paradigms.

    1. First, languages from the family of *Description Logics (DL)*, e.g., OWL-DL, are strict subsets of First Order Logic; the proposal of their use for modeling ontologies comes from (Baader, Horrocks and Sattler, 2004): they are described in detail in Chapter 14.

    2. The second comes from the tradition of logic programming with one prominent representative being F-Logic. Though logic programming (LP) often uses a syntax

comparable to First Order Logic, it assumes a different interpretations of formulae: LP selects only a subset of models to judge semantic entailment of formulae.

In the middle of the spectrum one can find some other relevant languages:

- Software Engineering techniques like Unified Modeling Language (UML) are used for modeling ontologies, in particular the lightweight ones; for heavyweight ontologies it is necessary to enrich UML with, for example, the Object Constraint Language (OCL), which is the language for describing constraints in UML. In UML class diagrams each class represents a concept. The instances of classes are represented by objects. Concept taxonomies are represented through generalization relationships. Binary relations are represented through association relationships.

- Database technologies are another possibility to represent ontologies using for example Entity-Relationship (ER) diagrams. Concepts can be represented using entities, which have attributes that are properties of the concept, with name and type. Relations between concepts are represented by relationships, which have a cardinality.

13.5 Applications

Database systems, Software Engineering and Artificial Intelligence are the three most important fields where ontologies have been used to construct solutions.

The main purpose for using ontologies is as means of integrating several platforms or applications, by looking for the most natural way to inter-communicate. So, it is important to have a set of concepts that form the vocabulary used by the applications and a set of rules for solving semantic heterogeneity. This allows transforming data from one application to another. Another use of ontologies is for domain modelling. Ontologies hope to represent an objective point of view of a part of the reality, and they include the main characteristics that would be used by any application that gives a particular solution in a modeled domain.

In Database systems, the ontologies help to model a specific domain and facilitate the integration with other databases, and improve information search.

In Software Engineering, a specific ontology could be taken as a reference point to validate a system acting over a particular domain.

In Artificial Intelligence ontologies help to ease the inference process.

Chapter 14

Knowledge Representation in Description Logics

Description Logic denotes a *family* of knowledge representation (KR) formalisms that model the application domain by defining the relevant concepts of the domain and using them to specify properties of objects and individuals in the domain (Baader and Nutt, 2003). Description Logics received attention recently because they provide a formal framework for the Web ontology language OWL, proposed as a standard (cf. Section 13.4). The history of Description Logics goes back to the discussion about knowledge representation formalisms in the 1980s. At the heart of the discussion was the categorization into *non-logic-based* and *logic-based formalisms*.

The non-logic-based formalisms claimed to be closer to one's intuition and easier to comprehend: they include semantic networks, frames, rule-based representations. Most of them lack a consistent semantics and adopt ad-hoc reasoning procedures.

The second category borrows the basic syntax, semantics and proof theory of First Order Logic, which is considered to be able to describe facts about the real world, so these formalisms have a solid foundation. The full power of First Order Logic was not necessary to achieve an adequate level of expressiveness. As a result, research on the so-called *terminological systems* began. Recently, the term Description Logics (DLs) was adopted to emphasize the importance of the underlying logical system. It is considered to define *subsets of First Order Logic* (FOL). Like FOL, syntax defines which collections of symbols are legal expressions in a Description Logic, and semantics determines the meaning. Unlike FOL, a DL may have several well known syntactic variants.

Section 14.1 introduces the basic concepts about DLs general syntax, with a dedicated subsection relative to $\mathcal{SHOIN}^{(\mathbf{D})}$. Section 14.2 explains general semantics, principles of the satisfaction of axioms, translation of DL axioms to first order logic predicates, semantics of $\mathcal{SHOIN}^{(\mathbf{D})}$ DL. Section 14.3 discusses the kinds of reasoning that one can perform on a DL knowledge base and the practical available algorithmic approaches, among which `Pellet`.

14.1 Syntax

The basic syntactic building blocks are the following three disjoint sets:

- *atomic concepts*, which denote types, categories, or classes of entities, usually characterized by common properties, e.g., $Cat, Country, Doctor$; they are equivalent to FOL unary predicates;

- *atomic roles*, which denote binary relationships between individuals of a domain, e.g., $hasParent, loves, locatedIn$; they are equivalent to FOL binary predicates;

- *individuals*, that correspond to all names used to denote singular entities (be they persons, objects or anything else) in the domain, like $Mary, Boston, Italy$; they are equivalent to FOL constants.

According to a convention widely adopted, we capitalize concept names' initial whereas individual and role names are written with lower case initial. Camelcase is used for names corresponding to multi-word units in natural language.

Elementary descriptions are atomic concepts and atomic roles, which constitute the *vocabulary* or *signature* of an application domain. Complex descriptions of concepts and roles can be built from them inductively with concept and role *constructors*, the range of which is dependent on the particular Logic. Some constructors are related to logical constructors in First Order Logic, other constructors have no corresponding construction in FOL, including restrictions on roles, inverse, transitivity and functionality for example. In abstract notation, A denotes an atomic concept and C, D denote concept descriptions (complex concepts); P denotes an atomic role and R a role description (complex role); a denote an individual.

Concept and Role constructors

For **concepts**, the available operators usually include some or all of the standard logical connectives, *conjunction* (denoted $\sqcap$), *disjunction* (denoted $\sqcup$) and *negation* (denoted $\neg$). In addition, the universal concept *top* (denoted $\top$, and equivalent to $\mathsf{A}\sqcup\neg\mathsf{A}$) and the incoherent concept *bottom* (denoted $\bot$, and equivalent to $\mathsf{A}\sqcap\neg\mathsf{A}$) are often predefined. *Top* contains all the individuals of the domain, while *bottom* is the empty concept.

Other commonly supported operators include restricted forms of quantification called *existential role restrictions* (denoted $\exists R.C$) and *universal role restrictions* (denoted $\forall R.C$). Some DLs also support *qualified number restrictions* (denoted $\leq n.\mathsf{P}C$ and $\geq n.\mathsf{P}C$), operators that place cardinality restrictions on the roles relating instances of a concept to instances of some other concept. Cardinality restrictions are often limited to the forms $\leq n.\mathsf{P}\top$ and $\geq n.\mathsf{P}\top$, that are called *unqualified number restrictions*, or simply number restrictions, and are often abbreviated to $\leq n.\mathsf{P}$ and $\geq n.\mathsf{P}$. The roles that can appear in cardinality restriction concepts are usually restricted to being atomic.

Role forming operators may also be supported, and in some very expressive logics roles can be expressions formed using union (denoted $\sqcup$), composition (denoted $\circ$), reflexive-transitive closure (denoted *) and identity operators (denoted *id*), possibly augmented with the inverse (also known as converse) operator (denoted $^-$). In most implemented systems, however, roles are restricted to being atomic names.

Given these constructors, we now inductively define *complex concepts or concepts expressions* (also simply called *concepts*).

Let $\mathbf{N_C}$, $\mathbf{N_R}$ and $\mathbf{N_I}$ be sets of *atomic concepts* (or *concept names*), *roles* and *individuals*, respectively. Then the ordered triple $(\mathbf{N_C}, \mathbf{N_R}, \mathbf{N_I})$ is the signature.

1. The following are concepts:
   - $\top$ (top)
   - $\bot$ (bottom)
   - every $\mathsf{A} \in \mathbf{N_C}$ (all atomic concepts are concepts)
   - for every finite set $\{a_1, \ldots, a_n\} \in \mathbf{N_I}$ of individual names, $\{a_1, \ldots, a_n\}$ is a concept; they are called nominal concepts
2. If C and D are concepts and $R \in \mathbf{N_R}$ then the following are concepts:

- $(C \sqcap D)$ (the intersection of two concepts is a concept)
- $(C \sqcup D)$ (the union of two concepts is a concept)
- $\neg C$ (the complement of a concept is a concept)
- $\exists R.C$ (the existential restriction of a concept by a role is a concept)
- $\forall R.C$ (the universal restriction of a concept by a role is a concept)
- for a natural number n, $\exists R.Self$ (self restriction, which expresses reflexivity of a role); $\geq nR$ (at-least restriction) and $\leq nR$ (at-most restriction) (the unqualified number restrictions on roles are concepts); $\geq nR.C$ and $\leq nR.C$ (the qualified number restrictions on roles are concepts)

In Table 14.1 are illustrated some examples of complex concepts.

Table 14.1: Examples of Description Logic concept expressions.

Construct	Example	Meaning
intersection	Person $\sqcap$ Female	those persons that are female
union	Mother $\sqcup$ Father	individuals are mother or father
complement	$\neg$Male	those individuals who are not males
$\{a_1, ..., a_n\}$	{john, mary}	the set of individuals $john, mary$
$\forall R.C$	$\forall$hasChild.Female	those individuals all of whose children are female
$\exists R.C$	$\exists$hasChild.Female	those individuals whose child is a female
$\exists R.\{a\}$	$\exists$citizenOf.{USA}	those individuals who are USA citizens
$\exists R.Self$	$\exists$likes.Self	those individuals who are narcist (like themselves)
$\geq nR$(minCardinality)	$\geq$ 2hasChild	those individuals who have at least 2 children
$\leq nR$(maxCardinality)	$\leq$ 1hasChild	those individuals who have no more than one child
$\geq nR.C$	$\geq$ 2hasChild.Female	those individuals who have at least 2 daughters
$\leq nR.C$	$\leq$ 1hasChild.Male	those individuals who have no more than one son

Knowledge Bases

A KR system based on Description Logic provides facilities to set up knowledge bases, to reason about their content, and to manipulate them. A knowledge base (KB) comprises two components, the intensional knowledge (TBox and RBox), i.e., general knowledge about the problem domain, and extensional knowledge (ABox), i.e., knowledge about a specific situation. The TBox introduces the *terminology*, i.e., the vocabulary of an application domain, while the *ABox* contains assertions about named individuals in terms of this vocabulary.

TBox

The TBox (terminological box) contains all the **concept** definitions. Moreover, it is built through declarations that describe general properties of concepts. *Terminological axioms* make statements about how concepts are related to each other. The axioms of a TBox can be divided into:

- *definitions*: $C \equiv D$
- *subsumptions*: $C \sqsubseteq D$

where C, D are concepts.

Definitions Axioms of the first kind are called *concept equalities*, since they state that a concept C is equivalent to another concept D (atomic or complex). Definitions are used to introduce symbolic names for complex descriptions. For instance, by the axiom

$$\mathsf{Mother} \equiv \mathsf{Woman} \sqcap \exists \mathsf{hasChild}.\mathsf{Person}.$$

we associate to the description on the right-hand side the name Mother. Symbolic names may be used as abbreviations in other descriptions. If, for example, we have defined Father analogously to Mother, we can define Parent as

$$\mathsf{Parent} \equiv \mathsf{Mother} \sqcup \mathsf{Father}.$$

We call a finite set of definitions $\mathcal{T}$ a *terminology or TBox* if no symbolic name is defined more than once, that is, if for every atomic concept A there is at most one axiom whose left-hand side is A. We divide the atomic concepts in $\mathcal{T}$ into two sets, the *name symbols* $\mathcal{N}_{\mathcal{T}}$ that occur on the left-hand side of some axiom and the *base symbols* $\mathcal{B}_{\mathcal{T}}$ that occur only on the right-hand side of axioms. Name symbols are often called *defined* concepts and base symbols *primitive* concepts. We expect that the terminology defines the name symbols in terms of the base symbols.

Subsumptions For certain concepts we may be unable to define them completely. In this case, we can still state necessary conditions for concept membership using an inclusion. In particular, axioms of the second kind are called *concept inclusions* since state that a concept C is a subclass of the concept D and is often read "C is subsumed by D". We call an inclusion whose left-hand side is atomic a *specialization*. Sometimes, this axiom type is also referred to as an *is-a* relationship (e.g. "a cat is a mammal" would be a typical verbalization of $\mathsf{Cat} \sqsubseteq \mathsf{Mammal}$). We use $C \equiv D$ to abbreviate $C \sqsubseteq D$ and $D \sqsubseteq C$.

For example, if one thinks that the definition of Woman as $\mathsf{Woman} \equiv \mathsf{Person} \sqcap \mathsf{Female}$ is not satisfactory, but if one also feels that is not able to define the concept in all detail, one can require that every woman is a person with the specialization

$$\mathsf{Woman} \sqsubseteq \mathsf{Person}.$$

A set of axioms $\mathcal{T}$ is a *generalized terminology* if the left-hand side of each axiom is an atomic concept and for every atomic concept there is at most one axiom where it occurs on the left-hand side.

A *TBox* $\mathcal{T}$ is a finite set of *general concept inclusion axioms* (GCIs). The kind of axioms that can appear in $\mathcal{T}$ depends on the DL.

RBox

The RBox (Role box) is a set of statements about the characteristics of roles. A *role* is either a universal role U, an atomic role $R \in \mathbf{N_R}$ or the inverse R^- of an atomic role R. The universal role interconnects any two individuals of the domain and also every individual with itself. We use $\mathbf{N_R^-}$ to denote the set of all inverses of roles in $\mathbf{N_R}$.

An RBox $\mathcal{R}$ is a finite set of statements of the form

- $Func(R)$ or $R \in \mathbf{F}$, where $\mathbf{F} \subseteq \mathbf{N_R}$ is the set of *functional* roles (e.g., since one can have at most one father, the role $hasFather$ is functional);
- $Trans(R)$ or $R \in \mathbf{N_{R_+}}$, where $\mathbf{N_{R_+}} \subseteq \mathbf{N_R}$ is the set of *transitive* roles (e.g., the role $partOf$);
- $R \sqsubseteq S$, called *role inclusions* (e.g. $isComponent \sqsubseteq partOf$); $R \equiv S$, called *role equivalence*, which is an abbreviation for $(R \sqsubseteq S)$ and $(S \sqsubseteq R)$. R and S are roles in $\mathbf{N_R} \cup \mathbf{N_R}^-$.

Statements in $\mathcal{R}$ are called *role axioms*. The kinds of role axioms that can appear in $\mathcal{R}$ depend on the expressiveness the Description Logic. Many DLs, e.g. $\mathcal{ALC}$, do not provide any role axioms at all; for the $\mathcal{S}$-family of DLs, however, the RBox is a very important component in a DL knowledge base, since $\mathcal{S}$ itself provides transitive role axioms.

ABox

The ABox (assertional box) provides the world description, a specific state of affairs of an application domain in terms of concepts and roles. Some of the concept and role atoms in the ABox may be defined names of the TBox. In the ABox, one introduces individuals (instances), by giving them names, and one asserts properties of these individuals. We denote individual names as a, b, c. Using concepts C and roles R, one can make assertions of the following kinds in an ABox:

1. $a : C$, called *concept assertions*, stating that a belongs to C;
2. $(a, b) : R$, called *role assertions*, stating that c is a filler of the role R for b, i.e., b is R-related to c;
3. *equality assertions* $a = b$ between individuals;
4. *inequality axioms* $a \neq b$ between individuals.

An ABox, denoted as $\mathcal{A}$, is a finite set of such assertions. Sometimes, it is convenient to allow individual names (also called *nominals*) not only in the ABox, but also in the description language. Some concept constructors employing individuals occur in systems and have been investigated in the literature. The most basic one is the set (or *one-of*) constructor, written $\{a_1, \dots, a_n\}$, where $a_1, \dots a_n$ are individual names, cf. subsection 14.1. With sets in the description language one can for instance define the concept of permanent members of the UN security council as $\{CHINA, FRANCE, RUSSIA, UK, USA\}$.

In Table 14.2 are illustrated some examples of TBox, RBox and ABox axioms.

Table 14.2: Examples of $axioms$ of a DL Knowledge Base.

Construct	Example	Box
Subsumption	$\mathsf{Human} \sqsubseteq \mathsf{Animal} \sqcap \mathsf{Biped}$	TBox
Definition	$\mathsf{Man} \equiv \mathsf{Human} \sqcap \mathsf{Male}$	TBox
Role inclusion	$\mathsf{hasDaughter} \sqsubseteq \mathsf{hasChild}$	RBox
Role equiv. & Inversion	$\mathsf{hasChild} \equiv \mathsf{hasParent}^-$	RBox
Role incl. & Transitivity	$\mathsf{ancestor}^+ \sqsubseteq \mathsf{ancestor}$	RBox
Individuals Equality	$\mathsf{PresidentBush} = \mathsf{GWBush}$	ABox
Individuals Inequality	$\mathsf{john} \neq \mathsf{peter}$	ABox

Description Logics Nomenclature

There is a well-established naming convention for DLs. The naming scheme for mainstream DLs can be summarized as follows:

$$((\mathcal{ALC} \mid \mathcal{FL} \mid \mathcal{EL} \mid \mathcal{S})\,[\,\mathcal{H}\,] \mid \mathcal{SR})\,[\,\mathcal{O}\,][\,\mathcal{I}\,][\,\mathcal{F} \mid \mathcal{E} \mid \mathcal{U} \mid \mathcal{N} \mid \mathcal{Q}\,]^{(\mathcal{D})}$$

The meaning of the name constituents is as follows:

- $\mathcal{ALC}$ is an abbreviation for *attributive language with complements*. This is the base language which allows atomic negation, concept intersection, complex concept negation (letter $\mathcal{C}$), universal restrictions, limited existential quantification. This DL disallows RBox axioms as well as role inverses, cardinality constraints, nominal concepts, and self concepts.

- $\mathcal{FL}$ is an abbreviation for *frame based description language*. This DL allows concept intersection, universal restrictions, limited existential quantification, role restriction. $\mathcal{FL}^-$ is a sub-language of $\mathcal{FL}$, which is obtained by disallowing role restriction. $\mathcal{FL}_o$ is a sub-language of $\mathcal{FL}^-$, which is obtained by disallowing limited existential quantification.

- $\mathcal{EL}$ allows concept operators and concept axioms ($\sqsubseteq, \equiv$), but no role/axioms operators. $\mathcal{EL}^{++}$ is an alias for $\mathcal{ELRO}$.

- By $\mathcal{S}$ we denote $\mathcal{ALC}$ where we additionally allow transitivity statements. The name goes back to the name of a modal logic called S.

- $\mathcal{ALC}$ and $\mathcal{S}$ can be extended by role hierarchies (obtaining $\mathcal{ALCH}$ or $\mathcal{SH}$) which allow for simple role inclusions, i.e., role chain axioms of the form $R \sqsubseteq S$.

- $\mathcal{SR}$ denotes $\mathcal{ALC}$ extended with all kinds of RBox axioms as well as self concepts, e.g., $hasParent \circ hasBrother \sqsubseteq hasUncle$.

- The letter $\mathcal{O}$ in the name of a DL indicates that nominal concepts are supported, e.g. $\{Italy\}$.

- When a DL contains $\mathcal{I}$ then it features role inverses, e.g. $isChildOf \equiv hasChild^-$.

- The letter $\mathcal{F}$ at the end of a DL name enables support for role functionality statements which can be expressed as $\leq 1R.\top$, e.g. $\leq 1 hasMother$.

- The letter $\mathcal{E}$ enables full existential quantification.
- The letter $\mathcal{U}$ allows concept union.
- $\mathcal{N}$ at the end of a DL name allows for unqualified cardinality restrictions, i.e., concepts of the shape $\geq 2 hasChild$ and $\leq 3 hasChild$.
- $\mathcal{Q}$ indicates support for arbitrary qualified cardinality restrictions, i.e., $\geq 2 hasChild.Doctor$.
- $^{(\mathcal{D})}$ indicates the use of datatype properties.

Example 28 *Some examples belonging to the family of Description Logics are (M., 2011):*

- *$\mathcal{ALC}$, which is a centrally important Description Logic;*
- *$\mathcal{SHOIN}^{(\mathcal{D})}$: it is a type of Description Logic that provides a high level of expressivity and offers full negation, disjunction within inverse roles and a restricted form of existential quantification; it is therefore called "concept description". It additionally supports reasoning with concrete data-types. At present, OWL DL is correspondent to $\mathcal{SHOIN}^{(\mathcal{D})}$. The Protégé ontology editor supports $\mathcal{SHOIN}^{(\mathcal{D})}$.*
- *$\mathcal{SHIQ}^{(\mathcal{D})}$: it is distinguished from $\mathcal{SHOIN}^{(\mathcal{D})}$ essentially by not supporting nominal concepts (or named objects), allowing qualified number restrictions of the concept and simple roles. There is a mapping or translation from DAML+OIL to the $\mathcal{SHIQ}^{(\mathcal{D})}$ language. $\mathcal{SHIQ}$ is the logic $\mathcal{ALC}$ plus extended cardinality restrictions, and transitive and inverse roles.*
- *$\mathcal{SHIF}^{(\mathcal{D})}$: it is just $\mathcal{SHOIN}^{(\mathcal{D})}$ with the exclusion of the oneOf constructor and the inclusion of the (at-least) and (at-most) constructors limited to 0 and 1. In fact, OWL Lite can be translated to $\mathcal{SHIF}^{(\mathcal{D})}$ to allow for reasoning.*
- *Three major bioinformatic terminology bases,* Snomed, Galen*, and* GO*, are expressible in $\mathcal{EL}$ (with additional role properties).*

Syntax of $\mathcal{SHOIN}^{(\mathbf{D})}$

This subsection illustrates the syntax of $\mathcal{SHOIN}^{(\mathbf{D})}$ DL, which will be the subject of Chapter 16.

The Description Logic $\mathcal{SHOIN}$ is the logic underlying OWL-DL, and results from $\mathcal{ALC}$ plus all constructs and syntax of the $\mathcal{S}$, $\mathcal{H}$, $\mathcal{O}$, $\mathcal{I}$ and $\mathcal{N}$ languages:

- $\mathcal{S}$: Role transitivity (e.g. $\mathsf{Trans(ancestor)}$)
- $\mathcal{H}$: Role hierarchy (e.g. $\mathsf{parent} \sqsubseteq \mathsf{ancestor}$)
- $\mathcal{O}$: Nominals of the form $\{a\}$ and $\{a_1, \dots, a_n\}$ (one-of construct) (cf. subsection 14.1)
- $\mathcal{I}$: Role Inverses (e.g. parent^-)
- $\mathcal{N}$: Unqualified number restrictions

A knowledge base KB in $\mathcal{SHOIN}$ consists of a TBox $\mathcal{T}$, an RBox $\mathcal{R}$ and an ABox $\mathcal{A}$.

The Description Logic $\mathcal{SHOIN}^{\mathbf{(D)}}$ is a generalization of $\mathcal{SHOIN}$ by **datatypes**, such as strings and integers. The elementary ingredients are as follows. We assume a set of *data values*, a set of *elementary datatypes*, and a set of *datatype predicates*, where each datatype predicate has a predefined arity $n \geq 1$. A *datatype* is an elementary datatype or a finite set of data values. So we can define four disjoint sets $\mathbf{N_C}, \mathbf{N_{R_A}}, \mathbf{N_{R_D}}, \mathbf{N_I}$ for atomic concepts, abstract roles, datatype roles and individuals, respectively.
For example, over the integers, $\geq_{20}$ may be a unary predicate denoting the set of integers greater or equal to 20, and thus $\mathsf{Person} \sqcap \exists \mathsf{age}. \geq_{20}$ may denote a person whose age is at least 20.

To consider datatypes we extend:

- The inductive definition of *concepts*. If D is an n-ary datatype predicate and $T, T_1, ..., T_n \in R_D$, then $\exists T_1, ..., T_n.D$, $\forall T_1, ..., T_n.D$, $\geq nT$, and $\leq nT$ are concepts (called datatype exists, value, at-least, and at-most restriction, respectively) for an integer $n \geq 0$. For example, we may write the concept

  $$\mathsf{Flower} \sqcap \exists \mathsf{hasPetalWidth}. \geq_{\mathsf{20mm}} \sqcap \exists \mathsf{hasPetalWidth}. \leq \mathsf{40mm} \sqcap \exists \mathsf{hasColor.Red}$$

  to denote the set of flowers having petal's dimension within 20mm and 40mm (where we assume that every flower has exactly one associated petal width) whose color is red. Here, $\geq_{20mm}$ and $\leq_{40mm}$ are datatype predicates.

- the RBox content. It consists of a finite set of transitivity axioms and role inclusion axioms $R \sqsubseteq S$, where either $R, S \in \mathbf{N_{R_A}} \cup \mathbf{N_{R_A^-}}$ or $R, S \in \mathbf{N_{R_D}}$.

- the ABox content. It is a finite set of axioms as specified in subsection 14.1 plus role membership axioms $(a, v) : T$, where $a \in \mathbf{N_I}$ and v is a data value.

14.2 Semantics

Like for any other logic, the definition of a formal semantics for DLs aims at providing a consequence relation that determines whether an axiom logically follows from (also: is entailed by) a given set of axioms. The semantics of Description Logics is defined in a *model-theoretic* way and concepts are given a *set-theoretic* interpretation: a concept is interpreted as a set of individuals and roles are interpreted as sets of pairs of individuals. The domain of interpretation can be chosen arbitrarily, and it can be infinite. The non-finiteness of the domain and the open-world assumption are distinguishing features of Description Logics.

One central notion is that of an **interpretation**. An interpretation, normally denoted with $\mathcal{I}$, provides

- a nonempty set $\Delta^{\mathcal{I}}$, called the *domain* or also universe of discourse, which can be understood as the entirety of individuals or things existing in the 'world' that $\mathcal{I}$ represents,
- a function $\cdot^{\mathcal{I}}$, called *interpretation function*, which connects the vocabulary elements (i.e., the individual, concept, and role names) to $\Delta^{\mathcal{I}}$, by providing
  - for each individual name $\mathsf{a} \in \mathbf{N_I}$ a corresponding individual $\mathsf{a}^{\mathcal{I}} \in \Delta^{\mathcal{I}}$ from the domain,
  - for each atomic concept $\mathsf{A} \in \mathbf{N_C}$ a corresponding set $\mathsf{A}^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}}$ of domain elements (as opposed to the domain itself, $\mathsf{A}^{\mathcal{I}}$ is allowed to be empty), and
  - for each atomic role $\mathsf{R} \in \mathbf{N_R}$ a corresponding (also possibly empty) set $\mathsf{R} \subseteq \Delta^{\mathcal{I}} \times \Delta^{\mathcal{I}}$ of ordered pairs of domain elements,

where $\mathbf{N_I}, \mathbf{N_C}, \mathbf{N_R}$ are respectively the set of individual names, of concept names and of role names. Figure 14.1 depicts this definition graphically. For domain elements $\delta, \delta' \in \Delta^{\mathcal{I}}$, the intuitive meaning of $\delta \in A^{\mathcal{I}}$ is that the individual δ belongs to the class described by the concept name A, while $(\delta, \delta') \in \mathsf{R}^{\mathcal{I}}$ means that δ is connected to δ' by the relation denoted by the role name R.

To avoid confusion, it is important to strictly separate syntactic notions (referring to the vocabulary and axioms) from the semantic notions (referring to the domain and domain elements). Individual names, concept names and role names are syntactic entities and so are roles and concepts. Individuals are elements of $\Delta^{\mathcal{I}}$ and hence semantic entities. In order to refer to the semantic counterparts of concepts and roles, one would use the terms *concept extension*

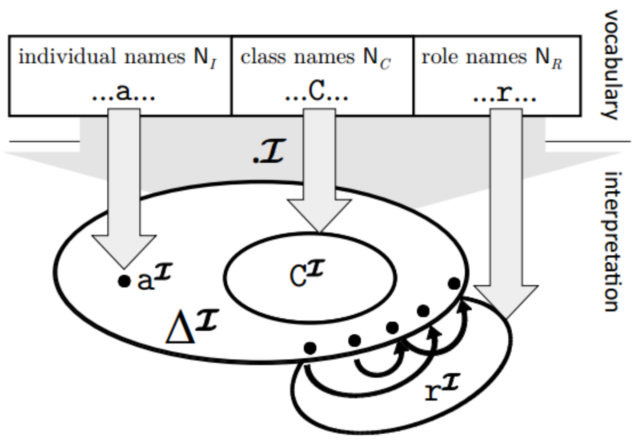


Figure 14.1: Structure of DL interpretations.

or *role extension*, respectively. Single elements of the extension of a concept or role are also called *concept instances* or *role instances*.

The domain *is not required to be finite*, but can also be an infinite set. It is also possible to consider only interpretations with finite domains, but then one explicitly talks about finite models or finite satisfiability. There are logics where infinite interpretations are "dispensable" as there are always finite ones that do the same job, these logics are said to have the *finite model property*. $\mathcal{SHOIN}$ does not have the finite model property.

Example 29 *As an example of an interpretation, with an infinite domain, consider the following vocabulary:*

- $\mathsf{N_I} = \{\mathsf{zero}\}$
- $\mathsf{N_C} = \{\mathsf{Prime}, \mathsf{Positive}\}$
- $\mathsf{N_R} = \{\mathsf{hasSuccessor}, \mathsf{lessThan}, \mathsf{multipleOf}\}$

We define $\mathcal{I}$ as follows: let $\Delta^{\mathcal{I}} = \mathbb{N} = \{0, 1, 2, ...\}$, i.e., the set of all natural numbers including zero.

Furthermore, we let $\mathsf{zero}^{\mathcal{I}} = 0$, as well as $\mathsf{Prime}^{\mathcal{I}} = \{n | n \textit{ is a prime number}\}$ and $\mathsf{Positive}^{\mathcal{I}} = \{n | n > 0\}$.

For the roles, we define:

- $\mathsf{hasSuccessor}^{\mathcal{I}} = \{(n, n+1) \mid n \in \mathbb{N}\}$
- $\mathsf{lessThan}^{\mathcal{I}} = \{(n, n') \mid n < n',\ n, n' \in \mathbb{N}\}$

- $\mathsf{multipleOf}^{\mathcal{I}} = \{(n, n') \mid \exists k.n = k \cdot n',\ n, n', k \in \mathbb{N}\}$

We have seen that an interpretation determines the semantic counterparts of vocabulary elements. However, in order to determine the truth of complex axioms, it is necessary to also find the counterparts of complex concepts and roles. The semantics of a complex language expression can be obtained from the semantics of its constituents (thereby following the principle of compositional semantics): atomic concepts are subsets of the interpretation domain, while the semantics of the other concepts is then specified on the basis of the construct. Formally, this is done by *extending the interpretation function* to these complex expressions:

1. $\cdot^{\mathcal{I}}$ is extended from **role** names to roles by letting $u^{\mathcal{I}} = \Delta^{\mathcal{I}} \times \Delta^{\mathcal{I}}$ (that is: the *universal role* interconnects any two individuals of the domain and also every individual with itself), and the set of all pairs (δ, δ') of domain elements for which (δ', δ) is contained in $R^{\mathcal{I}}$ is assigned to inverted role names R^{-}.

2. $\cdot^{\mathcal{I}}$ is extended to **concept** descriptions this way

   - $\top$ is the concept which is true for every individual of the domain, hence $\top^{\mathcal{I}} = \Delta^{\mathcal{I}}$
   - $\bot$ is the concept which has no instances, hence $\bot^{\mathcal{I}} = \emptyset$
   - $\{a_1, \ldots, a_n\}$ is the concept containing exactly the individuals denoted by $a_1, \ldots, a_n$, therefore $\{a_1, \ldots, a_n\}^{\mathcal{I}} = \{a_1^{\mathcal{I}}, \ldots, a_n^{\mathcal{I}}\}$
   - $\neg C$ is supposed to denote the set of all those domain individuals that are not contained in the extension of C, i.e., $(\neg C)^{\mathcal{I}} = \Delta^{\mathcal{I}} \setminus C^{\mathcal{I}}$
   - $C \sqcap D$ is the concept comprising all individuals that are simultaneously in C and D, thus $(C \sqcap D)^{\mathcal{I}} = C^{\mathcal{I}} \cap D^{\mathcal{I}}$
   - $C \sqcup D$ contains individuals being present in C or D (or both), therefore $(C \sqcup D)^{\mathcal{I}} = C^{\mathcal{I}} \cup D^{\mathcal{I}}$
   - $\forall R.C$ denotes the set of individuals $\delta \in \Delta^{\mathcal{I}}$ with the following property: whenever δ is connected to some domain individual $\delta' \in \Delta^{\mathcal{I}}$ via the relation denoted by R, then δ' belongs to the extension of the concept C, formally: $(\forall R.C)^{\mathcal{I}} = \{\delta \in \Delta^{\mathcal{I}} \mid \forall \delta' \in \Delta^{\mathcal{I}}.((\delta, \delta') \in R^{\mathcal{I}} \rightarrow \delta' \in C^{\mathcal{I}})\}$
   - $\exists R.C$ is the concept that holds for an individual $\delta \in \Delta^{\mathcal{I}}$ exactly if there is some domain individual $\delta' \in \Delta^{\mathcal{I}}$ such that δ is connected to δ' via the relation denoted

by R and δ' belongs to the extension of the concept C, formally: $(\exists R.C)^{\mathfrak{I}} = \{\delta \in \Delta^{\mathfrak{I}} \mid \exists \delta' \in \Delta^{\mathfrak{I}}.((\delta, \delta') \in R^{\mathfrak{I}} \wedge \delta' \in C^{\mathfrak{I}})\}$

- $\exists R.Self$ comprises those domain individuals which are R-related to themselves, thus we let $(\exists R.Self)^{\mathfrak{I}} = \{x \in \Delta^{\mathfrak{I}} \mid (x, x) \in R^{\mathfrak{I}}\}$
- $\leq nR$ refers to the domain elements $\delta \in \Delta^{\mathfrak{I}}$ for which no more than n individuals exist to which δ is R-related, formally: $(\leq nR)^{\mathfrak{I}} = \{\delta \in \Delta^{\mathfrak{I}} \mid \#\{\delta' \in \Delta^{\mathfrak{I}} \mid (\delta, \delta') \in R^{\mathfrak{I}}\} \leq n\}$ ($\#S$ is used to denote the cardinality of a set S),
- $\leq nR.C$ refers to the domain elements $\delta \in \Delta^{\mathfrak{I}}$ for which no more than n individuals exist to which δ is R-related and that are in the extension of C, formally: $(\leq nR.C)^{\mathfrak{I}} = \{\delta \in \Delta^{\mathfrak{I}} \mid \#\{\delta' \in \Delta^{\mathfrak{I}} \mid (\delta, \delta') \in R^{\mathfrak{I}} \wedge \delta' \in C^{\mathfrak{I}}\} \leq n\}$,
- $\geq nR$ and $\geq nR.C$, duals to the case before, denote those domain elements having at least n such R-related elements: $(\geq nR)^{\mathfrak{I}} = \{\delta \in \Delta^{\mathfrak{I}} \mid \#\{\delta' \in \Delta^{\mathfrak{I}} \mid (\delta, \delta') \in R^{\mathfrak{I}}\} \geq n\}$; $(\geq nR.C)^{\mathfrak{I}} = \{\delta \in \Delta^{\mathfrak{I}} \mid \#\{\delta' \in \Delta^{\mathfrak{I}} \mid (\delta, \delta') \in R^{\mathfrak{I}} \wedge \delta' \in C^{\mathfrak{I}}\} \geq n\}$.

Satisfaction of Axioms

The final purpose of the extended interpretation function is to determine the satisfaction of axioms. In the following, we define when an axiom E is true (holds), given a specific interpretation $\mathfrak{I}$. If this is the case, we also say that $\mathfrak{I}$ is a model of E or that $\mathfrak{I}$ satisfies E and we write $\mathfrak{I} \models E$.

- A role inclusion axiom $R \sqsubseteq S$ holds in $\mathfrak{I}$ ($\mathfrak{I} \models R \sqsubseteq S$) iff $R^{\mathfrak{I}} \subseteq S^{\mathfrak{I}}$
- A role transitivity statement $Trans(R)$ is true in $\mathfrak{I}$ iff $R^{\mathfrak{I}}$ is transitive, i.e., if, for every individual x, y, z, $(x, y) \in R^{\mathfrak{I}}, (y, z) \in R^{\mathfrak{I}} \rightarrow (x, z) \in R^{\mathfrak{I}}$
- A general concept inclusion $C \sqsubseteq D$ is satisfied by $\mathfrak{I}$, if every instance of C is also an instance of D. An alternative wording would be that the extension of C is contained in the extension of D, formally $C^{\mathfrak{I}} \subseteq D^{\mathfrak{I}}$
- A general concept equality $C \equiv D$ is satisfied by $\mathfrak{I}$, if the instances of C and D refer to the same set of domain elements
- A concept assertion $a : C$ holds in $\mathfrak{I}$ ($\mathfrak{I} \models a : C$) if the individual with the name a is an instance of the concept C, that is $a^{\mathfrak{I}} \in C^{\mathfrak{I}}$

- A role assertion $(a, b) : R$ holds in $\mathcal{I}$ if the individual denoted by a is R-connected to the individual denoted by b, i.e. the extension of R contains the corresponding pair of domain elements: $(a^{\mathcal{I}}, b^{\mathcal{I}}) \in R^{\mathcal{I}}$
- The equality statement $a = b$ holds in $\mathcal{I}$ if the individual names a and b refer to the same domain individual, i.e. $a^{\mathcal{I}} = b^{\mathcal{I}}$; $\mathcal{I}$ is a model of $a \neq b$ exactly if it is not a model of $a = b$ $(a^{\mathcal{I}} \neq b^{\mathcal{I}})$

Now that we have defined when an interpretation $\mathcal{I}$ is a model of an axiom, we can easily extend this notion to whole knowledge bases: $\mathcal{I}$ is a model of a given knowledge base $\mathcal{KB}$ (also: $\mathcal{I}$ satisfies $\mathcal{KB}$), written $\mathcal{I} \models \mathcal{KB}$, if it satisfies all the axioms of $\mathcal{KB}$, i.e., if $\mathcal{I} \models E$ for every $E \in \mathcal{KB}$. In particular:

- An interpretation $\mathcal{I}$ is a model of a Tbox $\mathcal{T}$ (denoted by $\mathcal{I} \models \mathcal{T}$) iff it satisfies all GCIs of $\mathcal{T}$.
- An interpretation $\mathcal{I}$ is a model of a RBox $\mathcal{R}$ (denoted by $\mathcal{I} \models \mathcal{R}$) iff it satisfies all role inclusion axioms of $\mathcal{R}$.
- An interpretation $\mathcal{I}$ is a model of an ABox $\mathcal{A}$ (denoted by $\mathcal{I} \models A$) iff it satisfies all assertions in $\mathcal{A}$. An ABox $\mathcal{A}$ is consistent with respect to a Rbox $\mathcal{R}$ and a Tbox $\mathcal{T}$ if there is a model $\mathcal{I}$ for $\mathcal{R}$ and $\mathcal{T}$ such that $\mathcal{I} \models A$.

A knowledge base $\mathcal{KB}$ is called *satisfiable* or *consistent* if it has a model, and *unsatisfiable* or *inconsistent* or *contradictory* otherwise.

An axiom E is a *logical consequence* of (also *entailed by*) a knowledge base $\mathcal{KB}$ (written: $\mathcal{KB} \models E$) if every model of $\mathcal{KB}$ is also a model of E, i.e. for every $\mathcal{I}$ with $\mathcal{I} \models \mathcal{KB}$, it also holds $\mathcal{I} \models E$.

A concept C is *satisfiable* relative to $\mathcal{KB}$ iff there exists an interpretation $\mathcal{I}$ such that $C^{\mathcal{I}} \neq \emptyset$.

Semantics via Embedding into FOL

Most description logics are fragments of First Order predicate Logic (FOL). This statement may be somewhat misleading since, from a syntax point of view, most DL axioms are not FOL formulae. However, DL interpretations have the same structure as FOL interpretations if one conceives individual names as constants, concept names as unary predicates and role names as binary predicates. Under this assumption, one can define an easy syntactic translation π which, applied to a DL axiom E, yields a FOL sentence $\pi(E)$ such that the model sets of E and $\pi(E)$ coincide, that is an interpretation $\mathcal{I}$ is a model of E exactly if it is a model of $\pi(E)$. An atomic concept A is translated into the formula $A(x)$; the constructors intersection, union, and negation are translated into logical conjunction, disjunction, and negation, respectively. Consequently, every reasoning problem in a DL is easily transferable to an equivalent reasoning problem in FOL. The semantics of Description Logics can - as an alternative to the previously introduced way - be defined by reducing it to the semantics of FOL via the mentioned translation.

We provide here a definition of π. Every knowledge base $\mathcal{KB}$ thus translates via π to a theory $\pi(\mathcal{KB})$ in First Order predicate Logic with equality. We define

$$\pi(\mathcal{KB}) = \bigcup_{E \in \mathcal{KB}} \pi(E),$$

i.e., we translate every axiom of the knowledge base separately into a FOL sentence. How exactly $\pi(E)$ is defined depends on the type of the axiom E.

First we have to define auxiliary translation functions $\pi_{\mathbf{R}} : \mathbf{R} \times Var \times Var \rightarrow FOL$ for roles and $\pi_{\mathbf{C}} : \mathbf{C} \times Var \rightarrow FOL$ for concepts (where $Var = \{x_0, x_1, ...\}$ is a set of variables):

$$\begin{array}{rcl}
\pi_{\mathbf{R}}(u, x_i, x_j) & = & \mathbf{true} \\
\pi_{\mathbf{R}}(R, x_i, x_j) & = & R(x_i, x_j) \\
\pi_{\mathbf{R}}(R^-, x_i, x_j) & = & R(x_j, x_i) \\
\pi_{\mathbf{C}}(\mathsf{A}, x_i) & = & \mathsf{A}(x_i) \\
\pi_{\mathbf{C}}(\top, x_i) & = & \mathbf{true} \\
\pi_{\mathbf{C}}(\bot, x_i) & = & \mathbf{false} \\
\pi_{\mathbf{C}}(\{a_1, \ldots, a_n\}, x_i) & = & \bigvee_{1 \le j \le n} x_i = a_j \\
\pi_{\mathbf{C}}(\neg C, x_i) & = & \neg \pi_{\mathbf{C}}(C, x_i) \\
\pi_{\mathbf{C}}(C \sqcap D, x_i) & = & \pi_{\mathbf{C}}(C, x_i) \wedge \pi_{\mathbf{C}}(D, x_i) \\
\pi_{\mathbf{C}}(C \sqcup D, x_i) & = & \pi_{\mathbf{C}}(C, x_i) \vee \pi_{\mathbf{C}}(D, x_i) \\
\pi_{\mathbf{C}}(\exists R.C, x_i) & = & \exists x_{i+1}.(\pi_{\mathbf{R}}(R, x_i, x_{i+1}) \wedge \pi_{\mathbf{C}}(C, x_{i+1})) \\
\pi_{\mathbf{C}}(\exists R^-.C, x_i) & = & \exists x_{i+1}.(\pi_{\mathbf{R}}(R, x_{i+1}, x_i) \wedge \pi_{\mathbf{C}}(C, x_{i+1})) \\
\pi_{\mathbf{C}}(\forall R.C, x_i) & = & \forall x_{i+1}.(\pi_{\mathbf{R}}(R, x_i, x_{i+1}) \rightarrow \pi_{\mathbf{C}}(C, x_{i+1})) \\
\pi_{\mathbf{C}}(\forall R^-.C, x_i) & = & \forall x_{i+1}.(\pi_{\mathbf{R}}(R, x_{i+1}, x_i) \rightarrow \pi_{\mathbf{C}}(C, x_{i+1})) \\
\pi_{\mathbf{C}}(\exists R.\mathit{Self}, x_i) & = & \pi_{\mathbf{R}}(R, x_i, x_i) \\
\pi_{\mathbf{C}}(\ge nR.C, x_i) & = & \exists x_{i+1} ... x_{i+n}.(\bigwedge_{i+1 \le j < k \le i+n}(x_j \ne x_k) \wedge \\
 & & \bigwedge_{i+1 \le j \le i+n}(\pi_{\mathbf{R}}(R, x_i, x_j) \wedge \pi_{\mathbf{C}}(C, x_j))) \\
\pi_{\mathbf{C}}(\ge nR, x_i) & = & \exists x_{i+1} ... x_{i+n}.(\bigwedge_{i+1 \le j < k \le i+n}(x_j \ne x_k) \wedge \\
 & & \bigwedge_{i+1 \le j \le i+n} \pi_{\mathbf{R}}(R, x_i, x_j)) \\
\pi_{\mathbf{C}}(\ge nR^-, x_i) & = & \exists x_{i+1} ... x_{i+n}.(\bigwedge_{i+1 \le j < k \le i+n}(x_j \ne x_k) \wedge \\
 & & \bigwedge_{i+1 \le j \le i+n} \pi_{\mathbf{R}}(R, x_j, x_i)) \\
\pi_{\mathbf{C}}(\le nR.C, x_i) & = & \neg \pi_{\mathbf{C}}(\ge (n+1)R.C, x_i) \\
\pi_{\mathbf{C}}(\le nR, x_i) & = & \neg \pi_{\mathbf{C}}(\ge (n+1)R, x_i) \\
\pi_{\mathbf{C}}(\le nR^-, x_i) & = & \neg \pi_{\mathbf{C}}(\ge (n+1)R^-, x_i)
\end{array}$$

Obviously, the translation assigns a FOL formula with (at most) two free variables to a role and a FOL formula with (at most) one free variable to a concept.

Now it is possible to translate axioms:

$$\begin{array}{rcl}
\pi(R \sqsubseteq S) & = & \forall x_0, x_1(\pi_{\mathbf{R}}(R, x_0, x_1) \rightarrow \pi_{\mathbf{R}}(S, x_0, x_1)) \\
\pi(Trans(R)) & = & \forall x, y, z(\pi_{\mathbf{R}}(R, x, z) \wedge \pi_{\mathbf{R}}(R, z, y) \rightarrow \pi_{\mathbf{R}}(R, x, y)) \\
\pi(C \sqsubseteq D) & = & \forall x_0(\pi_{\mathbf{C}}(C, x_0) \rightarrow \pi_{\mathbf{C}}(D, x_0)) \\
\pi(\mathsf{a} : C) & = & \pi_{\mathbf{C}}(C, x_0)[x_0/a] = C(a) \\
\pi((\mathsf{a}, \mathsf{b}) : R) & = & \pi_{\mathbf{R}}(C, x_0, x_1)[x_0/a, x_1/b] = R(a, b) \\
\pi(a = b) & = & a = b \\
\pi(a \neq b) & = & a \neq b
\end{array}$$

We can now define instantiations of FOL formulas obtained by translating a DL knowledge base. Here we assume a fixed interpretation domain $\Delta^{\mathcal{I}}$ that is non-empty and possibly infinite. Given a predicate logic formula F and a domain $\Delta^{\mathcal{I}}$, a *substitution* θ is a set of couples x/a where x is a variable universally quantified in the outermost quantifier in F and $a \in \mathbf{N_I}$. The application of θ to F, indicated by $F\theta$, is called an *instantiation of* F and is obtained by replacing x with a in F and by removing x from the external quantification for every couple x/a in θ. Moreover, given a substitution θ, let $Var(\theta) = \{x | x/a \in \theta\}$ be the set of variables of θ and let $\theta|_{Var} = \{x/i | x \in Var\}$ be the restriction of θ to the variables of Var. Formulas not containing variables are called *ground*. A substitution θ is *grounding* for a formula F if $F\theta$ is ground.

Semantics of $\mathcal{SHOIN}^{(\mathbf{D})}$

This subsection illustrates the semantics of $\mathcal{SHOIN}^{(\mathbf{D})}$, as done in Subsection 14.1 for the syntax. The $\mathcal{SHOIN}^{(\mathbf{D})}$ semantics is a simple generalization of all the previous definitions with *datatypes*, such as strings and integers.

A *datatype theory* $\mathbf{D} = (\Delta^{\mathbf{D}}, \cdot^{\mathbf{D}})$ consists of a datatype domain $\Delta^{\mathbf{D}}$ and a mapping $\cdot^{\mathbf{D}}$ that assigns to each data value an element of $\Delta^{\mathbf{D}}$, to each elementary datatype a subset of $\Delta^{\mathbf{D}}$, and to each datatype predicate of arity n a relation over $\Delta^{\mathbf{D}}$ of arity n. We extend $\cdot^{\mathbf{D}}$ to all datatypes by $\{v_1, ...\}^{\mathbf{D}} = \{v_1^{\mathbf{D}}, ...\}$.

Let $\mathbf{N_C}, \mathbf{N_{R_A}}, \mathbf{N_{R_D}}, \mathbf{N_I}$ be four disjoint sets of atomic concepts, abstract roles, datatype roles and individuals, respectively.

An *interpretation* $\mathcal{I} = (\Delta^{\mathcal{I}}, \cdot^{\mathcal{I}})$ relative to a datatype theory consists of a nonempty abstract domain $\Delta^{\mathcal{I}}$, disjoint from $\Delta^{\mathbf{D}}$, and an interpretation function $\cdot^{\mathcal{I}}$ that assigns to each $a \in \mathbf{N_I}$ an element in $\Delta^{\mathcal{I}}$, to each $C \in \mathbf{N_C}$ a subset of $\Delta^{\mathcal{I}}$, to each $R \in \mathbf{N_{R_A}}$ a subset of $\Delta^{\mathcal{I}} \times \Delta^{\mathcal{I}}$, to each $T \in \mathbf{N_{R_D}}$ a subset of $\Delta^{\mathcal{I}} \times \Delta^{\mathbf{D}}$ and to every data value, datatype, and datatype predicate the same value as $\cdot^{\mathbf{D}}$. The mapping $\cdot^{\mathcal{I}}$ is extended to all roles and concepts as usual:

$$\begin{array}{rcl}(\forall T_1, \ldots, T_n.d)^{\mathcal{I}} & = & \{x \in \Delta^{\mathcal{I}} \mid T_1^{\mathcal{I}}(x) \times \ldots \times T_n^{\mathcal{I}}(x) \subseteq d^{\mathcal{I}}\} \\ (\exists T_1, \ldots, T_n.d)^{\mathcal{I}} & = & \{x \in \Delta^{\mathcal{I}} \mid T_1^{\mathcal{I}}(x) \times \ldots \times T_n^{\mathcal{I}}(x) \cap d^{\mathcal{I}} \neq \emptyset\}\end{array}$$

The satisfaction of an axiom E in an interpretation $\mathcal{I}$ is defined, for a data value v, as: $\mathcal{I} \models (a, v) : T$ iff $(a^{\mathcal{I}}, v^{\mathbf{D}}) \in T^{\mathcal{I}}$.

14.3 Reasoning Tasks

A knowledge representation system based on DLs is able to perform specific kinds of reasoning. A knowledge base comprising TBox and ABox has a semantics that makes it equivalent to a set of axioms in First Order predicate Logic. Thus, like any other set of axioms, it contains implicit knowledge that can be made explicit through inferences. The different kinds of reasoning performed by a DL system are defined as logical inferences. In the following, we shall discuss these inferences, first for concepts, then for TBoxes and ABoxes. It will turn out that there is one main inference problem, namely the consistency check for ABoxes, to which all other inferences can be reduced.

The inference services provided by DL systems for **concept consistency and TBox reasoning** can be summarized as follows:

- *Concept Satisfiability or Consistency* (w.r.t a TBox): given a TBox $\mathcal{T}$, a concept C is called satisfiable with respect to $\mathcal{T}$, if it may contain individuals, i.e. there is a model $\mathcal{I}$ of $\mathcal{T}$ that maps C to a nonempty set, formally: $C^{\mathcal{I}} \neq \emptyset$. We get yes or no as an answer. A concept is unsatisfiable if $C^{\mathcal{I}} = \emptyset$, which can be rewritten into $C^{\mathcal{I}} \subseteq \emptyset$, and further into $C^{\mathcal{I}} \subseteq \bot^{\mathcal{I}}$ for every model $\mathcal{I}$ of $\mathcal{T}$. This means $\mathcal{I} \models C \sqsubseteq \bot$ for every model $\mathcal{I}$ of $\mathcal{T}$. Hence, unsatisfiability of a concept C with respect to a TBox can be decided by checking whether $\mathcal{T}$ entails the GCI $C \sqsubseteq \bot$.

- *Concept subsumption* (w.r.t. a TBox): given a TBox $\mathcal{T}$, a concept C is subsumed by a concept D if in every model of $\mathcal{T}$ the set denoted by C is a subset of the set denoted by D, formally: $C^{\mathcal{I}} \subseteq D^{\mathcal{I}}$ for every model $\mathcal{I}$ of $\mathcal{T}$. In this case we write $\mathcal{T} \models C \sqsubseteq D$. Algorithms that check subsumption are also employed to organize the concepts of a TBox in a taxonomy according to their generality.

- *Consistency* of a TBox: this task verifies that there exists at least one interpretation $\mathcal{I}$ for a given TBox $\mathcal{T}$ ($\mathcal{T} \not\models \perp$).

Traditionally, the basic reasoning mechanism provided by DL systems checked the subsumption of concepts. This is, in fact, sufficient to implement also the other inferences, as can be seen by the following reductions.

For concepts C, D we have:

- C is unsatisfiable $\Leftrightarrow$ C is subsumed by $\perp$;
- C and D are equivalent $\Leftrightarrow$ C is subsumed by D and D is subsumed by C;
- C and D are disjoint $\Leftrightarrow$ $C \cap D$ is subsumed by $\perp$.

The inference services for the ABox are:

- *ABox consistency* (w.r.t. a TBox): An ABox $\mathcal{A}$ is consistent with respect to a TBox $\mathcal{T}$, if there is an interpretation that is a model of both $\mathcal{A}$ and $\mathcal{T}$.
- *Instance check* w.r.t. an ABox, also called *Axiom entailment*: checking whether an assertion E is entailed by an ABox ($\mathcal{A} \models E$) can be seen as the prototypical reasoning task for querying knowledge. If E is of the form $C(a)$ - i.e. we want to check if a given individual a belongs to a particular concept C - we can reduce the instance check to the consistency problem for ABoxes because there is the following connection: $\mathcal{A} \models C(a)$ iff $\{\mathcal{A} \cup \neg C(a)\}$ is inconsistent. The problem of checking axiom entailment in general can be reduced to consistency checking, i.e., whether a concept is (un)satisfiable. The idea behind this reduction is proof by contradiction: we show that something holds by assuming the opposite and deriving a contradiction from that assumption. The correspondences for all types of axioms are given in Table 14.3.
- *Instance retrieval* is the problem of finding all individuals a mentioned in an ABox that are an instance of a given concept C w.r.t. a TBox, formally $\mathcal{A} \models C(a)$.
- The set of *fillers* of a role R for an individual i w.r.t. a TBox $\mathcal{T}$ and an ABox $\mathcal{T}$ is defined as $\{x \mid (\mathcal{T}, \mathcal{A}) \models (i, x) : R\}$.
- The set of *roles* between two individuals i and j w.r.t. a knowledge base $(\mathcal{T}, \mathcal{A})$ is defined as $\{R \mid (\mathcal{T}, \mathcal{A}) \models (i, j) : R\}$.

In many DL systems, there are some auxiliary supported queries: retrieval of concept names or individuals mentioned in a knowledge base, retrieval of the set of roles, retrieval of the role parents and children, retrieval of the set of individuals in the domain and in the range of a role, etc.

Table 14.3: Definition of axiom sets $\mathcal{A}_E$ s. t. $\mathcal{KB} \models E$ iff $\mathcal{KB} \cup \mathcal{A}_E$ is unsatisfiable.

E	$\mathcal{A}_E$
$R \sqsubseteq S$	$\{\neg S(\mathsf{x},\mathsf{y}), R(\mathsf{x},\mathsf{y})\}$
$C \sqsubseteq D$	$\{(C \sqcap \neg D(\mathsf{x})\}$
$C(\mathsf{a})$	$\{\neg C(\mathsf{a})\}$
$R(\mathsf{a},\mathsf{b})$	$\{\neg R(\mathsf{a},\mathsf{b})\}$
$\mathsf{a} = \mathsf{b}$	$\mathsf{a} \neq \mathsf{b}$
$\mathsf{a} \neq \mathsf{b}$	$\mathsf{a} = \mathsf{b}$

Other reasoning tasks, called non-standard, have a somewhat different goal:

- *Induction*: as opposed to the aforementioned deductive methods, inductive approaches usually take an amount of factual (assertional) data and try to generalize them by generating hypotheses expressed as terminological axioms or complex concepts. This task draws inspiration from inductive logic programming;

- *Abduction*: In ontology engineering, abductive reasoning services come handy when a wanted consequence (say E) is not entailed by the knowledge base $\mathcal{KB}$ and one wants to determine what information $\mathcal{KB}'$ is missing, such that $\mathcal{KB} \cup \mathcal{KB}' \models E$;

- *Explanation*: the goal is to give an account on the cause why some axiom is entailed by the knowledge base, in other words to give an explanation for it. More precisely, a justification for the entailment is a knowledge base $\mathcal{KB}' \subseteq \mathcal{KB}$ such that $\mathcal{KB}' \models E$. There might be more than one justification for an entailment.

Closed- vs. Open-world Semantics

Often, an analogy is established between databases on the one hand and DL knowledge bases on the other hand. The schema of a database is compared to the TBox and the instance with the actual data is compared to the ABox. However, the semantics of ABoxes differs from the usual semantics of database instances. While a database instance represents exactly one interpretation, namely the one where classes and relations in the schema are interpreted by the objects and tuples in the instance, an ABox represents many different interpretations, namely all its models. As a consequence, absence of information in a database instance is interpreted as negative information, while absence of information in an ABox only indicates lack of knowledge. For example, if the only assertion about Peter is $\mathsf{hasChild}(\mathsf{PETER}, \mathsf{HARRY})$, then in a database this is understood as a representation of the fact that Peter has only one child. In an ABox, the assertion only expresses that, in fact, Harry is a child of Peter. However, the ABox has several models, some in which Harry is the only child and others in which he has brothers or sisters. The only way of stating in an ABox that Harry is the only child is by adding the assertion $(\leq 1\mathsf{hasChild})(\mathsf{PETER})$. The semantics of ABoxes is therefore an *open-world* semantics, while the traditional semantics of databases is a *closed-world* semantics.

This view has consequences for the way queries are answered. A database (in the sense introduced above) is a listing of a single finite interpretation. Answering a query, represented by a complex concept C, over that database amounts to computing $C^{\mathcal{I}}$, which is equivalent to evaluate a formula in a fixed finite model. Since an ABox represents possibly infinitely many interpretations, namely its models, query answering is more complex.

Algorithmic Approaches

Various reasoning paradigms have been investigated with respect to their applicability to DLs. Most of them originate from well-known approaches for theorem proving in a first-order logic setting. However, in contrast to the unavoidable downside that reasoning methods for first-order logic cannot be sound, complete, and terminating, approaches to reasoning in DLs aim at being sound and complete decision procedures, whence the reasoning techniques have to guarantee termination.

In general, reasoning methods can be subdivided into model-theoretic methods on one hand and proof-theoretic methods on the other.

Model-theoretic methods essentially try to construct models of a given knowledge base in an organized way. If this succeeds, the knowledge base has obviously been shown to be satisfiable, if the construction fails, unsatisfiability has been established. Typical reasoning paradigms of that sort are tableau procedures and automata-based approaches.

Proof-theoretic approaches operate more on the syntactic side: starting out from a normalized version of the knowledge base, deduction rules are applied to derive further logical statements about a potential model. If, in the course of these derivations a contradiction is derived, the considered knowledge base has shown to be unsatisfiable.

The majority of state-of-the art OWL reasoners, such as `Pellet` (Sirin et al., 2007), `FaCT++`, or
`RacerPro` use *tableau* methods with good performance results, but even those successful systems are not applicable in all practical scenarios. This motivates the search for alternative reasoning approaches that employ different methods in order to address cases where tableau algorithms exhibit certain weaknesses. Successful examples in this respect are the works based on resolution and hypertableaux as well as consequence-based approaches.

In Chapter 17 we will use `Pellet` as an OWL-DL reasoner to return explanations of queries on a (probabilistic) ontology, so a brief illustration of its main services is reported. For a complete description of its architecture and functionalities see the main reference (Sirin et al., 2007).

The Tableau Algorithm

Tableau procedures aim at constructing a model that satisfies all axioms of the given knowledge base. The strategy here is to maintain a set D of elements representing domain individuals (including anonymous ones) and acquire information about their concept memberships and role interrelatedness. D is initialized by all the individual names and the according ABox facts. Normally, the partial model thus constructed does not satisfy all the TBox and RBox axioms. Thus, the intermediate model is "repaired" as required by the axioms. This may mean to establish new concept membership or role interrelatedness information about the maintained elements, yet sometimes it may also be necessary to extend the set of considered domain individuals. Now and again, it might be required to make case distinctions and backtrack later. If we arrive at a state, where the intermediate model satisfies all the axioms and hence does not need to be repaired further, the knowledge base is satisfiable. If the intermediate model contains overt contradictions (such as an element marked as instance of a concept C and its negation $\neg C$ or an element marked as an instance of $\perp$), we can be sure that repairing it further by adding more information will never lead to a proper model, hence we are in a "dead end" and we need to backtrack. If every alternative branch thus followed leads into such a "dead end", we can be sure that no model can exist. However, note that the continued "repairing" performed in a tableau procedure does not necessarily terminate, since performing one repair might cause the need for another repair and so forth ad infinitum. Therefore, in order to be applicable as a decision procedure, these infinite computations must be prevented to ensure termination. This can be achieved by a strategy called blocking, where certain domain elements are blocked (which essentially means that they are exempt from the necessity of being repaired) by other domain individuals which “look the same” in terms of concept memberships. For more advanced DLs, more complicated blocking strategies are needed.

Let’s see how the procedure, shown in Algorithm 13, works in detail.
Tableaux are *completion graphs* where each node a represents an individual a, labeled with the set of concepts $\mathcal{L}(a)$ it belongs to. Each edge $\langle a, b\rangle$ in the graph is labeled with the set of roles to which the couple (a, b) belongs. The reasoner repeatedly applies a set of consistency preserving *tableau expansion rules* until a clash (i.e., a contradiction) is detected or a clash-free graph is found to which no more rules are applicable. Some of the rules are non-deterministic, i.e., they generate a finite set of tableaux. Thus the algorithm keeps a set of tableaux that is consistent if there is any tableau in it that is consistent, i.e., that is clash-free.

Given a concept C, to prove the axiom $C(a)$ an individual a is assumed to be in $\neg C$, thus $\neg C$ is assigned to the label of a. The entailment of any type of axiom by a knowledge base can be checked by means of the tableau algorithm as shown in Table 14.3.

Formally, a **completion graph** for a knowledge base $\mathcal{KB}$ is a tuple $G = (V, E, \mathcal{L}, \dot{\neq})$ in which (V, E) is a directed graph. Each node $a \in V$ is labeled with a set of concepts $\mathcal{L}(a)$ and each edge $e = \langle a, b\rangle$ is labeled with a set $\mathcal{L}(e)$ of role names. The binary predicate $\dot{\neq}$ is used to specify the inequalities between nodes.

In order to manage non-determinism, the algorithm keeps a set T of completion graphs. T is initialized with a single completion graph G_0 that contains a node for each individual a asserted in the knowledge base, labeled with the nominal $\{a\}$ plus all concepts C such that $a : C \in \mathcal{KB}$, and an edge $e = \langle a, b\rangle$ labeled with R for each assertion $(a, b) : R \in \mathcal{KB}$.

At each step of the algorithm, an expansion rule is applied to a completion graph G from T: G is removed from T, the rule is applied and the results are inserted in T. The rules for $\mathcal{SHOIN}^{(\mathbf{D})}$ are shown in Figure 14.2. For example, if the rule $\rightarrow \sqcap$ is applied, a concept $C \sqcap D$ in the label of a node a causes C and D to be added to $\mathcal{L}(a)$, because the individual that a represents must be an instance of both C and D.

If a *non-deterministic* rule is applied to a graph G in T, then G is replaced by the resulting set of graphs. For example, if the disjunction $C \sqcup D$ is present in the label of a node, the rule

Algorithm 13 Tableau algorithm.

```
1: function TABLEAU($C, a, \mathcal{KB}$)
2:     Input: $C, a$ (the concept and the individual to test)
3:     Input: $\mathcal{KB}$ (the knowledge base)
4:     Output: $S$ (a set of axioms) or $null$
5:     Let $G_0$ be an initial completion graph from $\mathcal{KB}$ containing an anonymous individual $a$ and $\neg C \in \mathcal{L}(a)$
6:     $T \leftarrow \{G_0\}$                                   ▷ T: set of completion graphs
7:     repeat
8:         Select a rule $r$ applicable to a clash-free graph $G$ from $T$
9:         $T \leftarrow T \setminus \{G\}$
10:        Let $\mathcal{G} = \{G'_1, ..., G'_n\}$ be the result of applying $r$ to $G$
11:        $T \leftarrow T \cup \mathcal{G}$
12:    until All graphs in $T$ have a clash or no rule is applicable
13:    if All graphs in $T$ have a clash then
14:        $S \leftarrow \emptyset$
15:        for all $G \in T$ do
16:            let $s_G$ the result of $\tau$ for the clash of $G$
17:            $S \leftarrow S \cup s_G$
18:        end for
19:        $S \leftarrow S \setminus \{\neg C(a)\}$
20:        return $S$
21:    else
22:        return $null$
23:    end if
24: end function
```

$\rightarrow \sqcup$ generates two graphs, one in which C is added to the node's label and the other in which D is added to the node's label.

An **event** during the execution of the algorithm can be (Kalyanpur, 2006): 1) $Add(C, a)$, the addition of a concept C to $\mathcal{L}(a)$; 2) $Add(R, \langle a, b\rangle)$, the addition of a role R to $\mathcal{L}(\langle a, b\rangle)$; 3) $Merge(a, b)$, the merging of the nodes a, b; 4) $\dot{\neq}(a, b)$, the addition of the inequality $a \dot{\neq} b$ to the relation $\dot{\neq}$; 5) $Report(g)$, the detection of a clash g. We use $\mathcal{E}$ to denote the set of events recorded during the execution of the algorithm. A clash is either:

- a couple (C, a) where C and $\neg C$ are present in the label of a node, i.e. $\{C, \neg C\} \subseteq \mathcal{L}(a)$;
- a couple $(Merge(a, b), \dot{\neq}(a, b))$, where the events $Merge(a, b)$ and $\dot{\neq}(a, b)$ belong to $\mathcal{E}$.

Each time a clash is detected in a completion graph G, the algorithm stops applying rules to G. Once every completion graph in T contains a clash or no more expansion rules can be applied to it, the algorithm *terminates*. If all the completion graphs in the final set T contain a clash, the algorithm returns *unsatisfiable* as no model can be found. Otherwise, any one clash-free completion graph in T represents a possible model for the concept and the algorithm returns *satisfiable*.

The `Pellet` Reasoner

`Pellet` is the first complete OWL-DL consistency checker, that "takes a document as input, and returns one word being Consistent, Inconsistent, or Unknown". OWL-DL is a syntactic variant of the very expressive Description Logic $\mathcal{SHOIN}^{(\mathbf{D})}$. `Pellet` covers all of OWL-DL including inverse and transitive properties, cardinality restrictions, datatype reasoning for an extensive set of built-ins as well as user defined simple XML schema datatypes, enumerated classes (nominals) and instance assertions.

This practical OWL reasoner provides the "standard" set of Description Logic inference services, namely Consistency checking of an ontology (checking the consistency of an ABox with respect to a TBox), Concept satisfiability, Classification (creating the complete class hierarchy), Realization (finding the most specific classes that an individual belongs to). It is standard to reduce them all to Consistency checking, as `Pellet` does. These basic services can be accessed by querying the reasoner. Pellet also supports some less standard services.

The core of the system is the *tableaux* reasoner, which has only one functionality: checking the consistency of an ontology. According to the OWL model-theoretic semantics, an ontology is consistent if there is an interpretation that satisfies all the facts and axioms in the ontology. Such an interpretation is called a model of the ontology. The tableaux reasoner searches for such a model.

All other reasoning tasks can be defined in terms of consistency checking. For example, checking whether an individual is an instance of a concept or not can be tested by asserting that the individual is an instance of the complement of that class and then checking for (in)consistency.

`Pellet` is written in Java and is open source. It is used in a number of projects, from pure research to industrial settings.

```
$\rightarrow$ unfold: if $A \in \mathcal{L}(a)$, $A$ atomic and $(A \sqsubseteq D) \in K$, then
  if D $\notin \mathcal{L}(a)$, then $Add(D, \mathcal{L}(a))$
  $(D, a) := ((A, a) \cup \{A \sqsubseteq D\})$
$\rightarrow$ CE: if $(C \sqsubseteq D) \in K$, with $C$ not atomic, $a$ not blocked then
  if $(\neg C \sqcup D) \notin \mathcal{L}(a)$, then $Add((\neg C \sqcup D), a)$
  $((\neg C \sqcup D), a) := \{C \sqsubseteq D\}$
$\rightarrow \sqcap$: if $(C_1 \sqcap C_2) \in \mathcal{L}(a)$, $a$ is not indirectly blocked, then
  if $\{C_1, C_2\} \not\subseteq \mathcal{L}(a)$, then $Add(\{C_1, C_2\}, a)$
  $(C_i, a) := ((C_1 \sqcap C_2), a)$
$\rightarrow \sqcup$: if $(C_1 \sqcup C_2) \in \mathcal{L}(a)$, $a$ is not indirectly blocked, then
  if $\{C_1, C_2\} \cap \mathcal{L}(a) = \emptyset$, then
    Generate graphs $G_i := G$ for each $i \in \{1, 2\}$
    $Add(C_i, a)$ in $G_i$ for each $i \in \{1, 2\}$
    $(C_i, a) := ((C_1 \sqcup C_2), a)$
$\rightarrow \exists$: if $\exists S.C \in \mathcal{L}(a)$, $a$ is not blocked then
  if $a$ has no S-neighbour $b$ with $C \in \mathcal{L}(b)$,then create new node $b$, $Add(S, \langle a, b\rangle)$, $Add(C, b)$
  $(C, b) := ((\exists S.C), a)$;  $(S, \langle a, b\rangle) := ((\exists S.C), a)$
$\rightarrow \forall$: if $\forall(S.C) \in \mathcal{L}(a)$, $a$ is not indirectly blocked and there is an $S$-neighbor $b$ of $a$, then
  if $C \notin \mathcal{L}(b)$, then $Add(C, b)$
  $(C, b) := (((\forall S.C), a) \cup (S, \langle a, b\rangle))$
$\rightarrow \forall^+$: if $\forall(S.C) \in \mathcal{L}(a)$, $a$ is not indirectly blocked
  and there is an $R$-neighbor $b$ of $a$, $Trans(R)$ and $R \sqsubseteq S$, then
  if $\forall R.C \notin \mathcal{L}(b)$, then $Add(\forall R.C, b)$
  $((\forall R.C), b) := ((\forall S.C), a) \cup ((R, \langle a, b\rangle) \cup \{Trans(R)\} \cup \{R \sqsubseteq S\})$
$\rightarrow \geq$: if $(\geq nS) \in \mathcal{L}(a)$, $a$ is not blocked, then
  if there are no $n$ safe $S$-neighbors $b_1, ..., b_n$ of $a$ with $b_i \neq b_j$, then
    create $n$ new nodes $b_1, ..., b_n$; $Add(S, \langle a, b_i\rangle)$; $\dot{\neq}(b_i, b_j)$
  $(S, \langle a, b_i\rangle) := ((\geq nS), a)$;  $(\dot{\neq}(b_i, b_j)) := ((\geq nS), a)$
$\rightarrow \leq$: if $(\leq nS) \in \mathcal{L}(a)$, $a$ is not indirectly blocked and there are $m$ $S$-neighbors $b_1, ..., b_m$ of $a$ with $m > n$, then
  For each possible pair $b_i, b_j$, $1 \leq i, j \leq m; i \neq j$ then
    Generate a graph $G'$
    $(Merge(b_i, b_j)) := (((\leq nS), a) \cup (S, \langle a, b_1\rangle) ... \cup (S, \langle a, b_m\rangle))$
    if $b_j$ is a nominal node, then $Merge(b_i, b_j)$ in $G'$,
    else if $b_i$ is a nominal node or ancestor of $b_j$, then $Merge(b_j, b_i)$
    else $Merge(b_i, b_j)$ in $G'$
    if $b_i$ is merged into $b_j$, then for each concept $C_i$ in $\mathcal{L}(b_i)$,
    $(Add(C_i, \mathcal{L}(b_j))) := (Add(C_i, \mathcal{L}(b_i))) \cup (Merge(b_i, b_j))$
    (similarly for roles merged, and correspondingly for concepts in $b_j$ if merged into $b_i$)
$\rightarrow O$: if, $\{o\} \in \mathcal{L}(a) \cap \mathcal{L}(b)$ and not $a \dot{\neq} b$, then $Merge(a, b)$
  $(Merge(a, b)) := (\{o\}, a) \cup (\{o\}, b)$
  For each concept $C_i$ in $\mathcal{L}(a)$, $(Add(C_i, \mathcal{L}(b))) := (Add(C_i, \mathcal{L}(a))) \cup (Merge(a, b))$
  (similarly for roles merged, and correspondingly for concepts in $\mathcal{L}(b)$)
$\rightarrow NN$: if $(\leq nS) \in \mathcal{L}(a)$, $a$ nominal node, $b$ blockable S-predecessor of $a$ and there is no $m$
    s.t. $1 \leq m \leq n$, $(\leq mS) \in \mathcal{L}(a)$ and there exist $m$ nominal S-neighbours $c_1, ..., c_m$ of $a$ s.t. $c_i \dot{\neq} c_j$, $1 \leq j \leq m$,
  then generate new $G_m$ for each $m$, $1 \leq m \leq n$ and do the following in each $G_m$:
      $Add(\leq mS, a)$, $((\leq mS), a) := ((\leq nS), a) \cup ((S, \langle b, a\rangle)$
      create $b_1, ..., b_m$; add $b_i \dot{\neq} b_j$ for $1 \leq i \leq j \leq m$. $(\dot{\neq}(b_i, b_j) := ((\leq nS), a) \cup (S, \langle b, a\rangle)$
      $Add(S, \langle a, b_i\rangle)$; $Add(\{o_i\}, b_i)$;
      $(S, \langle a, b_i\rangle) := ((\leq nS), a) \cup (S, \langle b, a\rangle)$; $(\{o_i\}, b_i) := ((\leq nS), a) \cup (S, \langle b, a\rangle)$
```

Figure 14.2: $\mathcal{SHOIN}^{(\mathbf{D})}$ Tableau expansion rules.

Part V

Probability in Description Logics (DLs)

Chapter 15

Probabilistic Extensions for DLs

Description Logics have been extended by features not available in the basic framework, but considered important for using them as a modeling language. Examples concern: concrete domain constraints; modal, epistemic, and temporal operators; probabilities and fuzzy logic; defaults. These extensions are “non-classical” in the sense that defining their semantics is not obvious and requires an extension of the model-theoretic framework considered until now.

In order to represent *vague and uncertain knowledge*, different approaches based on probabilistic (Heinsohn, 1994; Jaeger, 1994; Koller et al., 1997; Lukasiewicz and Straccia, 2008; Yelland, 2000), possibilistic (Hollunder, 1994), and fuzzy logics (Straccia, 1998, 2001; Tresp and Molitor, 1998) have been proposed, since Description Logics whose semantics is based on classical first-order logic cannot express that kind of knowledge.

We review here the **probabilistic extensions** that have been proposed lately, before presenting our probabilistic approach applied to the $\mathcal{SHOIN}^{(\mathbf{D})}$ Description Logic in the next Chapter. First, how to extend the terminological (TBox) formalism is considered.

In classical Description Logics, one has very restricted means of expressing (and testing for) relationships between concepts. Given two concepts C and D, subsumption tells whether C is contained in D, and the satisfiability test (applied to $C \sqcap D$) tells us whether C and D are disjoint. Relationships that are in-between (e.g., 90% of all Cs are Ds) can neither be expressed nor be derived.

This deficiency is overcome in (Heinsohn, 1994; Jaeger, 1994) by allowing for *probabilistic terminological axioms* of the form

$$P(C \mid D) = p,$$

where C, D are concept descriptions and $0 < p < 1$ is a real number. (Heinsohn, 1994) actually uses a different notation and allows for more expressive axioms stating that $P(C \mid D)$ belongs to an interval $[p_l; p_u]$, with $0 \leq p_l \leq p_u \leq 1$ for the Description Logic $\mathcal{ALC}$. Such an axiom states that the conditional probability for an object known to be in D to belong to C is p. A given finite interpretation $\mathcal{I}$ satisfies $P(C \mid D) = p$ iff

$$\frac{|(C \sqcap D)^{\mathcal{I}}|}{|D^{\mathcal{I}}|} = p.$$

More generally, the formal semantics of the extended language is defined in terms of probability measures on the set of all concept descriptions.

Given a knowledge base $\mathcal{P}$ consisting of probabilistic terminological axioms, the main inference task is then to derive optimal bounds for additional conditional probabilities: $\mathcal{P} \models P(C|D) \in [p, q]$ iff in all probability measures satisfying $\mathcal{P}$ the conditional probability belongs to the interval $[p, q]$. One is interested in finding the maximal p and minimal q such that $\mathcal{P} \models P(C|D) \in [p, q]$ is true. (Heinsohn, 1994) introduces local inference rules that can be used to derive bounds for conditional probabilities, but these rules are not complete, that is, in general they are not sufficient to derive the optimal bounds. (Jaeger, 1994) only describes a naive method for computing optimal bounds. A more sophisticated version of that method reduces the inference problem to a linear optimization problem.

(Jaeger, 1994) also extends the assertional formalism by allowing for *probabilistic assertions* of the form

$$P(C(a)) = p,$$

where C is a concept description, a an individual name, and p a real number between 0 and 1. This kind of probabilistic statement is quite different from the one introduced by the terminological formalism. Whereas probabilistic terminological axioms state *statistical information*, which is usually obtained by observing a large number of objects, probabilistic assertions express a *degree of belief* in assertions for specific individuals. The formal semantics of probabilistic assertions is again defined with the help of probability measures on the set of all concept descriptions, one for each individual name. Intuitively, the measure for a tells for each concept C how likely it is (believed to be) that a belongs to C.

Given a knowledge base $\mathcal{P}$ consisting of probabilistic terminological axioms and assertions, the main inference task is now to derive optimal bounds for additional probabilistic assertions. However, if the probabilistic terminological axioms are supposed to have an impact on this inference problem, the semantics as sketched until now is not sufficient. In fact, until now there is no connection between the probability measure used for the terminological part and the measures for the assertional part. (Jaeger, 1994) uses cross entropy minimization in order to give a formal meaning to this intuition. Until now, there is no algorithm for computing optimal bounds for $P(C(a))$, given a knowledge base consisting of probabilistic terminological axioms and assertions.

The work reported in (Koller et al., 1997), which is restricted to the terminological component, has a focus that is quite different. In the previous works, the probabilistic terminological axioms provide constraints on the set of admissible probability measures, that may still be satisfied by a large set of distributions. In contrast, (Koller et al., 1997) present a framework for the specification of a unique probability distribution on the set of all concept descriptions (modulo equivalence). Since there are infinitely many such descriptions, providing such a (finite) specification is a nontrivial task. They employ Bayesian networks as the basic representation language for the required probabilistic specifications. The probability $P(C)$ of a concept description C can then be computed by using inference algorithms developed for Bayesian networks. The complexity of this computation is linear in the length of C.

(Yelland, 2000) also combines Bayesian networks and Description Logics. In contrast to (Koller et al., 1997), this work extends Bayesian networks by Description Logic features rather than the other way round. The Description Logic used is rather inexpressive, but this allows the author to avoid restrictions on the network that had to be imposed by (Koller et al., 1997).

The distinction between assertions with statistical information and assertions expressing a degree of belief dates back to (Halpern, 1990)'s work, which presented two approaches to giving semantics to first-order logics of probability. The first approach puts a probability on the domain and is appropriate for giving semantics to formulas involving *statistical* information such as "The probability that a randomly chosen bird flies is greater than 0.9". It is equivalent to say that 90% of the individuals in a population have the property P of flying. The second approach puts a probability on possible worlds, and is appropriate for giving semantics to formulas describing degrees of belief, such as "The probability that Tweety (a particular bird) flies is greater than 0.9". The first statement seems to assume only one possible world (the real one), and some probability distribution over the set of birds: if we consider a bird chosen at random, with probability greater than 0.9 it will fly. The second statement implicitly assumes the existence of a number of possibilities (in some of which Tweety flies, while in others doesn't), with some probability over these possibilities.

(Halpern, 1990) also shows how the two approaches can be combined in one framework, allowing simultaneous reasoning, for example to express the statement "The probability that Tweety flies is greater than the probability that a randomly chosen bird flies."

(Ding and Peng, 2004) proposes a probabilistic extension of OWL that admits a translation into Bayesian networks. This semantics assigns a probability distribution $P(a)$ over individuals, i.e.
$\sum_a P(a) = 1$, and assigns a probability to a class C as $P(C) = \sum_{a \in C} P(a)$.

PR-OWL (Carvalho et al., 2010; Costa et al., 2008) is an upper ontology that provides a framework for building probabilistic ontologies. It allows to use the first-order probabilistic logic MEBN (Laskey and Costa, 2005) for representing uncertainty in ontologies.

In (Giugno and Lukasiewicz, 2002; Lukasiewicz, 2002, 2008) the authors use probabilistic lexicographic entailment from probabilistic default reasoning. They use the DL P-$\mathcal{SHIQ}^{(\mathcal{D})}$ and allow both terminological and assertional probabilistic knowledge about instances of concepts and roles. Probabilistic knowledge is expressed using *conditional constraints* of the form $(D|C)[l, u]$ as previously seen in (Heinsohn, 1994). `PRONTO` (Klinov, 2008) is a system that allows to perform inference in this semantics; in particular it is the first probabilistic Nilsson-style (see below) Description Logic reasoner capable of processing knowledge bases containing about a thousand of probabilistic axioms.

Similarly to (Jaeger, 1994), the terminological knowledge is interpreted statistically while the assertional knowledge is interpreted in an epistemic way by assigning degrees of beliefs to assertions. Moreover it also allows to express default knowledge about concepts that can be overridden in subconcepts and whose semantics is given by Lehmann's lexicographic default entailment. These works are based on Nilsson's probabilistic logic (Nilsson, 1986), where a probabilistic interpretation Pr defines a probability distribution over the set of interpretations Int. The probability of a logical formula F according to Pr, denoted $Pr(F)$, is the sum of all $Pr(I)$ such that $I \in Int$ and $I \models F$. A probabilistic knowledge base $\mathcal{KB}$ is a set of probabilistic formulas of the form $F \geq p$. A probabilistic interpretation Pr satisfies $F \geq p$ iff $Pr(F) \geq p$. Pr satisfies $\mathcal{KB}$, or Pr is a model of $\mathcal{KB}$, iff Pr satisfies all $F \geq p \in \mathcal{KB}$. $Pr(F) \geq p$ is a tight logical consequence of $\mathcal{KB}$ iff p is the infimum of $Pr(F)$ subject to all models Pr of $\mathcal{KB}$. Computing tight logical consequences from probabilistic knowledge bases can be done by solving a linear optimization problem.

Other approaches, such as (d'Amato et al., 2008; Gottlob et al., 2011), combine a lightweight ontology language, *DL-Lite* and *Datalog+/-* respectively, with graphical models, Bayesian networks and Markov networks respectively. In both cases, an ontology is composed of a set of annotated axioms and a graphical model and the annotations are sets of assignments of random variables from the graphical model. The semantics is assigned by considering the possible worlds of the graphical model and by stating that an axiom holds in a possible world if the assignments in its annotation hold. The probability of a conclusion is then the sum of the probabilities of the possible worlds where the conclusion holds.

Chapter 16

Probabilistic DLs under the Distribution Semantics

This chapter is dedicated to presenting a new approach for the integration of probability theory and DLs, that draws on the Distribution Semantics (Sato, 1995) described in Chapter 9. The integrated framework is applied to $\mathcal{SHOIN}^{(\mathbf{D})}$, that is the basis of the OWL-DL language, and takes the name of `DISPONTE` for ***DIstribution Semantics for Probabilistic ONTologiEs*** (Bellodi et al., 2011),(Riguzzi et al., 2012a), (Riguzzi et al., 2012b). This approach is also inspired by (Halpern, 1990) since `DISPONTE` allows to represent both statistical and epistemic (i.e., about degree of belief) information and combine them in hybrid forms. Syntax and semantics are illustrated in Sections 16.1 and 16.2 respectively. Inference under `DISPONTE` semantics is presented with several examples in Section 16.3.

16.1 Syntax

The basic idea of `DISPONTE` is to annotate axioms with a probability and assume that each axiom is independent of the others. We have followed an approach similar to (Halpern, 1990) for the assignment of probabilities.

A *probabilistic knowledge base* $\mathcal{KB}$ is a set of certain axioms or probabilistic axioms.

- *Certain axioms* take the form of regular DL axioms;
- *Probabilistic axioms* take the form

$$p ::_{Var} E \tag{16.1}$$

Axiom	Variables allowed in the subscript
ABox axiom	none
$C \sqsubseteq D$	x
$R \sqsubseteq S$	x, y
$Trans(R)$	x, y, z

Table 16.1: Variables which have to be instantiated for each kind of axiom.

where p is a real number in $[0, 1]$, Var is a set of variables from $\{x, y, z\}$ and E is a DL axiom. Var is usually written as a string, so xy indicates the subset $\{x, y\}$. If Var is empty, then the :: symbol has no subscript. The variables in Var must appear in the FOL version of E. Variables allowed by the different types of axioms are shown in Table 16.1.

In order to give a semantics to such probabilistic knowledge bases, we consider their translation into First Order predicate Logic and then we use the model-theoretic semantics of the resulting theory. The translation functions for roles and concepts are described in Section 14.2, where the set $Var = \{x_0, x_1, x_2\}$ corresponds to the set here referred as $\{x, y, z\}$.

in order to associate independent Boolean random variables to (instantiations of) the FOL formulas. By assigning values to every random variable we obtain a *world*: in particular, a *world* is identified by the set of FOL formulas whose random variables is assigned value 1. We fix a domain $\Delta^{\mathcal{I}}$ of interpretation and each individual a appearing in $\mathcal{KB}$ is replaced with $a^{\mathcal{I}}$. Every formula translated from a *certain* axiom is included in a world w. For each *probabilistic* axiom, we generate all the substitutions for the variables of the equivalent predicate logic formula that are indicated in the subscript. There may be an infinite number of instantiations. Each instantiated formula may be included or not in w.
In this way we obtain a FOL theory to which a model-theoretic semantics may be assigned.

Var in Formula (16.1) indicates the set of variables of the axiom that should be replaced by random individuals. In other words, it indicates which instantiated forms of the axiom should be considered. Similarly to (Halpern, 1990), this allows to assign a different interpretation to the probabilistic axioms depending on the variables that have to be instantiated and allows for a fine-grained modeling of the domain.

If Var is empty, the probability p can be interpreted as an *epistemic probability*, i.e., as the degree of our belief in axiom E, while if Var is equal to the set of all variables appearing in E (given in Table 16.1), p can be interpreted as a *statistical probability*, i.e., as information regarding random individuals from the domain. If Var is nor empty neither the set of all allowed variables, an hybrid interpretation can be given, in which a degree of belief is assigned to instantiations of the axiom with random individuals.

Probabilistic concept assertions

A *probabilistic concept assertion*

$$p :: a : C$$

means that we have degree of belief p in $C(a)$, i.e., we believe with probability p that the individual a belongs to concept C. The statement that "Tweety flies with probability 0.9" of (Halpern, 1990) can be expressed as

$$0.9 :: tweety : Flies$$

A *probabilistic concept inclusion axiom* of the form

$$p :: C \sqsubseteq D \tag{16.2}$$

represents the fact that we believe in the truth of $C \sqsubseteq D$ with probability p.
A probabilistic concept inclusion axiom of the form

$$p ::_x C \sqsubseteq D \tag{16.3}$$

instead means that a random individual x of class C has probability p of belonging to D.

The first two examples use p as an epistemic probability, while the third one represents the statistical information that a fraction p of the individuals of C belongs to D. In this way, the overlap between C and D is quantified by the probability p. For example, the statement that "90% of birds fly"' (Halpern, 1990) can be expressed as

$$0.9 ::_x Bird \sqsubseteq Flies \tag{16.4}$$

The difference between axioms 16.2 and 16.3 is that, if two individuals belong to class C, the probability that they both belong to D according to (16.2) is p, since p represents the truth of the formula as a whole, while according to (16.3) is $p \cdot p$, since *each* randomly chosen individual has probability p of belonging to class D and the two events are independent.

On the other hand, if a query Q to a knowledge base containing Formula (16.3) can be proved true in two ways, using axiom $C \sqsubseteq D$ instantiated with individual a or instantiated with individual b, and no other probabilistic axiom is used for deriving the query, the truth of the query is given by the disjunction of two independent random variables (associated to the two instantiations) each having probability p of being true. Thus the probability of the query will result in $P(Q) = p + p - p \cdot p$. If the knowledge base contains axiom (16.2) instead, the probability of the query would be $P(Q) = p$.

The larger the number of variables specified in Var is, the more fine-grained is the model of the domain, in which different ways of reaching a conclusion are taken into account and each provides a contribution to the probability. This results in considering more probable conclusions that have multiple supporting derivations at the expense of complexity, since more random variables must be considered.

Example 30 *Consider the knowledge base $\mathcal{KB}$:*

$$\begin{array}{lll} 0.7 & ::_x & Schoolchild \sqsubseteq European \\ 0.4 & ::_x & Schoolchild \sqsubseteq OnlyChild \\ 0.6 & ::_x & European \sqsubseteq GoodInMath \\ 0.5 & ::_x & OnlyChild \sqsubseteq GoodInMath \end{array}$$

It states that 70% of school children are Europeans, 40% of school children are only children, 60% of Europeans are good in math and 50% of only children are good in math.

Probabilistic role assertions

A *role inclusion axiom* $R \sqsubseteq S$ can be subscripted with:

- *nothing*:

  $$p :: R \sqsubseteq S$$

  p expresses a degree of belief in the inclusion in its entirety.

- xy:

  $$p ::_{xy} R \sqsubseteq S$$

  given a random couple of individuals a and b, if $R(a, b)$ holds, then $S(a, b)$ holds with probability p. In other words, a randomly chosen couple of individuals which is R-related, has probability p of being S-related.

- x or y:

$$p ::_x R \sqsubseteq S$$

given a random individual x, we have degree of belief p in the formula

$$\forall y.R(x, y) \rightarrow S(x, y)$$

- a *transitivity axiom* can be subscripted with all subsets of $\{x, y, z\}$:

$$p ::_{xyz} Trans(R) \tag{16.5}$$

means that, given three random individuals a, b and c, if $R(a, b)$ and $R(b, c)$ hold, then $R(a, c)$ holds with probability p, i.e., the formula

$$R(a, b) \wedge R(b, c) \rightarrow R(a, c) \tag{16.6}$$

has degree of belief p. Note that if two different instantiations of the transitivity formula are used to derive a query, they are considered as independent random variables with axiom (16.5).

Instead, the probabilistic transitivity axiom

$$p' ::_{xy} Trans(R) \tag{16.7}$$

indicates that we consider versions in which the variables x and y are instantiated: given a random couple of individuals a and b, we have degree of belief p' in the formula

$$\forall z.R(a, b) \wedge R(b, z) \rightarrow R(a, z)$$

Note that we may have the same axiom with different subscripts in the knowledge base. In this case, each probabilistic axiom represents independent evidence for the instantiated versions.

If Formula (16.6) is found to be necessary to entail a query and the knowledge base contains both (16.5) and (16.7), the probability of such a formula is given by the disjunction of two Boolean random variables, one with probability p and the other with probability p'.

Example 31 *The knowledge base*

$$\begin{array}{rcl} & & kevin : \forall friend.Person \\ & & (kevin, laura) : friend \\ & & (laura, diana) : friend \\ 0.4 & ::_{xyz} & Trans(friend) \end{array}$$

means that all individuals in the $friend$ relation with $kevin$ are persons, $kevin$ is a friend of $laura$, $laura$ is a friend of $diana$ and given three randomly chosen individuals a, b and c, there is 40% probability that if a is a friend of b and b is a friend of c, a will be a friend of c. In particular, we have 40% probability that, if $kevin$ is $laura$'s friend and $laura$ is $diana$'s friend, then $kevin$ is $diana$'s friend. Since the first two are certain facts, $kevin$ is $diana$'s friend with probability 40%.

16.2 Semantics

While we follow (Halpern, 1990) with respect to the syntax and to the kinds of information captured by a probabilistic statement, the semantics in this context is only defined on the basis of *possible worlds*, rather than on probability structures with two separate probability measures, one over the individuals of the domain and the other over possible worlds. The full machinery of (Halpern, 1990) is not required because possible worlds correspond to sets of formulas rather than to interpretations and the language is much simpler as it does not allow unlimited nesting of the operator w, used by (Halpern, 1990) to indicate a statement's probability.

Instead, the DISPONTE semantics for $\mathcal{SHOIN}^{(\mathbf{D})}$ is based on *the Distribution Semantics for Probabilistic Logic Programs* (PLP), described in Chapter 9. Since the domain $\Delta^{\mathcal{I}}$ may be infinite, we have to apply the Distribution Semantics for PLP *with function symbols*, that has an infinite domain of interpretation as well. Here we follow the approach of (Poole, 2000).

An *atomic choice* in this context is a triple (F_i, θ_j, k) where F_i is the formula obtained by translating the i_{th} probabilistic axiom, θ_j is a substitution and $k \in \{0, 1\}$; θ_j instantiates the variables indicated in the Var subscript of the ith probabilistic axiom, i.e., $Var(\theta_j) = Var$ in 16.1, while k indicates whether $F_i\theta_j$ is chosen to be included in a world (k = 1) or not (k = 0). Note that, differently from the Distribution Semantics for PLP, substitutions need not ground formulas but this is not a core requirement of the semantics.

A *composite choice* κ is a consistent set of atomic choices, i.e., $(F_i, \theta_j, k) \in \kappa, (F_i, \theta_j, m) \in \kappa \Rightarrow k = m$ (only one decision for each formula). The probability of composite choice κ is $P(\kappa) = \prod_{(F_i,\theta_j,1)\in\kappa} p_i \prod_{(F_i,\theta_j,0)\in\kappa}(1 - p_i)$, where p_i is the probability associated to axiom F_i.

A *selection* σ is a total composite choice, i.e., it contains an atomic choice (F_i, θ_j, k) for every instantiation $F_i\theta_j$ of every probabilistic axiom of the theory. Since the domain may be infinite, selections may, too. Let us indicate with $\mathcal{S}_{\mathcal{K}}$ the set of all selections. A selection σ identifies a theory w_σ called a *world* in this way: $w_\sigma = \mathcal{C} \cup \{F_i\theta_j | (F_i, \theta_j, 1) \in \sigma\}$ where $\mathcal{C}$ is the set of the certain axioms translated in FOL. Let $\mathcal{W}_{\mathcal{K}}$ be the set of all worlds. A composite choice κ identifies a set of worlds $\omega_\kappa = \{w_\sigma | \sigma \in \mathcal{S}_{\mathcal{K}}, \sigma \supseteq \kappa\}$. We define the set of worlds identified by a set of composite choices K as $\omega_K = \bigcup_{\kappa \in K} \omega_\kappa$.

Properties of Composite Choices

We review in the following a few interesting properties of composite choices for the purposes of inference tasks.

- A composite choice κ is an **explanation** for a query Q if Q is entailed by every world of ω_κ. A set K of composite choices is *covering* with respect to Q if every world $w_\sigma \in \mathcal{S}_{\mathcal{K}}$ in which Q is entailed is such that $w_\sigma \in \omega_K$.

- Two composite choices κ_1 and κ_2 are **incompatible** if their union is inconsistent. For example, the composite choices $\kappa_1 = \{(F_i, \theta_j, 1)\}$ and $\kappa_2 = \{(F_i, \theta_j, 0)\}$ are incompatible.

  A set K of composite choices is **mutually incompatible** if for all $\kappa_1 \in K, \kappa_2 \in K, \kappa_1 \neq \kappa_2 \Rightarrow \kappa_1$ and κ_2 are incompatible. For example

  $$K = \{\kappa_1, \kappa_2\} \tag{16.8}$$

  with

  $$\kappa_1 = \{(F_i, \theta_j, 1)\}$$

  and

  $$\kappa_2 = \{(F_i, \theta_j, 0), (F_l, \theta_m, 1)\} \tag{16.9}$$

  is mutually incompatible.

  We define *the probability of a mutually incompatible set K of composite choices* as

  $$P(K) = \sum_{\kappa \in K} P(\kappa) \tag{16.10}$$

- Two sets of composite choices K_1 and K_2 are **equivalent** if $\omega_{K_1} = \omega_{K_2}$, i.e., if they identify the same set of worlds. For example, K in (16.8) is equivalent to

  $$K' = \{\kappa'_1, \kappa'_2\} \tag{16.11}$$

with

$$\kappa'_1 = \{(F_i, \theta_j, 1)\}$$

and

$$\kappa'_2 = \{(F_l, \theta_m, 1)\} \tag{16.12}$$

- If $F\theta$ is an instantiated formula and κ is a composite choice such that $\kappa \cap \{(F, \theta, 0), (F, \theta, 1)\} = \emptyset$, the **split of** κ **on** $F\theta$ is the set of composite choices $S_{\kappa,F\theta} = \{\kappa \cup \{(F, \theta, 0)\}, \kappa \cup \{(F, \theta, 1)\}\}$. It is easy to see that κ and $S_{\kappa,F\theta}$ identify the same set of possible worlds, i.e., that $\omega_\kappa = \omega_{S_{\kappa,F\theta}}$. For example, the split of κ'_2 in (16.12) on $F_i\theta_j$ contains κ_2 of Formula (16.9) and $\{(F_i, \theta_j, 1), (F_l, \theta_m, 1)\}$.

Following (Poole, 2000), we can prove the following results.

Theorem 1 (Splitting algorithm) *Given a finite set K of finite composite choices, there exists a finite set K' of mutually incompatible finite composite choices such that K and K' are equivalent.*

Proof 1 *Given a finite set of finite composite choices K, there are two possibilities to form a new set K' of composite choices so that K and K' are equivalent:*

1. ***removing dominated elements**: if $\kappa_1, \kappa_2 \in K$ and $\kappa_1 \subset \kappa_2$, let $K' = K \setminus \{\kappa_2\}$.*
2. ***splitting elements**: if $\kappa_1, \kappa_2 \in K$ are compatible (and neither is a superset of the other), there is a $(F, \theta, k) \in \kappa_1 \setminus \kappa_2$. We replace κ_2 by the split of κ_2 on $F\theta$. Let $K' = K \setminus \{\kappa_2\} \cup S_{\kappa_2,F\theta}$.*

In both cases $\omega_K = \omega_{K'}$. If we repeat this two operations until neither of them is applicable we obtain a splitting algorithm (see Figure 14) that terminates because K is a finite set of finite composite choices. The resulting set K' is mutually incompatible and is equivalent to the original set. For example, the splitting algorithm applied to K' of Formula (16.11) can result in K of Formula (16.8).

Theorem 2 *If K_1 and K_2 are both mutually incompatible finite sets of finite composite choices such that they are equivalent, then $P(K_1) = P(K_2)$.*

Proof 2 *The theorem is the same as Lemma A.8 in (Poole, 1993). We report here the proof for the sake of clarity.*

Algorithm 14 Splitting algorithm to generate a set K' of *mutually incompatible* composite choices, equivalent to the input set K.

```
1: procedure SPLIT($K$)
2:     Input: finite set of composite choices $K$
3:     Output: mutually incompatible set $K'$ of composite choices, equivalent to $K$
4:     loop
5:         if $\exists \kappa_1, \kappa_2 \in K$ and $\kappa_1 \subset \kappa_2$ then
6:             $K \leftarrow K \setminus \{\kappa_2\}$
7:         else
8:             if $\exists \kappa_1, \kappa_2 \in K$ compatible then
9:                 choose $(F, \theta, k) \in \kappa_1 \setminus \kappa_2$
10:                $K \leftarrow K \setminus \{\kappa_2\} \cup S_{\kappa_2,F\theta}$        ▷ $S_{\kappa_2,F\theta}$ is the split of $\kappa_2$ on $F\theta$
11:            else
12:                exit and return $K$
13:            end if
14:        end if
15:    end loop
16: end procedure
```

Consider the set D of all instantiated formulas $F\theta$ that appear in an atomic choice in either K_1 or K_2. This set is finite. Each composite choice in K_1 and K_2 has atomic choices for a subset of D. For both K_1 and K_2, we repeatedly replace each composite choice κ of K_1 and K_2 with its split K' on an $F_i\theta_j$ from D that does not appear in κ. This procedure does not change the total probability as the probabilities of $(F_i, \theta_j, 0)$ and $(F_i, \theta_j, 1)$ sum to 1.

At the end of this procedure the two sets of composite choices will be identical. In fact, any difference can be extended to a possible world belonging to ω_{K_1} but not to ω_{K_2} or vice versa.

For example, K in (16.8) and $K'' = \{\kappa''_1, \kappa''_2\}$ with $\kappa''_1 = \{(F_i, \theta_j, 1), (F_l, \theta_m, 0)\}$ and $\kappa''_2 = \{(F_l, \theta_m, 1)\}$ of (16.9) are equivalent and are both mutually incompatible. Their probabilities are

$$P(K) = p_i + (1 - p_i)p_l = p_i + p_l - p_i p_l$$

and

$$P(K'') = p_i(1 - p_l) + p_l = p_i + p_l - p_i p_l$$

Note that if we compute the probability of K' in (16.11) with Formula (16.10) we would obtain $p_i + p_l$ which is different from the probabilities of K and K'' above, even if K' is equivalent to K and K''. The reason is that K' is not mutually exclusive.

Probability Measure

(Kolmogorov, 1950) defined probability functions (or measures) μ as real-valued functions over a σ-algebra Ω of subsets of a set $\mathcal{W}$ called the *sample space*. $\langle \mathcal{W}, \Omega, \mu \rangle$ is called a *probability space*. The set Ω of subsets of $\mathcal{W}$ is a σ-algebra of $\mathcal{W}$ iff

1. $\mathcal{W} \in \Omega$,
2. Ω is closed under complementation, i.e., $\omega \in \Omega \rightarrow (\mathcal{W} \setminus \omega) \in \Omega$, and
3. Ω is closed under countable union, i.e., if $\omega_i \in \Omega$ for $i = 1, 2, \ldots$ then $\bigcup_i \omega_i \in \Omega$.

The elements of Ω are called measurable sets. Not every subset of $\mathcal{W}$ need be present in Ω.

Given a sample space $\mathcal{W}$ and an algebra Ω of subsets of $\mathcal{W}$, a **probability measure** is a function $\mu : \Omega \rightarrow \mathbb{R}$ that satisfies the following axioms:

1. $\mu(\omega) \geq 0$ for all $\omega \in \Omega$,
2. $\mu(\mathcal{W}) = 1$,
3. μ is countably additive, i.e., if $O = \{\omega_1, \omega_2, \ldots\} \subseteq \Omega$ is a countable collection of pairwise disjoint sets, then $\cup_{\omega \in O} \omega = \sum_i \mu(\omega_i)$.

Here the finite additivity version of probability spaces (Halpern, 2003) is assumed. In this version, we impose a stronger condition on Ω, namely that it is an algebra: condition (3) above is replaced by (3$'$) Ω is closed under *finite* union, i.e., $\omega_1 \in \Omega, \omega_2 \in \Omega \rightarrow (\omega_1 \cup \omega_2) \in \Omega$. In this case, a measure μ must satisfy the following modification of axiom (3): (3$'$) μ is finitely additive, i.e., $\omega_1 \cap \omega_2 = \emptyset \rightarrow \mu(\omega_1 \cup \omega_2) = \mu(\omega_1) + \mu(\omega_2)$ for all $\omega_1, \omega_2 \in \Omega$.

We now define a different unique probability measure $\mu : \Omega_{\mathcal{K}} \rightarrow [0, 1]$ where $\Omega_{\mathcal{K}}$ is defined as the algebra of sets of *worlds identified by finite sets of finite composite choices*: $\Omega_{\mathcal{K}} = \{\omega_K | K \text{ is a finite set of finite composite choices}\}$. It is easy to see that $\Omega_{\mathcal{K}}$ is an algebra over $\mathcal{W}_{\mathcal{K}}$.

μ is defined by $\mu(\omega_K) = P(K')$ where K' is a mutually incompatible set of composite choices equivalent to K. $\langle \mathcal{W}_{\mathcal{K}}, \Omega_{\mathcal{K}}, \mu \rangle$ is a probability space according to Kolmogorov's definition.

16.3 Inference

The basic inference task of probabilistic ontologies in $\mathcal{SHOIN}^{(\mathbf{D})}$ DL under the Distribution Semantics is calculating probabilities of queries, i.e., axioms regarding concept and roles, according to a knowledge base $\mathcal{KB}$.

The probability of a query Q - according to the probability measure μ just defined in the previous subsection - is given by $P(Q) = \mu(\{w|w \in \mathcal{W}_{\mathcal{K}} \wedge w \models Q\})$. If Q has a finite set K of finite explanations such that K is covering then $\{w|w \in \mathcal{W}_{\mathcal{K}} \wedge w \models Q\} = \omega_K \in \Omega_{\mathcal{K}}$ and $P(Q)$ is well-defined. The problem of computing the probability of a query can thus be reduced to that of *finding a covering set of explanations K and then making it mutually incompatible*, so that the probability can be computed with a summation as in Formula (16.10). To obtain a mutually incompatible set of explanations, the splitting algorithm can be applied.

Alternatively, given a covering set K of explanations (not necessarily mutually incompatible) for a query Q, we can define the Disjunctive Normal Form (DNF) Boolean formula f_K

$$f_K(\mathbf{X}) = \bigvee_{\kappa \in K} \bigwedge_{(F_i,\theta_j,1)} X_{ij} \bigwedge_{(F_i,\theta_j,0)} \overline{X_{ij}} \tag{16.13}$$

The variables $\mathbf{X} = \{X_{ij} \mid \exists k\ (F_i, \theta_j, k) \in \kappa, \kappa \in K\}$ are independent Boolean random variables. The probability that $f_K(\mathbf{X})$ assumes value 1 is equal to $P(Q)$. We can now apply *knowledge compilation* to the propositional formula $f_K(\mathbf{X})$ (Darwiche and Marquis, 2002), i.e., translate it to a target language that allows to answer queries in polynomial time. A target language that was found to give good performances is the one of Binary Decision Diagrams (BDD). From a BDD we can compute the probability of the query $P(Q)$ with a dynamic programming algorithm that is linear in the size of the BDD (De Raedt et al., 2007). (Riguzzi, 2009) showed that this approach is faster than the splitting algorithm. For a detailed description of BDDs see Section 7.2.

A BDD performs a Shannon expansion of the Boolean formula $f_K(\mathbf{X})$, so that if X is the variable associated with the root level of a BDD, the formula $f_K(\mathbf{X})$ can be represented as $f_K(\mathbf{X}) = X \wedge f_K^X(\mathbf{X}) \vee \overline{X} \wedge f_K^{\overline{X}}(\mathbf{X})$ where $f_K^X(\mathbf{X})$ ($f_K^{\overline{X}}(\mathbf{X})$) is the formula obtained from $f_K(\mathbf{X})$ by setting X to 1 (0). Now the two disjuncts are mutually exclusive and the probability of $f_K(\mathbf{X})$ can be computed as $P(f_K(\mathbf{X})) = P(X)P(f_K^X(\mathbf{X})) + (1 - P(X))P(f_K^{\overline{X}}(\mathbf{X}))$. In this way BDDs make the explanations mutually incompatible.

Having built the BDD representing the Boolean function of Boolean variables $f_K(\mathbf{X})$, in order to compute its probability and making inference, the dynamic programming algorithm traverses the diagram from the leaves, as shown in Figure 15, which it is recalled from subsection 9.2.

Algorithm 15 Probability of a Boolean function computed by traversing its BDD.

```
1:  function BDD_PROBABILITY($node\ n$)
2:      Input: a BDD node
3:      Output: the probability of the Boolean function encoded by the BDD
4:      if $n$ is 1-terminal then
5:          return 1
6:      end if
7:      if $n$ is 0-terminal then
8:          return 0
9:      end if
10:     let $X$ be $v(n)$                    ▷ $v(n)$ is the variable associated with node $n$
11:     let $h$ and $l$ be the high and low children of $n$
12:     $P_h$ =BDD_PROBABILITY($h$)
13:     $P_l$ ←BDD_PROBABILITY($l$)
14:     return $P(X) \cdot P_h + (1 - P(X)) \cdot P_l$
15: end function
```

Examples

In the following we show how inference is performed over different probabilistic knowledge bases.

Example 32 *The following probabilistic knowledge base is inspired by the* `people+pets` *ontology proposed in (Patel-Schneider et al., 2003):*

$$\begin{array}{rcl} & & \exists hasAnimal.Pet \sqsubseteq NatureLover \\ & & (kevin, fluffy) : hasAnimal \\ & & (kevin, tom) : hasAnimal \\ 0.4 & :: & fluffy : Cat \\ 0.3 & :: & tom : Cat \\ 0.6 & :: & Cat \sqsubseteq Pet \end{array}$$

The $\mathcal{KB}$ indicates that the individuals that own an animal which is a pet are nature lovers and that $kevin$ owns the animals $fluffy$ and tom. Moreover, we believe in the fact that $fluffy$ and

tom are cats and that cats are pets with a certain probability.
The predicate logic formulas (without external quantifiers) equivalent to the probabilistic axioms are

$$\begin{aligned} F_1 &= Cat(\mathit{fluffy}) \\ F_2 &= Cat(tom) \\ F_3 &= Cat(x) \rightarrow Pet(x) \end{aligned}$$

A covering set of explanations for the ***query axiom*** $Q = kevin : NatureLover$ *is* $K = \{\kappa_1, \kappa_2\}$ *where* $\kappa_1 = \{(F_1, \emptyset, 1), (F_3, \emptyset, 1)\}$ *and* $\kappa_2 = \{(F_2, \emptyset, 1), (F_3, \emptyset, 1)\}$.

P(Q) may be computed by means of two alternatives:

1. *An equivalent mutually incompatible set K' of explanations can be obtained by applying the splitting algorithm. In this case $K' = \{\kappa'_1, \kappa'_2\}$ where*
   $\kappa'_1 = \{(F_1, \emptyset, 1), (F_3, \emptyset, 1), (F_2, \emptyset, 0)\}$ *and*
   $\kappa'_2 = \{(F_2, \emptyset, 1), (F_3, \emptyset, 1)\}$.

   So $P(Q) = 0.4 \cdot 0.6 \cdot 0.7 + 0.3 \cdot 0.6 = 0.348$.

2. *If we associate the random variables X_{11} with $(F_1, \emptyset)$, X_{21} with $(F_2, \emptyset)$ and X_{31} with $(F_3, \emptyset)$, the BDD associated with the set K of explanations is shown in Figure 16.1.*

   By applying the dynamic programming algorithm 15 we get

$$\begin{aligned} \text{BDD\_PROBABILITY}(n_3) &= 0.6 \cdot 1 + 0.4 \cdot 0 = 0.6 \\ \text{BDD\_PROBABILITY}(n_2) &= 0.4 \cdot 0.6 + 0.6 \cdot 0 = 0.24 \\ \text{BDD\_PROBABILITY}(n_1) &= 0.3 \cdot 0.6 + 0.7 \cdot 0.24 = 0.348 \end{aligned}$$

   so $P(Q) = \text{PROB}(n_1) = 0.348$.

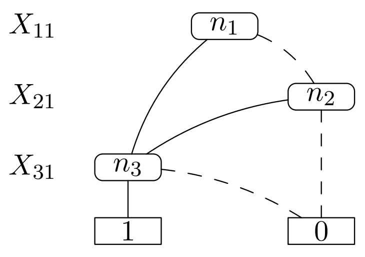


Figure 16.1: BDD for Example 32.

Example 33 *If we replace the axiom*

$$0.6 :: Cat \sqsubseteq Pet$$

in Example 32 with

$$0.6 ::_x Cat \sqsubseteq Pet$$

we are expressing the knowledge that 60% of cats are pets. In this case the query would have the explanations $K = \{\kappa_1, \kappa_2\}$ *where*
$\kappa_1 = \{(F_1, \emptyset, 1), (F_3, \{x/\mathit{fluffy}\}, 1)\}$ *and*
$\kappa_2 = \{(F_2, \emptyset, 1), (F_3, \{x/tom\}, 1)\}$.

P(Q) may be computed by means of two alternatives:

1. *An equivalent mutually incompatible set* K' *of explanations obtained by applying the splitting algorithm is* $K' = \{\kappa'_1, \kappa'_2, \kappa'_3\}$ *where*
   $\kappa'_1 = \{(F_1, \emptyset, 1), (F_3, \{x/\mathit{fluffy}\}, 1), (F_2, \emptyset, 0)\}$,
   $\kappa'_2 = \{(F_1, \emptyset, 1), (F_3, \{x/\mathit{fluffy}\}, 1), (F_2, \emptyset, 1), (F_3, \{x/tom\}, 0)\}$ *and*
   $\kappa'_3 = \{(F_2, \emptyset, 1), (F_3, \{x/tom\}, 1)\}$.

   So $P(Q) = 0.4 \cdot 0.6 \cdot 0.7 + 0.4 \cdot 0.6 \cdot 0.3 \cdot 0.4 + 0.3 \cdot 0.6 = 0.3768$.

2. *If we associate the random variables* X_{11} *with* $(F_1, \emptyset)$*,* X_{21} *with* $(F_2, \emptyset)$*,* X_{31} *with* $(F_3, \{x/\mathit{fluffy}\})$ *and* X_{32} *to* $(F_3, \{x/tom\})$*, the BDD associated with the set K of explanations is shown in Figure 16.2.*

By applying Algorithm 15 we get

$$\begin{aligned}
\text{BDD\_PROBABILITY}(n_4) &= 0.6 \cdot 1 + 0.4 \cdot 0 = 0.6 \\
\text{BDD\_PROBABILITY}(n_3) &= 0.3 \cdot 0.6 + 0.7 \cdot 0 = 0.18 \\
\text{BDD\_PROBABILITY}(n_2) &= 0.6 \cdot 1 + 0.4 \cdot 0.18 = 0.672 \\
\text{BDD\_PROBABILITY}(n_1) &= 0.4 \cdot 0.672 + 0.6 \cdot 0.18 = 0.3768
\end{aligned}$$

so $P(Q) = \text{PROB}(n_1) = 0.3768$.

Example 34 *Let us consider a slightly different knowledge base:*

$$\begin{array}{lll}
0.5 & ::_x & \exists hasAnimal.Pet \sqsubseteq NatureLover \\
 & & (kevin, \mathit{fluffy}) : hasAnimal \\
 & & (kevin, tom) : hasAnimal \\
 & & \mathit{fluffy} : Cat \\
 & & tom : Cat \\
0.6 & ::_x & Cat \sqsubseteq Pet
\end{array}$$

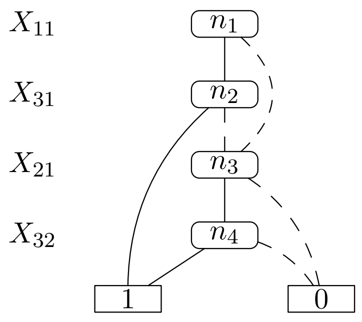


Figure 16.2: BDD for Example 33.

Here the ABox assertions are certain, the overlap between cats and pets is defined as in Example 33 and moreover we say that 50% of people who have an animal that is a pet are nature lovers. The predicate logic formulas (without external quantifiers) equivalent to the probabilistic axioms are

$$\begin{aligned} F_1 &= \exists y.hasAnimal(x,y) \land Pet(y) \rightarrow NatureLover(x) \\ F_2 &= Cat(x) \rightarrow Pet(x) \end{aligned}$$

A covering set of explanations for the ***query axiom*** $Q = kevin : NatureLover$ *is* $K = \{\kappa_1, \kappa_2\}$ *where*
$\kappa_1 = \{(F_1, \{x/kevin\}, 1), (F_2, \{x/fluffy\}, 1)\}$ *and*
$\kappa_2 = \{(F_1, \{x/kevin\}, 1), (F_2, \{x/\ tom\}, 1)\}$.

P(Q) may be computed by means of two alternatives:

1. *An equivalent mutually incompatible set K' of explanations obtained by applying the splitting algorithm is $K' = \{\kappa'_1, \kappa'_2\}$ where*
   $\kappa'_1 = \{(F_1, \{x/kevin\}, 1), (F_2, \{x/fluffy\}, 1), (F_2, \{x/tom\}, 0)\}$ *and*
   $\kappa'_2 = \{(F_1, \{x/kevin\}, 1), (F_2, \{x/tom\}, 1)\}$.
   So $P(Q) = 0.5 \cdot 0.6 \cdot 0.4 + 0.5 \cdot 0.6 = 0.42$.

2. *If we associate the random variables X_{31} with $(F_1, \{x/kevin\})$, X_{11} with $(F_2, \{x/fluffy\})$ and X_{21} with $(F_2, \{x/tom\})$, the BDD associated with the set K of explanations is shown in Figure 16.1.*

   By applying Algorithm 15 we get

$$\begin{aligned} \text{BDD\_PROBABILITY}(n_3) &= 0.5 \cdot 1 + 0.5 \cdot 0 = 0.5 \\ \text{BDD\_PROBABILITY}(n_2) &= 0.6 \cdot 0.5 + 0.4 \cdot 0 = 0.3 \\ \text{BDD\_PROBABILITY}(n_1) &= 0.6 \cdot 0.5 + 0.4 \cdot 0.3 = 0.42 \end{aligned}$$

so $P(Q) = \textsc{Prob}(n_1) = 0.42$.

Example 35 *Let us consider the knowledge base from Example 30:*

$$\begin{array}{lll}0.7 & ::_x & Schoolchild \sqsubseteq European \\ 0.4 & ::_x & Schoolchild \sqsubseteq OnlyChild \\ 0.6 & ::_x & European \sqsubseteq GoodInMath \\ 0.5 & ::_x & OnlyChild \sqsubseteq GoodInMath\end{array}$$

The predicate logic formulas (without external quantifiers) equivalent to the probabilistic axioms are:

$$\begin{array}{lll}F_1 & = & Schoolchild(x) \rightarrow European(x) \\ F_2 & = & Schoolchild(x) \rightarrow OnlyChild(x) \\ F_3 & = & European(x) \rightarrow GoodInMath(x) \\ F_4 & = & OnlyChild(x) \rightarrow GoodInMath(x)\end{array}$$

A covering set of explanations for the ***query axiom*** $Q = Schoolchild \sqsubseteq GoodInMath$ *is* $K = \{\kappa_1, \kappa_2\}$ *where* $\kappa_1 = \{(F_1, \{x/a\}, 1), (F_3, \{x/a\}, 1)\}$ *and*
$\kappa_2 = \{(F_2, \{x/a\}, 1), (F_4, \{x/a\}, 1)\}$*, where* a *is an anonymous member of* $\Delta^{\mathcal{I}}$.

P(Q) may be computed by means of two alternatives:

1. *After splitting we get* $K' = \{\kappa'_1, \kappa'_2, \kappa'_3\}$ *where*
   $\kappa'_1 = \{(F_1, \{x/a\}, 1), (F_3, \{x/a\}, 1)\}$,
   $\kappa'_2 = \{(F_1, \{x/a\}, 0), (F_2, \{x/a\}, 1), (F_4, \{x/a\}, 1)\}$ *and*
   $\kappa'_3 = \{(F_1, \{x/a\}, 1), (F_3, \{x/a\}, 0), (F_2, \{x/a\}, 1), (F_4, \{x/a\}, 1)\}$.
   So $P(Q) = 0.7 \cdot 0.6 + 0.3 \cdot 0.4 \cdot 0.5 + 0.7 \cdot 0.6 \cdot 0.5 = 0.536$.

2. *If we associate the random variables* X_{11} *with* $(F_1, \{x/a\})$, X_{21} *with* $(F_3, \{x/a\})$, X_{31} *with* $(F_2, \{x/a\})$ *and* X_{32} *with* $(F_4, \{x/a\})$*, the BDD associated with the set* K *of explanations is shown in Figure 16.2.*

   By applying Algorithm 15 we get

$$\begin{array}{lll}\textsc{Bdd\_Probability}(n_4) & = & 0.5 \cdot 1 + 0.5 \cdot 0 = 0.5 \\ \textsc{Bdd\_Probability}(n_3) & = & 0.4 \cdot 0.5 + 0.6 \cdot 0 = 0.2 \\ \textsc{Bdd\_Probability}(n_2) & = & 0.6 \cdot 1 + 0.4 \cdot 0.2 = 0.68 \\ \textsc{Bdd\_Probability}(n_1) & = & 0.7 \cdot 0.68 + 0.3 \cdot 0.2 = 0.536\end{array}$$

   so $P(Q) = \textsc{Prob}(n_1) = 0.536$.

Example 36 *Let us consider the knowledge base of Example 31:*

$$\begin{array}{lll} & & kevin : \forall friend.Person \\ & & (kevin, laura) : friend \\ & & (laura, diana) : friend \\ 0.4 & ::_{xyz} & Trans(friend) \end{array}$$

The predicate logic formula (without external quantifiers) equivalent to the transitivity probabilistic axiom is

$$F_1 \quad = \quad friend(x, y) \land friend(y, z) \rightarrow friend(x, z)$$

A covering set of explanations for the ***query axiom*** $Q = diana : Person$ *is* $K = \{\kappa_1\}$ *where* $\kappa_1 = \{(F_1, \{x/kevin, y/laura, z/diana\}, 1)\}$*, so* $P(Q) = 0.4$*.*

Example 37 *The following knowledge base contains transitivity and subrole axioms:*

$$\begin{array}{lll} & & kevin : \forall kin.Person \\ & & (kevin, laura) : friend \\ & & (laura, diana) : friend \\ 0.8 & ::_{xy} & friend \sqsubseteq kin \\ 0.4 & ::_{xyz} & Trans(friend) \end{array}$$

The subrole axiom states that, given two randomly chosen individuals a *and* b*, there is 80% probability that if* a *is a friend of* b *then* a *is kin to* b*. The predicate logic formulas (without external quantifiers) equivalent to the probabilistic axioms are* F_1 *as in Example 36 and*

$$F_2 \quad = \quad friend(x, y) \rightarrow kin(x, y)$$

A covering set of explanations for the ***query axiom*** $Q = diana : Person$ *is* $K = \{\kappa_1\}$ *where* $\kappa_1 = \{(F_1, \{x/kevin, y/laura, z/diana\}, 1), (F_2, \{x/kevin, y/diana\}, 1)\}$*.*
So $P(Q) = 0.4 \cdot 0.3 = 0.12$*.*

Chapter 17

The Probabilistic Reasoner **BUNDLE**

This chapter presents the algorithm BUNDLE for *Binary decision diagrams for Uncertain reasoNing on Description Logic thEories*, that performs inference over DISPONTE $\mathcal{SHOIN}^{(\mathbf{D})}$ DL. It exploits an underlying reasoner such as Pellet (Sirin et al., 2007) that returns explanations for queries, introduced in subsection 14.3. BUNDLE, whose preliminary version appeared in (Riguzzi et al., 2012c), uses the inference techniques developed for Probabilistic Logic Programs under the Distribution Semantics, in particular Binary Decision Diagrams.
BUNDLE is available for download from `http://sites.unife.it/ml/bundle` together with the dataset used in the experiments.

Section 17.1 describes the algorithms on which Pellet is based to return explanations for queries; Section 17.2 shows how these algorithms have been modified to BUNDLE needs. The complete system is summarized in Section 17.3. BUNDLE's complexity is dealt with in Section 17.4, while the results of its application on a real world dataset, in comparison with the system PRONTO, are illustrated in Section 17.5.

The problem of finding explanations for a query has been investigated by various authors (Horridge et al., 2009; Kalyanpur, 2006; Kalyanpur et al., 2007; Schlobach and Cornet, 2003). (Schlobach and Cornet, 2003) call it **axiom pinpointing** and consider it as a non-standard reasoning service useful for debugging ontologies. In particular, (Schlobach and Cornet, 2003) define *minimal axiom sets* or *MinAs* for short.

Definition 21 (MinA) *Let $\mathcal{KB}$ be a knowledge base and E an axiom that follows from it, i.e., $\mathcal{KB} \models E$. We call a set $M \subseteq \mathcal{KB}$ a* minimal axiom set *or* MinA *for E in $\mathcal{KB}$ if $M \models E$ and it is minimal w.r.t. set inclusion.*

The problem of enumerating all *MinAs* is called MIN-A-ENUM and is characterized by:
Input: A knowledge base $\mathcal{KB}$ and an axiom E such that $\mathcal{KB} \models E$.
Output: The set ALL-MINAS($E, \mathcal{KB}$) of all MinAs for E in $\mathcal{KB}$.

The set of all MinAs can be used to derive a covering set of explanations. Axiom pinpointing has been thoroughly discussed in (Halaschek-Wiener et al., 2006; Kalyanpur et al., 2005a, 2007, 2005b) for the purpose of tracing derivations and debugging ontologies. The techniques proposed in these papers have been integrated into the `Pellet` reasoner (Sirin et al., 2007). `Pellet` solves MIN-A-ENUM by finding a single MinA by means of a tableau algorithm and then uses a *hitting set tree* algorithm to find all the other *MinAs*.

`BUNDLE` is based on `Pellet` and uses it for solving the MIN-A-ENUM problem. However, `BUNDLE` needs, besides ALL-MINAS($E, \mathcal{KB}$), also the individuals to which axioms were applied for each probabilistic axiom appearing in ALL-MINAS($E, \mathcal{KB}$). We call this problem **instantiated axiom pinpointing** and `Pellet` has been modified to solve it.

In the following, first `Pellet` is illustrated for solving MIN-A-ENUM (Section 17.1), then the modified version of `Pellet` for solving instantiated axiom pinpointing follows (Section 17.2). Finally we summarize the whole `BUNDLE` algorithm in Section 17.3.

17.1 Axiom Pinpointing in `Pellet`

The algorithm for computing a *single MinA* (Function SINGLEMINA in Algorithm 16) takes advantage of (1) Function TABLEAU (Algorithm 13) and (2) Function BLACKBOXPRUNING (Algorithm 17). TABLEAU exploits the "tableau algorithm" (Schmidt-Schauß and Smolka, 1991), introduced in subsection 14.3: it tries to prove the unsatisfiability of a concept C by showing that the assumption of non empty C leads to contradiction. This is done by assuming that C has an instance and by trying to build a model for the knowledge base. If no model can be built, then C is unsatisfiable, otherwise the model is a counter example for C unsatisfiability.

Function TABLEAU

In order to find a *MinA* `Pellet` modifies the tableau expansion rules so that a *tracing function* τ is updated as well (Halaschek-Wiener et al., 2006; Kalyanpur, 2006; Kalyanpur et al., 2005a).

τ associates sets of axioms with events in the derivation. The **tracing function** τ maps each event $\varepsilon \in \mathcal{E}$ to a fragment of $\mathcal{KB}$. For example, ($\tau(Add(C, a))$,$\tau(Add(R, \langle a, b\rangle))$) is the

Algorithm 16 Algorithm for the computation of a *single* minimal axiom set *MinA*.

```
function SINGLEMINA($C, a, \mathcal{KB}$)
    Input: $C$ (the concept to be tested for unsatisfiability, an individual $a$)
    Input: $\mathcal{KB}$ (the knowledge base)
    Output: $S$ (a MinA for the unsatisfiability of $C$ w.r.t. $\mathcal{KB}$) or null
    $S \leftarrow$TABLEAU($C, a, \mathcal{KB}$)                              ▷ cf. Alg. 13
    if $S = null$ then
        return $null$
    else
        return BLACKBOXPRUNING($C, a, S$)
    end if
end function
```

set of axioms needed to explain the event $Add(C, a)$ ($Add(R, \langle a, b\rangle)$). We can also define τ for couples (concept, individual) and (role, couple of individuals) as $\tau(C, a) = \tau(Add(C, a))$ and $\tau(R, \langle a, b\rangle) = \tau(Add(R, \langle a, b\rangle))$ respectively.
The function τ is initialized as the empty set for all the elements of its domain except for $\tau(C, a)$ and $\tau(R, \langle a, b\rangle)$ to which the values $\{a : C\}$ and $\{(a, b) : R\}$ are assigned, if $a : C$ and $(a, b) : R$ are in the ABox respectively. The expansion rules (Figure 17.1) add axioms to values of τ. For a clash g of the form (C, a), $\tau(Report(g)) = \tau(Add(C, a)) \cup \tau(Add(\neg C, a))$. For a clash of the form $(Merge(a, b), \dot{\neq}(a, b))$, $\tau(Report(g)) = \tau(Merge(a, b)) \cup \tau(\dot{\neq}(a, b))$.

If $g_1, ..., g_n$ are the clashes, one for each of the elements of the final set of tableaux and $\tau(Report(g_i)) = s_{g_i}$, the output of Function TABLEAU is $S = \bigcup_{i \in \{1,...,n\}} s_{g_i} \setminus \{\neg C(a)\}$ where $C(a)$ is the assertion to test. However, this set may be redundant because additional axioms are also included in τ (Kalyanpur, 2006), e.g., during the $\rightarrow\leq$ rule; these axioms are responsible for each of the S successor edges.

Function BLACKBOXPRUNING

The set S, returned by Function TABLEAU in the previous phase, is pruned using a "black-box approach" shown in Algorithm 17 (Kalyanpur, 2006). This algorithm executes a loop on S, from which it removes an axiom at each iteration and checks whether the concept C turns satisfiable w.r.t. S, in which case the axiom is reinserted into S. The process continues until all axioms in S have been tested and then returns S.

The output S of Function SINGLEMINA is guaranteed to be a *MinA*, as established by Theorem 3 (Kalyanpur, 2006), where ALL-MINAS($C, a, \mathcal{KB}$) stands for the set of MinAs in

```
$\rightarrow$ unfold: if $A \in \mathcal{L}(a)$, $A$ atomic and $(A \sqsubseteq D) \in K$, then
    if D $\notin \mathcal{L}(a)$, then $Add(D, \mathcal{L}(a))$
    $\tau(D, a) := (\tau(A, a) \cup \{A \sqsubseteq D\})$
$\rightarrow$ CE: if $(C \sqsubseteq D) \in K$, with $C$ not atomic, $a$ not blocked then
    if $(\neg C \sqcup D) \notin \mathcal{L}(a)$, then $Add((\neg C \sqcup D), a)$
    $\tau((\neg C \sqcup D), a) := \{C \sqsubseteq D\}$
$\rightarrow \sqcap$: if $(C_1 \sqcap C_2) \in \mathcal{L}(a)$, $a$ is not indirectly blocked, then
    if $\{C_1, C_2\} \not\subseteq \mathcal{L}(a)$, then $Add(\{C_1, C_2\}, a)$
    $\tau(C_i, a) := \tau((C_1 \sqcap C_2), a)$
$\rightarrow \sqcup$: if $(C_1 \sqcup C_2) \in \mathcal{L}(a)$, $a$ is not indirectly blocked, then
    if $\{C_1, C_2\} \cap \mathcal{L}(a) = \emptyset$, then
        Generate graphs $G_i := G$ for each $i \in \{1, 2\}$
        $Add(C_i, a)$ in $G_i$ for each $i \in \{1, 2\}$
        $\tau(C_i, a) := \tau((C_1 \sqcup C_2), a)$
$\rightarrow \exists$: if $\exists S.C \in \mathcal{L}(a)$, $a$ is not blocked then
    if $a$ has no S-neighbor $b$ with $C \in \mathcal{L}(b)$,then
        create new node $b$, $Add(S, \langle a, b\rangle)$, $Add(C, b)$
    $\tau(C, b) := \tau((\exists S.C), a)$;  $\tau(S, \langle a, b\rangle) := \tau((\exists S.C), a)$
$\rightarrow \forall$: if $\forall(S.C) \in \mathcal{L}(a)$, $a$ is not indirectly blocked and there is an $S$-neighbor $b$ of $a$, then
    if $C \notin \mathcal{L}(b)$, then $Add(C, b)$
    $\tau(C, b) := (\tau((\forall S.C), a) \cup \tau(S, \langle a, b\rangle))$
$\rightarrow \forall^+$: if $\forall(S.C) \in \mathcal{L}(a)$, $a$ is not indirectly blocked and there is an $R$-neighbor $b$ of $a$, $Trans(R)$ and $R \sqsubseteq S$, then
    if $\forall R.C \notin \mathcal{L}(b)$, then $Add(\forall R.C, b)$
    $\tau((\forall R.C), b) := \tau((\forall S.C), a) \cup (\tau(R, \langle a, b\rangle) \cup \{Trans(R)\} \cup \{R \sqsubseteq S\})$
$\rightarrow \geq$: if $(\geq nS) \in \mathcal{L}(a)$, $a$ is not blocked, then
    if there are no $n$ safe $S$-neighbors $b_1, ..., b_n$ of $a$ with $b_i \neq b_j$, then
        create $n$ new nodes $b_1, ..., b_n$; $Add(S, \langle a, b_i\rangle)$; $\dot{\neq}(b_i, b_j)$
    $\tau(S, \langle a, b_i\rangle) := \tau((\geq nS), a)$;  $\tau(\dot{\neq}(b_i, b_j)) := \tau((\geq nS), a)$
$\rightarrow \leq$: if $(\leq nS) \in \mathcal{L}(a)$, $a$ is not indirectly blocked and there are $m$ $S$-neighbors $b_1, ..., b_m$ of $a$ with $m > n$, then
    For each possible pair $b_i, b_j$, $1 \leq i, j \leq m; i \neq j$ then
        Generate a graph $G'$
        $\tau(Merge(b_i, b_j)) := (\tau((\leq nS), a) \cup \tau(S, \langle a, b_1\rangle) ... \cup \tau(S, \langle a, b_m\rangle))$
        if $b_j$ is a nominal node, then $Merge(b_i, b_j)$ in $G'$,
        else if $b_i$ is a nominal node or ancestor of $b_j$, then $Merge(b_j, b_i)$
        else $Merge(b_i, b_j)$ in $G'$
        if $b_i$ is merged into $b_j$, then for each concept $C_i$ in $\mathcal{L}(b_i)$,
        $\tau(Add(C_i, \mathcal{L}(b_j))) := \tau(Add(C_i, \mathcal{L}(b_i))) \cup \tau(Merge(b_i, b_j))$
        (similarly for roles merged, and correspondingly for concepts in $b_j$ if merged into $b_i$)
$\rightarrow O$: if, $\{o\} \in \mathcal{L}(a) \cap \mathcal{L}(b)$ and not $a \dot{\neq} b$, then $Merge(a, b)$
    $\tau(Merge(a, b)) := \tau(\{o\}, a) \cup \tau(\{o\}, b)$
    For each concept $C_i$ in $\mathcal{L}(a)$, $\tau(Add(C_i, \mathcal{L}(b))) := \tau(Add(C_i, \mathcal{L}(a))) \cup \tau(Merge(a, b))$
    (similarly for roles merged, and correspondingly for concepts in $\mathcal{L}(b)$)
$\rightarrow NN$: if $(\leq nS) \in \mathcal{L}(a)$, $a$ nominal node, $b$ blockable S-predecessor of $a$ and there is no $m$
        s.t. $1 \leq m \leq n$, $(\leq mS) \in \mathcal{L}(a)$ and there exist $m$ nominal S-neighbors $c_1, ..., c_m$ of $a$ s.t. $c_i \dot{\neq} c_j$, $1 \leq j \leq m$,
    then generate new $G_m$ for each $m$, $1 \leq m \leq n$ and do the following in each $G_m$:
            $Add(\leq mS, a)$, $\tau((\leq mS), a) := \tau((\leq nS), a) \cup (\tau(S, \langle b, a\rangle)$
            create $b_1, ..., b_m$; add $b_i \dot{\neq} b_j$ for $1 \leq i \leq j \leq m$. $\tau(\dot{\neq}(b_i, b_j) := \tau((\leq nS), a) \cup \tau(S, \langle b, a\rangle)$
            $Add(S, \langle a, b_i\rangle)$; $Add(\{o_i\}, b_i)$;
            $\tau(S, \langle a, b_i\rangle) := \tau((\leq nS), a) \cup \tau(S, \langle b, a\rangle)$; $\tau(\{o_i\}, b_i) := \tau((\leq nS), a) \cup \tau(S, \langle b, a\rangle)$
```

Figure 17.1: `Pellet` tableau expansion rules.

Algorithm 17 Black-box pruning algorithm.

```
1: function BLACKBOXPRUNING($C, a, S$)
2:     Input: $C, a$ (the concept and the individual to test)
3:     Input: $S$ (the set of axioms to be pruned)
4:     Output: $S$ (the pruned set of axioms)
5:     for all axioms $E \in S$ do
6:         $S \leftarrow S - \{E\}$
7:         if $C(a) \cup S$ is satisfiable then
8:             $S \leftarrow S \cup \{E\}$
9:         end if
10:    end for
11:    return $S$
12: end function
```

which C is unsatisfiable.

Theorem 3 *Let $C(a)$ be an entailed assertion w.r.t. $\mathcal{KB}$ and let S be the output of the algorithm* SINGLEMINA *with input C, a, $\mathcal{KB}$; then $S \in$* ALL-MINAS$(C, a, \mathcal{KB})$.

Proof 3 *We need to prove that the output S' of Function* TABLEAU *includes at least one explanation, i.e., $S \cup \{C(a)\}$ is unsatisfiable.*
Let $\mathcal{E}$ be the sequence of events generated by TABLEAU *with inputs C, a and $\mathcal{KB}$. Let T', $\mathcal{E}'$ be the corresponding sets of completion graphs and events generated. For each event $\varepsilon_i \in \mathcal{E}$, it is possible to perform ε_i in the same sequence as before. This is because, for each event ε_i, the set of axioms in $\mathcal{KB}$ responsible for ε_i have been included in the output S' by construction of the tracing function τ in Figure 17.1. Thus, given $\mathcal{E}' = \mathcal{E}$, a clash occurs in each of the completion graphs in T' and the algorithm finds $S \cup \{C(a)\}$ unsatisfiable.*
BLACKBOXPRUNING *removes axioms while keeping the unsatisfiability.*

Hitting Set Algorithm

Function SINGLEMINA returns a single *MinA*. To compute all MinAs, Pellet uses the *hitting set algorithm* (Reiter, 1987).

Formally, let us consider a *universal set U* and a set of *conflict sets $CS \subseteq \mathcal{P}U$*, where $\mathcal{P}$ denotes the powerset operator. The set $HS \subseteq U$ is a *hitting set* for CS if each $S_i \in CS$ contains at least one element of HS, i.e. if $C_i \cap HS \neq \emptyset$ for all $1 \leq i \leq n$. We say that HS is a *minimal hitting set* for CS if HS is a hitting set for CS and no $HS' \subset HS$ is a hitting set for CS. The *hitting set problem* with input CS, U is to compute all the minimal hitting sets for CS.

Reiter's algorithm for solving this problem (Reiter, 1987) constructs a labeled tree called *Hitting Set Tree* (HST). In an HST a node v is labeled with OK or X or a set $\mathcal{L}(v) \in CS$ and an edge e is labeled with an element of U. Let $H(v)$ be the set of edge labels on the path from the root of the HST to node v. For each element $E \in \mathcal{L}(v)$, v has a successor w connected to v by an edge with E in its label. If $\mathcal{L}(v) = OK$, then $H(v)$ is a hitting set for CS.

The algorithm, described in detail in (Kalyanpur, 2006) and shown in Algorithm 18, starts from a *MinA* S and initializes an HST with S as the label of its root v. Then it selects an arbitrary axiom E in S, it removes it from $\mathcal{KB}$, generating a new knowledge base $\mathcal{KB}' = \mathcal{KB} - \{\mathcal{E}\}$, and it tests the unsatisfiability. If $\mathcal{KB}'$ is unsatisfiable, we obtain a new explanation for $C(a)$. The algorithm adds a new node w in the tree and a new edge $\langle v, w\rangle$, then it assigns this new explanation to the label of w and the axiom E to the label of the edge. The algorithm repeats this process until the unsatisfiability test returns negative, in which case it labels the new node with OK. The algorithm also eliminates extraneous unsatisfiability tests based on previous results: once a hitting set path is found, any superset of that path is guaranteed to be a hitting set as well, and thus no additional unsatisfiability test is needed for that path, as indicated by X in the label of the node. When the HST is fully built, all leaves of the tree are labeled with OK or X.

The distinct non-leaf nodes of the tree collectively represent the set ALL-MINAS for the unsatisfiability of C.

Example 38 *Let us consider a knowledge base $\mathcal{KB}$ with ten axioms and an entailed assertion $C(a)$. For the purpose of the example, we denote the axioms in $\mathcal{KB}$ with natural numbers. Suppose* ALL-MINAS$(C, a, \mathcal{KB})$ *is*

$$\text{ALL-MINAS}(C, a, \mathcal{KB}) = \{\{1, 2, 3\}, \{1, 5\}, \{2, 3, 4\}, \{4, 7\}, \{3, 5, 6\}, \{2, 7\}\}$$

Figure 17.2 shows the HST generated by the algorithm. It starts by computing a single explanation, in our case with the tableau algorithm, that returns $S = \{2, 3, 4\}$. The next step is to initialize a hitting set tree HST with a root node v and S as its label. Then, the algorithm selects an arbitrary axiom in S, say 2, generates a new node w and a new edge $\langle v, w\rangle$ with axiom 2 as its label. The algorithm tests the unsatisfiability of $\mathcal{KB} - \{2\}$. If it is unsatisfiable, as in our case, we obtain a new explanation for unsatisfiability of $\mathcal{KB} - \{2\}$, say $\{1, 5\}$. We add this set to CS and also assign it to the label of the new node w.

The algorithm repeats this process - i.e. removing an axiom, adding a node and checking unsatisfiability - until the unsatisfiability test turns negative, in which case we mark the new node with OK. Then, it recursively repeats these operations until the HST is fully built.

Algorithm 18 Hitting Set Tree Algorithm for computing all minimal axiom sets ALL-MINAS.

```
procedure HITTINGSETTREE($C, \mathcal{KB}, CS, HS, w, \alpha, p$)
    Input: $C$ (concept to be tested for satisfiability)
    Input: $\mathcal{KB}$ (knowledge base)
    Input/Output: $CS$ (a set of conflict sets, initially containing a single explanation)
    Input/Output: $HS$ (a set of Hitting Sets)
    Input: $w$ (the last node added to the Hitting Set Tree)
    Input: $E$ (the last axiom removed from $\mathcal{KB}$)
    Input: $p$ (the current edge path)
    if there exists a set $h \in HS$ s.t. $(\mathcal{L}(p) \cup \{E\}) \subseteq h$ then
        $\mathcal{L}(w) \leftarrow X$
        return
    else
        if $C$ is unsatisfiable w.r.t. $\mathcal{KB}$ then
            $m \leftarrow$SINGLEMINA($C, \mathcal{KB}$)
            $CS \leftarrow CS \cup \{m\}$
            create a new node $w'$ and set $\mathcal{L}(w') \leftarrow m$
            if $w \neq null$ then
                create an edge $e = \langle w, w' \rangle$ with $\mathcal{L}(e) = E$
                $p \leftarrow p \cup e$
            end if
            loop for each axiom $F \in \mathcal{L}(w')$
                HITTINGSETTREE($A, (\mathcal{KB} - \{F\}), CS, HS, w', F, p$)
            end loop
        else
            $\mathcal{L}(w) \leftarrow OK$
            $HS \leftarrow HS \cup \mathcal{L}(p)$
        end if
    end if
end procedure
```

The correctness and completeness of the hitting set algorithm is given by the following theorem.

Theorem 4 *(Kalyanpur, 2006) Let $\mathcal{KB} \models C(a)$, then the set of explanations returned by the hitting set algorithm (we will call it* EXPHST$(C, a, \mathcal{KB})$*) is equal to the set of all explanations of $C(a)$ w.r.t. $\mathcal{KB}$, so*

$$\text{EXPHST}(C, a, \mathcal{KB}) = \text{ALL-MINAS}(\mathcal{C}, , \mathcal{KB})$$

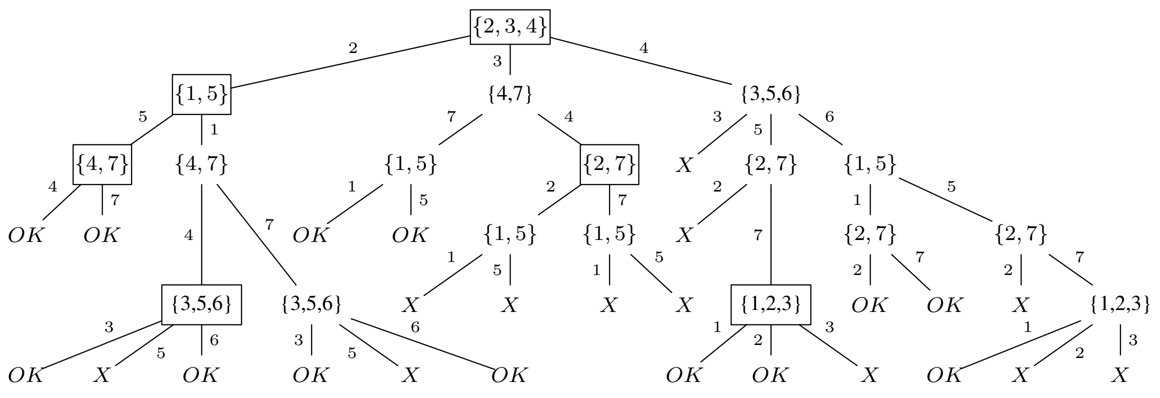


Figure 17.2: Finding ALL-MINAS$(C, a, \mathcal{KB})$ using the Hitting Set Algorithm: each distinct node is outlined in a box and represents a set in ALL-MINAS$(C, a, \mathcal{KB})$.

17.2 Instantiated Axiom Pinpointing

In instantiated axiom pinpointing we are interested in *instantiated minimal sets of axioms* that entail an axiom. We call this type of explanations *InstMinA*.

An *instantiated axiom set* is a finite set $\mathcal{F} = \{(F_1, \theta_1), \dots, (F_n, \theta_n)\}$ where $F_1, \dots, F_n$ are axioms and $\theta_1, \dots, \theta_n$ are substitutions.

Given two instantiated axiom sets $\mathcal{F} = \{(F_1, \theta_1), \dots, (F_n, \theta_n)\}$ and $\mathcal{E} = \{(E_1, \delta_1), \dots, (E_m, \delta_m)\}$, we say that $\mathcal{F}$ **precedes** $\mathcal{E}$, written $\mathcal{F} \preceq \mathcal{E}$, iff, for each $(F_i, \theta_i) \in \mathcal{F}$, there exists an $(E_j, \delta_j) \in \mathcal{E}$ and a substitution η such that $F_j\theta_j = E_i\delta_i\eta$.

Definition 22 (InstMinA) *Let $\mathcal{KB}$ be a knowledge base and E an axiom that follows from it, i.e., $\mathcal{KB} \models E$. We call $\{(F_1, \theta_1), \dots, (F_n, \theta_n)\}$ an* instantiated minimal axiom set *or* InstMinA *for E in $\mathcal{KB}$ if $\{F_1\theta_1, \dots, F_n\theta_n\} \models E$ and is minimal w.r.t. precedence.*

Minimality w.r.t. precedence means that axioms in a InstMinA are as instantiated as possible.

We call INST-MIN-A-ENUM the problem of enumerating all InstMinAs:

Problem: INST-MIN-A-ENUM
Input: A knowledge base $\mathcal{KB}$, and an axiom E such that $\mathcal{KB} \models E$.
Output: The set ALL-INSTMINAS$(E, \mathcal{KB})$ of all *InstMinAs* for E in $\mathcal{KB}$.

```
$\rightarrow$ *unfold*: **if** $A \in \mathcal{L}(a)$, $A$ atomic and $(A \sqsubseteq D) \in K$, **then**
    **if** D $\notin \mathcal{L}(a)$, **then** $Add(D, \mathcal{L}(a))$
    $\tau(D, a) := \tau(A, a) \cup \{(A \sqsubseteq D, a)\}$
$\rightarrow$ *CE*: **if** $(C \sqsubseteq D) \in K$, with $C$ not atomic, $a$ not blocked **then**
    **if** $(\neg C \sqcup D) \notin \mathcal{L}(a)$, **then** $Add(\neg C \sqcup D, a)$
    $\tau(\neg C \sqcup D, a) := \{(C \sqsubseteq D, a)\}$
$\rightarrow \forall$: **if** $\forall(S_1, C) \in \mathcal{L}(a_1)$, $a_1$ is not indirectly blocked and there is an $S_1$-neighbor $b$ of $a_1$, **then**
    **if** $C \notin \mathcal{L}(b)$, **then** $Add(C, b)$
    **if** there is a chain of individuals $a_2, \dots, a_n$ and roles $S_2, \dots, S_n$ such that
    $\bigcup_{i=2}^{n}\{(Trans(S_{i-1}), a_i, a_{i-1}), (S_{i-1} \sqsubseteq S_i, a_i)\} \subseteq \tau(\forall S_1.C, a_1)$
    and $\neg\exists a_{n+1} : \{(Trans(S_n), a_{n+1}, a_n), (S_n \sqsubseteq S_{n+1}, a_{n+1})\} \subseteq \tau(\forall S_1.C, a_1)$ **then**
        $\tau(C, b) := \tau(\forall S_1.C, a_1) \setminus \bigcup_{i=2}^{n}\{(Trans(S_{i-1}), a_i, a_{i-1}), (S_{i-1} \sqsubseteq S_i, a_i)\}$
        $\bigcup_{i=2}^{n}\{(Trans(S_{i-1}), a_i, a_{i-1}, b), (S_{i-1} \sqsubseteq S_i, a_i, b)\} \cup \tau(S_1, \langle a_1, b\rangle)$
    **else**
        $\tau(C, b) := \tau(\forall S_1.C, a_1) \cup \tau(S_1, \langle a_1, b\rangle)$
$\rightarrow \forall^+$: **if** $\forall(S.C) \in \mathcal{L}(a)$, $a$ is not indirectly blocked and there is an $R$-neighbor $b$ of $a$, $Trans(R)$ and $R \sqsubseteq S$, **then**
    **if** $\forall R.C \notin \mathcal{L}(b)$, **then** $Add(\forall R.C, b)$
    $\tau(\forall R.C, b) := \tau(\forall S.C, a) \cup \tau(R, \langle a, b\rangle) \cup \{(Trans(R), a, b), (R \sqsubseteq S, a)\}$
```

Figure 17.3: BUNDLE tableau expansion rules modified in Pellet.

In order to solve INST-MIN-A-ENUM, the Tableau expansion rules have been modified to return a set of pairs (axiom, substitution) instead of a set of axioms only.
In particular, we modified the rules $\rightarrow$ *unfold* , $\rightarrow$ *CE*, $\rightarrow\ \forall$ and $\rightarrow\ \forall^+$ as shown in Figure 17.3, where $(A \sqsubseteq D, a)$ is the abbreviation of $(A \sqsubseteq D, \{x/a\})$, $(Trans(R), a, b, c)$ of $(Trans(R), \{x/a, y/b, z/c\})$, $(Trans(R), a, b)$ of $(Trans(R), \{x/a, y/b\})$ and $(R \sqsubseteq S, a)$ of $(R \sqsubseteq S, \{x/a\})$, with a, b, c individuals and x, y, z variables.

The tracing function τ now stores, together with information regarding concepts and roles, also information concerning *individuals* involved in the expansion rules, which will be returned at the end of the derivation process together with the axioms. For rules $\rightarrow$ *unfold* and $\rightarrow CE$, the individual to which the subsumption axiom is applied is the one associated with the node. For rule $\rightarrow \forall^+$, the individuals considered are those connected by the role R, while rule $\rightarrow \forall$ makes a distinction between the case in which $\forall S_1.C$ was added to $\mathcal{L}(a_1)$ by $\forall^+$ or not. In the first case, it fully instantiates the transitivity and subrole axioms. In the latter case, it simply combines the explanation of $\forall S_1.C(a_1)$ with that of $(a_1, b) : S_1$.

Function BUNDLESINGLEMINA, shown in Algorithm 19, is BUNDLE version of Function SINGLEMINA and differs from it because it calls specialized versions of Functions TABLEAU and BLACKBOXPRUNING (indicated with the prefix BUNDLE) and it takes as input an extra argument, $BannedInstAxioms$.

Function BUNDLETABLEAU

Function BUNDLETABLEAU, shown in Algorithm 20, differs from TABLEAU because it uses the expansion rules of Figure 17.3 and takes an extra argument, $BannedInstAxioms$, that is used to specify a set of instantiated axioms to be avoided when expanding the tableau.
For the moment we assume that BUNDLESINGLEMINA is called with an empty set $BannedInstAxioms$, the case of a non empty set will be explained below. In this case the behavior of BUNDLETABLEAU is simply that of TABLEAU with an updated set of rules.

Algorithm 19 BUNDLE SINGLEMINA algorithm, a modified version of Algorithm 16 for the BUNDLE system.

```
1: function BUNDLESINGLEMINA($C, a, \mathcal{KB}, BannedInstAxioms$)
2:     Input: $C, a$ (the concept and individual to test)
3:     Input: $\mathcal{KB}$ (knowledge base)
4:     Input: $BannedInstAxioms$ (set of banned instantiated axioms)
5:     Output: $S$ (a MinA for $C(a)$) or $null$
6:     $S \leftarrow$BUNDLETABLEAU($C, a, \mathcal{KB}, BannedInstAxioms$)
7:     if $S = null$ then
8:         return $null$
9:     else
10:        return BUNDLEBLACKBOXPRUNING($C, S, BannedInstAxioms$)
11:    end if
12: end function
```

The following example clarifies how the rules $\rightarrow \forall$ and $\rightarrow \forall^+$ work.

Example 39 *Let us consider the knowledge base presented in Example 36 with the query $Q = diana : Person$.*

1. *BUNDLE starts from the tableau shown in Figure 17.4a.*

2. *It applies the $\rightarrow \forall^+$ rule to $kevin$, adding $\forall friend.Person$ to the label of $laura$. In this case $friend$ is considered as a subrole of itself. The tracing function τ is updated as:*

   $\tau(\forall friend.Person, laura) = \{$
   $(kevin : \forall friend.Person),$
   $((kevin, laura) : friend),$
   $(Trans(friend), kevin, laura)\}$

   equivalent to the following predicate logic theory:

Algorithm 20 BUNDLE TABLEAU algorithm, a modified version of Algorithm 13 for the BUNDLE system.

```
1: function BundleTableau($C, a, \mathcal{KB}, BannedInstAxioms$)
2:     Input: $C, a$ (the concept and individual to test)
3:     Input: $\mathcal{KB}$ (knowledge base)
4:     Input: $BannedInstAxioms$ (set of banned instantiated axioms)
5:     Output: $S$ (a set of axioms)
6:     Let $G_0$ be an initial completion graph from $\mathcal{KB}$ containing an anonymous individual $a$ and $\neg C \in \mathcal{L}(a)$
7:     $T \leftarrow \{G_0\}$
8:     repeat
9:         Select a rule $r$ applicable to a clash-free graph $G$ from $T$ such that no axiom
10:        from $BannedInstAxioms$ is added to $\tau$
11:        $T \leftarrow T \setminus \{G\}$
12:        Let $\mathcal{G} = \{G'_1, ..., G'_n\}$ be the result of applying $r$ to $G$
13:        $T \leftarrow T \cup \mathcal{G}$
14:    until All graphs in $T$ have a clash or no rule is applicable
15:    if All graphs in $T$ have a clash then
16:        $S \leftarrow \emptyset$
17:        for all $G \in T$ do
18:            let $s_G$ be the result of $\tau$ for the clash of $G$
19:            $S \leftarrow S \cup s_G$
20:        end for
21:        $S \leftarrow S \setminus \{\neg C(a)\}$
22:        return $S$
23:    else
24:        return $null$
25:    end if
26: end function
```

$$\begin{aligned}
&\tau(\forall friend.Person, laura) = \{\\
&\quad \forall y.friend(kevin, y) \rightarrow Person(y),\\
&\quad friend(kevin, laura),\\
&\quad \forall z.friend(kevin, laura) \wedge friend(laura, z) \rightarrow friend(kevin, z)\}
\end{aligned}$$

3. *BUNDLE applies the $\rightarrow \forall$ rule to $laura$ adding $Person$ to diana. The tracing function τ is modified as:*

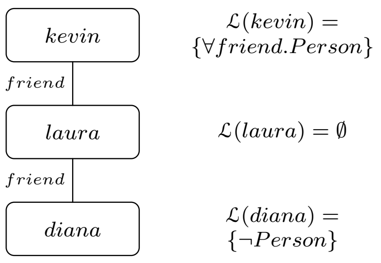
$$\begin{aligned}
&\tau(Person, diana) = \{\\
&\quad (kevin : \forall friend.Person),\\
&\quad ((kevin, laura) : friend), ((laura, diana) : friend),\\
&\quad (Trans(friend), kevin, laura, diana)\}
\end{aligned}$$

equivalent to the following predicate logic theory:

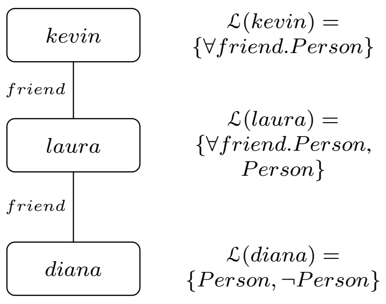
$$\begin{aligned}&\tau(Person, diana) = \{\\ &\quad \forall y.friend(kevin, y) \rightarrow Person(y),\\ &\quad friend(kevin, laura),\\ &\quad friend(laura, diana),\\ &\quad friend(kevin, laura) \wedge friend(laura, diana) \rightarrow friend(kevin, diana)\}\end{aligned}$$

4. *At this point the tableau contains a clash so the algorithm stops and returns the* $MinA = \tau(Person, diana) \cup \tau(\neg Person, diana) \setminus \{diana : \neg Person\} = \tau(Person, diana)$*.*

The final tableau is shown in Figure 17.4b.


$kevin$
$friend$
$laura$
$friend$
$diana$
$\mathcal{L}(kevin) = \{\forall friend.Person\}$
$\mathcal{L}(laura) = \emptyset$
$\mathcal{L}(diana) = \{\neg Person\}$

(a) Initial Tableau.


$kevin$
$friend$
$laura$
$friend$
$diana$
$\mathcal{L}(kevin) = \{\forall friend.Person\}$
$\mathcal{L}(laura) = \{\forall friend.Person, Person\}$
$\mathcal{L}(diana) = \{Person, \neg Person\}$

(b) Final Tableau.

Figure 17.4: Completion Graphs for Example 36. Nominals are omitted from node labels for brevity.

Example 40 *Let us consider the knowledge base*

$$\begin{array}{l} kevin : \forall kin.Person \\ (kevin, laura) : relative \\ (laura, diana) : ancestor \\ (diana, andrea) : ancestor \\ Trans(relative) \\ Trans(ancestor) \\ relative \sqsubseteq kin \\ ancestor \sqsubseteq relative \end{array}$$

The query $andrea : Person$ *has the* $InstMinA$ *(in predicate logic):*

$\tau(Person, andrea) = \{$
$\forall y.kin(kevin, y) \rightarrow Person(y),$
$relative(kevin, laura),$
$ancestor(laura, diana),$
$ancestor(diana, andrea),$
$relative(kevin, laura) \wedge relative(laura, andrea) \rightarrow relative(kevin, andrea),$
$ancestor(laura, diana) \wedge ancestor(diana, andrea) \rightarrow ancestor(laura, andrea),$
$relative(kevin, andrea) \rightarrow kin(kevin, andrea),$
$ancestor(laura, andrea) \rightarrow relative(laura, andrea)\}$

We can prove the analogous of Theorem 3 for our modified tableau algorithm. In the following, by $\{(E_1, \theta_1), ..., (E_n, \theta_n)\} \models E$ we mean $\{E_1\theta_1, ..., E_n\theta_n\} \models E$.

Theorem 5 *Let* $C(a)$ *be such that* $\mathcal{KB} \models C(a)$ *and let* S *be the output of Function* BUNDLETABLEAU *with input* $C, a, \mathcal{KB}$*, then* $S \in$ ALL-INSTMINAS$(C(a), \mathcal{KB})$.

Proof 4 *Following the proof of Theorem 3, we need to prove that the output* S *of* BUNDLETABLEAU *(before it is pruned) includes one explanation, i.e.,* $S \cup \{C(a)\}$ *is unsatisfiable. The sequence of events generated by the tableau algorithm of Figure 14.2 is the same as the one generated by the algorithm with the rules of Figure 17.3 since only the construction of* τ *has changed. To prove that* τ*, applied to an event, returns a set of instantiated axioms that entails the event, we proceed by induction on the number of rule applications. We have to do this only for the rules that have been modified.*

Let us consider the case of one rule application.

For rule $\rightarrow unfold$*, from* $A \in \mathcal{L}(a)$ *and* $A \sqsubseteq D$ *we conclude that* $D \in \mathcal{L}(a)$ *and we set* $\tau(D, a) = \tau(A, a) \cup \{(A \sqsubseteq D, a)\}$*. Since this is the first rule application, then* $\tau(A, a) = \{a : A\}$*. From* $A(a)$ *and* $A(a) \rightarrow D(a)$ *if follows that* $D(a)$ *is true.*

For rule $\rightarrow CE$*, from* $C \sqsubseteq D$ *we conclude that* $\neg C \sqcup D \in \mathcal{L}(a)$ *and we set* $\tau(\neg C \sqcup D, a) = \{(C \sqsubseteq D), a)\}$*. From* $C(a) \rightarrow D(a)$ *if follows that* $\neg C(a) \vee D(a)$*.*

For rule $\rightarrow \forall$*, since this is the first rule application,* $\bigcup_{i=2}^{n}\{(\mathit{Trans}(S_{i-1}), a_i, a_{i-1}), (S_{i-1} \sqsubseteq S_i, a_i)\} \subseteq \tau(\forall S_1.C, a_1)$ *does not hold because these axioms can be added only by rule* $\rightarrow \forall^+$*. Thus* τ *is modified as* $\tau(C, b) := \tau(\forall S_1.C, a_1) \cup \tau(S_1, \langle a_1, b\rangle)$*, resulting in* $\tau(C, b) = \{a_1 : \forall S_1.C, (a_1, b) : S_1)$*. From* $\forall y.S_1(a_1, y) \rightarrow C(y)$ *and* $S_1(a_1, b)$ *it follows that* $C(b)$*.*

For rule $\rightarrow \forall^+$*,* τ *is modified as*
$\tau(\forall R.C, b) := \tau(\forall S.C, a) \cup \tau(R, \langle a, b\rangle) \cup \{(\mathit{Trans}(R), a, b), (R \sqsubseteq S, a)\}$*, resulting in* $\tau(\forall R.C, b) := \{a : \forall S.C, (a, b) : R, (\mathit{Trans}(R), a, b), (R \sqsubseteq S, a)\}$*.*
From $R(a, b)$*,* $\forall z.R(a, b) \wedge R(b, z) \rightarrow R(a, z)$*,* $\forall y.R(a, y) \rightarrow S(a, y)$ *and* $\forall y.S(a, y) \rightarrow C(y)$ *it follows that* $\forall y.R(b, y) \rightarrow C(y)$*.*

For the inductive case*, suppose the thesis is true for* m *rules applications, we prove that is true for* $m + 1$ *rule applications. Again we have to do this only for the rules that have been modified.*

For rule $\rightarrow unfold$*, we set* $\tau(D, a) = \tau(A, a) \cup \{(A \sqsubseteq D), a)\}$*. For the inductive hypothesis* $\tau(A, a) \models A(a)$*, so from* $\tau(A, a)$ *and* $A(a) \rightarrow D(a)$ *if follows that* $D(a)$ *is true.*

For rule $\rightarrow CE$*, the same reasoning as in the base case can be applied.*

For rule $\rightarrow \forall$*, if*

$$\bigcup_{i=2}^{n}\{(\mathit{Trans}(S_{i-1}), a_i, a_{i-1}), (S_{i-1} \sqsubseteq S_i, a_i)\} \subseteq \tau(\forall S_1.C, a_1) \tag{17.1}$$

does not hold, we can apply the same reasoning as in the base case.
If (17.1) holds, $\tau(\forall S_1.C, a_1)$ *contains also* $\tau(S_{i-1}, \langle a_i, a_{i-1}\rangle)$ *added by previous applications of* $\rightarrow \forall^+$ *to* a_i *having* $\forall S_i.C \in \mathcal{L}(a_i)$ *for* $i = 2, \ldots, n$*. The completion graph thus looks as in Figure 17.5. We prove by induction on* n *that* $S_n(a_n, b)$ *holds. From this and the fact that* $\forall S_n.C \in \mathcal{L}(a_n)$ *we can conclude* $C(b)$ *holds.*

For the case of n = 2, $\tau(\forall S_1.C, a_1)$ *contains*

$$\tau(S_1, \langle a_2, a_1\rangle) \cup \{\forall z.S_1(a_2, a_1) \wedge S_1(a_1, z) \rightarrow S_1(a_2, z), \forall y.S_1(a_2, y) \rightarrow S_2(a_2, y)\}$$

If we replace y *and* z *with* b *we obtain*

$$\tau(S_1, \langle a_2, a_1\rangle) \cup \{S_1(a_2, a_1) \wedge S_1(a_1, b) \rightarrow S_1(a_2, b), S_1(a_2, b) \rightarrow S_2(a_2, b)\}$$

that, together with $\tau(S_1, \langle a_1, b\rangle)$*, entails* $S_2(a_2, b)$*.*

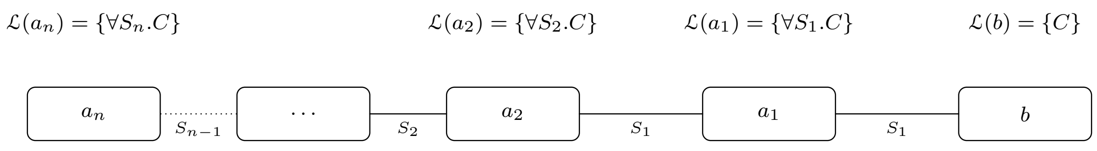

$\mathcal{L}(a_n) = \{\forall S_n.C\}$
$\mathcal{L}(a_2) = \{\forall S_2.C\}$
$\mathcal{L}(a_1) = \{\forall S_1.C\}$
$\mathcal{L}(b) = \{C\}$
a_n
S_{n-1}
$\dots$
S_2
a_2
S_1
a_1
S_1
b

Figure 17.5: Completion graph for rule $\rightarrow \forall$.

For the case of n, *suppose $S_{n-1}(a_{n-1}, b)$ holds. $\tau(\forall S_1.C, a_1)$ contains*

$$\tau(S_{n-1}, \langle a_n, a_{n-1}\rangle) \cup$$
$$\{\forall z.S_{n-1}(a_n, a_{n-1}) \wedge S_{n-1}(a_{n-1}, z) \rightarrow S_{n-1}(a_n, z), \forall y.S_{n-1}(a_n, y) \rightarrow S_n(a_n, y)\}$$

If we replace y and z with b we obtain

$$\tau(S_{n-1}, \langle a_n, a_{n-1}\rangle) \cup \{S_{n-1}(a_n, a_{n-1}) \wedge S_{n-1}(a_{n-1}, b) \rightarrow S_{n-1}(a_n, b), S_{n-1}(a_n, b) \rightarrow S_n(a_n, b)\}$$

that, together with the inductive hypothesis $S_{n-1}(a_{n-1}, b)$, entails $S_n(a_n, b)$.

It is clear that the expansion rules add only maximally instantiated axioms to τ, i.e., if $S = \{(F_1, \theta_1), \dots, (F_n, \theta_n)\}$ is returned by BUNDLETABLEAU*, no set $S' = \{(F'_1, \theta'_1), \dots, (F'_n, \theta'_n)\}$ exists such that S' entails the query, $F_i\theta_i\eta_i = F'_i\theta'_i$ for $i = 1, \dots, n$ and at least one η_i is non empty.*

Function BUNDLEBLACKBOXPRUNING

Since the instantiated axiom set S that is returned by BUNDLETABLEAU may contain redundant instantiated axioms as for TABLEAU, black-box pruning is applied. Function BUNDLEBLACKBOXPRUNING, shown in Algorithm 21, uses a specialized version of BUNDLETABLEAU, called BUNDLEINSTTABLEAU and shown in Algorithm 22, that takes as input also a set of instantiated axioms $InstAxioms$. BUNDLEINSTTABLEAU checks that every instantiated axiom added to τ belongs to $InstAxioms$, so that instantiated axioms can be removed one by one by the black-box algorithm in order to test their necessity.

Algorithm 21 `BUNDLE` black-box pruning algorithm, for pruning the output of Algorithm 20.

```
1:  function BUNDLEBLACKBOXPRUNING($C, a, S$)
2:      Input: $C, a$
3:      Input: $S$ (the set of instantiated axiom to be pruned)
4:      Input: $InstAxioms$ (set of instantiated axioms)
5:      Output: $S$ (the pruned set of axioms)
6:      for all axiom $(E, \theta) \in S$ do
7:          $S \leftarrow S - \{(E, \theta)\}$
8:          $\mathcal{KB} \leftarrow \{F | (F, \theta) \in S\}$
9:          if BUNDLEINSTTABLEAU($C, a, \mathcal{KB}, S$)= $null$ then
10:             $S \leftarrow S \cup \{(E, \theta)\}$
11:         end if
12:     end for
13:     return $S$
14: end function
```

Algorithm 22 `BUNDLE` TABLEAU for black-box pruning, called from Algorithm 21.

```
1:  function BUNDLEINSTTABLEAU($C, a, \mathcal{KB}, InstAxioms$)
2:      Input: $C, a$
3:      Input: $\mathcal{KB}$ (knowledge base)
4:      Input: $InstAxioms$ (set of instantiated axioms)
5:      Output: $S$ (a set of axioms)
6:      Let $G_0$ be an initial completion graph from $\mathcal{KB}$ containing an anonymous individual $a$ and $\neg C \in \mathcal{L}(a)$
7:      $T \leftarrow \{G_0\}$
8:      repeat
9:          Select a rule $r$ applicable to a clash-free graph $G$ from $T$ such all axioms added to $\tau$ are
10:         from $InstAxioms$
11:         $T \leftarrow T \setminus \{G\}$
12:         Let $\mathcal{G} = \{G'_1, ..., G'_n\}$ be the result of applying $r$ to $G$
13:         $T \leftarrow T \cup \mathcal{G}$
14:     until All graphs in $T$ have a clash or no rule is applicable
15:     if All graphs in $T$ have a clash then
16:         $S \leftarrow \emptyset$
17:         for all $G \in T$ do
18:             let $s_G$ be the result of $\tau$ for the clash of $G$
19:             $S \leftarrow S \cup s_G$
20:         end for
21:         $S \leftarrow S \setminus \{\neg C(a)\}$
22:         return $S$
23:     else
24:         return $null$
25:     end if
26: end function
```

BUNDLE Hitting Set Algorithm

Algorithm 23 BUNDLE Hitting Set Algorithm.

```
1: procedure BundleHittingSetTree($C, a, \mathcal{KB}, CS, HS, w, E, p, BannedInstAxioms$)
2:     Input: $C, a$
3:     Input: $\mathcal{KB}$ (knowledge base)
4:     Input: $CS$ (a set of conflict sets, initially containing a single explanation)
5:     Input: $HS$ (a set of Hitting Sets)
6:     Input: $w$ (the last node added to the Hitting Set Tree)
7:     Input: $\alpha$ (the last axiom removed from $\mathcal{KB}$)
8:     Input: $p$ (the current edge path)
9:     Input: $BannedInstAxioms$ (a set of instantiated axioms)
10:    if there exists a set $h \in HS$ s.t. $(\mathcal{L}(p) \cup \{E\}) \subseteq h$ then
11:        $\mathcal{L}(w) \leftarrow X$
12:        return
13:    else
14:        if $C$ is unsatisfiable w.r.t. $\mathcal{KB}$ then
15:            $m \leftarrow$BundleSingleMinA($C, a, \mathcal{KB}, BannedInstAxioms$)
16:            $CS \leftarrow CS \cup \{m\}$
17:            create a new node $w'$ and set $\mathcal{L}(w') \leftarrow m$
18:            if $w \neq null$ then
19:                create an edge $e = \langle w, w' \rangle$ with $\mathcal{L}(e) = E$
20:                $p \leftarrow p \cup e$
21:            end if
22:            loop for each $F\theta \in \mathcal{L}(w')$
23:                if $F$ is certain then
24:                    BundleHittingSetTree($A, (\mathcal{KB} - \{F\}), CS, HS, w', F, p, BannedInstAxioms$)
25:                else
26:                    BundleHittingSetTree($A, \mathcal{KB}, CS, HS, w', F\theta, p, BannedInstAxioms \cup \{F\theta\}$)
27:                end if
28:            end loop
29:        else
30:            $\mathcal{L}(w) \leftarrow OK$
31:            $HS \leftarrow HS \cup \mathcal{L}(p)$
32:        end if
33:    end if
34: end procedure
```

As in Pellet, to compute ALL-INSTMINAS($E, \mathcal{KB}$) we use the Hitting Set Algorithm that calls the BUNDLESINGLEMINA algorithm for computing single explanations. BUNDLEHITTINGSETTREE, shown in Algorithm 23, besides removing axioms from the knowledge base $\mathcal{KB}$, also keeps a set of instantiated banned axioms, $BannedInstAxioms$, where it stores the instantiated axioms that have to be removed from the knowledge base. This set is used by BUNDLESINGLEMINA and thus by BUNDLETABLEAU (Algorithm 20), in this way: before applying a rule, BUNDLETABLEAU checks whether one of the instantiated axioms to be added to τ is in $BannedInstAxioms$. If so, it does not apply the rule.

In BUNDLEHITTINGSETTREE, if the axiom to be removed is certain, the behavior is the same as in `Pellet`. If the axiom is probabilistic, BUNDLEHITTINGSETTREE adds the instantiated axiom to $BannedInstAxioms$ and calls BUNDLESINGLEMINA with this updated set. The correctness and completeness of this approach is proved by the following theorem, based on Theorem 4:

Theorem 6 *Let $C(a)$ be such that $\mathcal{KB} \models C(a)$, then the set of explanations returned by the hitting set algorithm (we will call it* INSTEXPHST$(C, a, \mathcal{KB})$*) is equal to the set of all explanations of $C(a)$ w.r.t. $\mathcal{KB}$, so*

$$\text{INSTEXPHST}(C, a, \mathcal{KB}) = \text{ALL-INSTMINAS}(C(a), \mathcal{KB})$$

Proof 5 *Theorem 4 can be applied to this case by observing that* BUNDLETABLEAU *behaves as if the knowledge base does not contain the instantiated axioms in $BannedInstAxioms$.*

17.3 Overall `BUNDLE`

`BUNDLE`, shown in Algorithm 24, first builds a data structure $PMap$ that associates each DL axiom E with a set of couples (Var, p), one for each probabilistic axiom $p ::_{Var} E$ in the knowledge base $\mathcal{KB}$. Then it calls Functions BUNDLESINGLEMINA and BUNDLEHITTINGSETTREE to compute all *MinAs* for $C(a)$. ALL-INSTMINAS$(C(a), \mathcal{KB})$ will be assigned to the set of conflict sets CS.

Algorithm 24 Function BUNDLE: computation of the probability of an axiom Q on a given ontology.

```
1: function BUNDLE($\mathcal{KB}, C, a$)
2:     Input: $\mathcal{KB}$ (knowledge base)
3:     Input: $C, a$
4:     Output: the probability of $C(a)$ w.r.t. $\mathcal{KB}$
5:     Build Map $PMap$ from DL axioms to sets of couples $(Var, probability)$
6:     $MinA \leftarrow$BUNDLESINGLAMINA($C, \mathcal{KB}, \emptyset$)
7:     $\mathcal{L}(root) \leftarrow MinA$; $CS \leftarrow \{MinA\}$; $HS \leftarrow \emptyset$
8:     loop for each axiom $F\theta \in \mathcal{L}(root)$
9:         if $F$ is certain then
10:            BUNDLEHITTINGSETTREE($C, (\mathcal{KB} - \{F\}), CS, HS, root, F, \emptyset, \emptyset$)
11:        else
12:            BUNDLEHITTINGSETTREE($C, \mathcal{KB}, CS, HS, root, F\theta, \emptyset, \{F\theta\}$)
13:        end if
14:    end loop
15:    Initialize $VarAxAnn$ to empty        ▷ $VarAxAnn$ is an array of triples $(Axiom, \theta, Prob)$
16:    $BDD \leftarrow$BDDZERO
17:    for all $MinA \in CS$ do
18:        $BDDE \leftarrow$BDDONE
19:        for all $(Ax, \theta) \in MinA$ do
20:            if $\mathcal{KB}$ contains a certain axiom $Ax$ then
21:                $BDDA \leftarrow$BDDONE
22:            else
23:                $Res \leftarrow$ the set of all couples $(Var, p)$ in $PMap(Ax)$ such that $Var \subseteq Var(\theta)$
24:                $BBDA \leftarrow$BDDZERO
25:                for all $(Var, p) \in Res$ do
26:                    $\theta' \leftarrow \theta|_{Var}$
27:                    Scan $VarAxAnn$ looking for $(Ax, \theta')$
28:                    if !found then
29:                        Add to $VarAxAnn$ a new cell containing $(Ax, \theta', p)$
30:                    end if
31:                    Let $i$ be the position of $(Ax, \theta', p)$ in $VarAxAnn$
32:                    $B \leftarrow$ BDDGETITHVAR($i$)
33:                    $BDDA \leftarrow$BDDOR($BDDA, B$)
34:                end for
35:            end if
36:            $BDDE \leftarrow$BDDAND($BDDE$,$BDDA$)
37:        end for
38:        $BDD \leftarrow$BDDOR($BDD$,$BDDE$)
39:    end for
40:    return BDD_PROBABILITY($BDD$)        ▷ $VarAxAnn$ is used to compute $P(X)$ in this function
41: end function
```

Two data structures are initialized: $VarAxAnn$ is an array that maintains the association between Boolean random variables (whose index is the array index) and triples $(\texttt{axiom}, \texttt{substitution}, \texttt{probability})$, and BDD stores a BDD. BDD is initialized to the Zero Boolean function.

Then BUNDLE performs three nested loops that build a BDD representing the set of explanations. To manipulate BDDs we used JavaBDD[1] that is an interface to a number of underlying BDD manipulation packages: as the underlying package we exploit CUDD.

In the outermost loop BUNDLE combines BDDs for different explanations. In the intermediate loop, BUNDLE generates the BDD for a single explanation, while in the innermost loop it generates the BDD associated to each axiom. Since the same axiom can appear multiple times with different Var annotations, for each instantiated axiom in a *MinA* the disjunction of random variables associated to all the applicable probabilistic axioms is computed, since the instantiated axiom is true if one of the axiom in the knowledge base is true.

In the outermost loop, $BDDE$ is initialized to the One Boolean function. In the intermediate loop, the couples $(\texttt{axiom}, \texttt{substitution})$ of a *MinA* are considered one by one. If the axiom is certain, the One Boolean function is conjoined with $BDDE$. Otherwise, the set of couples (Var, p) associated with the axiom, such that the variables in the substitution are a subset of Var, are extracted from $PMap$. Then, $BDDA$ is initialized to the Zero Boolean function and, for each couple (Var, p), the restriction of the substitution to Var is computed and the tuple $(\texttt{axiom}, \texttt{restrictedsubstitution}, \texttt{probability})$ is searched for in $VarAxAnn$ to see if it has already been assigned a random variable. If not, a cell is added to $VarAxAnn$ to store the tuple. At this point we know the tuple position i in $VarAxAnn$ and so the index of its Boolean variable X_i in the BDD. A BDD is built representing $X_i = 1$ with BDDGETITHVAR and it is disjointed with $BDDA$. At the end of the innermost loop, $BDDA$ is conjoined with $BDDE$ and, at the end of the intermediate loop, the BDD for the current explanation, $BDDE$, is disjointed with BDD. After the three cycles, function BDD_PROBABILITY of Algorithm 15 is called over BDD and its result is returned to the user.

[1]Available at `http://javabdd.sourceforge.net/`

Example 41 *Consider the knowledge base*

$$\begin{array}{rl}
 & kevin : \forall kin.Person \\
 & anna : \forall kin.Person \\
 & (kevin, laura) : friend \\
 & (anna, laura) : friend \\
 & Trans(friend) \\
0.8 \quad ::_x & friend \sqsubseteq kin
\end{array}$$

The query $laura : \forall friend.Person$ *has two* $InstMinAs$*, one is*

$$\begin{array}{l}
\{ \; \forall y.kin(kevin, y) \rightarrow Person(y), \\
\quad friend(kevin, laura), \\
\quad \forall z.friend(kevin, laura) \wedge friend(laura, z) \rightarrow friend(kevin, z), \\
\quad \forall y.friend(kevin, y) \rightarrow kin(kevin, y)\}
\end{array}$$

The other is

$$\begin{array}{l}
\{ \; \forall y.kin(anna, y) \rightarrow Person(y), \\
\quad friend(anna, laura), \\
\quad \forall z.friend(anna, laura) \wedge friend(laura, z) \rightarrow friend(anna, z), \\
\quad \forall y.friend(anna, y) \rightarrow kin(anna, y)\}
\end{array}$$

If we indicate with F *the formula of the only probabilistic axiom, we have the covering set of explanations* $K = \{\kappa_1, \kappa_2\}$ *with* $\kappa_1 = \{(F, \{x/kevin\}, 1\}$ *and* $\kappa_2 = \{(F, \{x/anna\}, 1)\}$*. Since* $Var = x$*, when building the BDD* $F\{x/kevin\}$ *and* $F\{x/anna\}$ *are associated with different random variables so the BDD computes the disjunction of the two variables and the probability of the query is* $0.8 + 0.8 - 0.8 \cdot 0.8 = 0.96$.

If the subscript of the probabilistic axiom is removed, then when building the BDD the two instantiated formulae are mapped to the same random variable, thus the BDD computes the disjunction of two equal variables obtaining the variable itself. Thus the probability of the query in this case is 0.8.

If the subscript of the probabilistic axiom is changed to xy*, then the two instantiated formulae are not valid forms of the axiom and the two explanations are discarded, leading to a 0 probability.*

17.4 Computational Complexity

The computational complexity of computing the probability of an axiom can be studied by considering the two problems that must be solved:

- The first problem is that of *axiom pinpointing*, whose computational complexity has been studied in a number of works (Peñaloza and Sertkaya, 2009, 2010a,b).

  (Baader et al., 2007) showed that there can be exponentially many *MinAs* for a very simple DL that is a subset of $\mathcal{SHOIN}^{(\mathbf{D})}$, thus the number of explanations for $\mathcal{SHOIN}^{(\mathbf{D})}$ may be even larger. Given this fact, we do not consider complexity with respect to the input only. We say an algorithm runs in *output polynomial time* (Johnson et al., 1988) if computes all the output in time polynomial in the overall size of the input and the output.

  Corollary 15 in (Peñaloza and Sertkaya, 2010b) shows that MINA-ENUM cannot be solved in output polynomial time for *DL-Lite*$_{bool}$ TBoxes unless $P = NP$. Since *DL-Lite*$_{bool}$ is a sublogic of $\mathcal{SHOIN}^{(\mathbf{D})}$, this result also holds for $\mathcal{SHOIN}^{(\mathbf{D})}$.

- The second problem is computing the *probability of a sum-of-products*, that is

  Problem: SUM-OF-PRODUCTS
  Input: Let S be a Boolean expression in disjunctive normal form (DNF), or a sum-of-products, in the variables $\{v_1, \dots, v_n\}$ and let $P(v_i)$ be the probability that v_i is true with $i = 1, \dots, n$.
  Output: The probability of S: $P(S)$, assuming all variables are independent.

  This problem was shown to be $\#P - hard$ (see e.g. (Rauzy et al., 2003)). The class $\#P$ (Valiant, 1979) describe counting problems associated with decision problems in NP. More formally, $\#P$ is the class of function problems of the form "compute $f(x)$", where f is the number of accepting paths of a nondeterministic Turing machine running in polynomial time.

  $\#P$ problems were shown very hard. First, a $\#P$ problem must be at least as hard as the corresponding NP problem. Second, (Toda, 1989) showed that a polynomial-time machine with a $\#P$ oracle ($\mathrm{P}^{\#\mathrm{P}}$) can solve all problems in PH, the entire polynomial hierarchy.

Given that the input of the SUM-OF-PRODUCTS problem is at least of exponential size, this means that computing the probability of an axiom from a $\mathcal{SHOIN}^{(\mathbf{D})}$ knowledge base is highly intractable.

However, the algorithms that have been proposed for solving the two problems were shown to be able to work on input of realistic size. For example, all *MinAs* have been found for various entailments over many real world ontologies within a few seconds (Kalyanpur, 2006; Kalyanpur et al., 2007). As regards the SUM-OF-PRODUCTS problem, algorithms based on BDDs were able to solve problems with hundred of thousand of variables (see e.g. the works on inference on Probabilistic Logic Programs (De Raedt et al., 2007; Kimmig et al., 2011; Riguzzi, 2007b, 2009; Riguzzi and Swift, 2010, 2012)). Moreover, Section 17.5 shows that in practice we can compute the probability of entailments on ontologies of realistic size.

17.5 Experiments

The experiments are directed to verify the performance of the probabilistic Description Logic reasoner `Bundle` in comparison with another state of the art system.

In the following a description of the dataset is provided before the experimental part.

Dataset

The dataset is a probabilistic ontology for breast cancer risk assessment (*BRCA*). The BRCA ontology was created as an attempt to model the problem of breast cancer risk assessment in a clear, ontological manner. The central idea behind the design the ontology was to reduce risk assessment to probabilistic entailment in $\mathcal{P} - \mathcal{SHIQ}^{(\mathbf{D})}$.

The ontology consists of two major parts: a classical OWL ontology and a probabilistic part that represents domain uncertainty. The ontology aims at modeling two types of risk of developing breast cancer. The probabilistic part contains conditional constraints of the form $(D \mid C)[l, u]$.

First, the ontology models *absolute* risk, i.e., the risk that can be measured without reference to specific categories of women. A statement like "an average woman has up to 12.3% of developing breast cancer in her lifetime" is an example. Such risk is modeled using subclasses of $\mathsf{WomanUnderAbsoluteBRCRisk}$. Subclasses distinguish between the risk of developing cancer over a lifetime vs. in the short term (e.g., ten years).

Second, the ontology models *relative* breast cancer risk. This is useful for representing the impact of various risk factors by describing how they increase or decrease the risk compared to an average woman. A statements like “having BRCA1 gene mutation increases the risk of developing breast cancer by a factor of four” is an example.

The ontology defines risk factors that are relevant to breast cancer using subclasses of RiskFactor. It makes the distinction between the factors that should be known to a woman, and those that can only be inferred on the basis of other factors or by examination, e.g., BRCA gene mutation, etc. It also defines different categories of women: first, those that have certain risk factors (subclasses of WomanWithRiskFactors); and, second, those defined in terms of the risk of developing cancer (subclasses of WomanUnderBRCRisk).

With this classical ontology, it is possible to assess the risk in terms of probabilistic entailment. The problem is to compute the conditional probability that a certain woman is an instance of some subclass of WomanUnderBRCRisk given probabilities that she is an instance of some subclasses of WomanWithRiskFactors. This requires probabilistic entailment of ABox axioms. In addition, it might also be useful to infer the generic probabilistic relationships between classes under WomanUnderBRCRisk and under WomanWithRiskFactors.

The $\mathcal{KB}$ contains a set of probabilistic ABox (PAbox) and TBox (PTbox) axioms. The PABox axioms define risk factors that are relevant to a particular individual. The PTBox axioms model generic probabilistic relationships between classes in the ontology, i.e., those that are assumed to hold for a randomly chosen individual.

The model represents absolute risk using the subclasses of WomanUnderAbsoluteBRCRisk as conclusions in conditional constraints. For example, the above statement that an average woman has risk up to 12.3% can be expressed as the following TBox axiom:

$$(WomanUnderAbsoluteBRCRisk \mid Woman)[0, 0.123].$$

Relative risk can be captured analogously by using the subclasses of WomanUnderRelativeBRCRisk as conclusions.

The model also allows to express various inter-relationships between risk factors. One possibility is to represent how the presence of one risk factor allows to guess on the presence of others. This is the principal method of inferring risk factors, i.e., those unknown to a woman. For example, BRCA gene mutation is more likely to be statistically developed by certain ethnic groups.

In addition, the model allows to represent how different risk factors strengthen or weaken the effect of each other. The classical part of the ontology provides classes that are combinations of multiple risk factors. For example, Woman50PlusMotherBRCA is a subclass of both WomanAged50Plus and WomanWithMotherBRCA, i.e., it represents women after the age of 50 whose mothers developed breast cancer in the past. The model can define the risk for such women to be much higher than if they had just one of the factors.
Informally, PTBox axioms for the combination of factors, such as:

$$(WomanUnderStrongBRCRisk|Woman50PlusMotherBRCA)[0.9, 1]$$

override the axioms for each individual factor, thus allowing the system to make a more relevant and objective inference.

Finally, the ontology contains a number of PABoxes that represent risk factors for specific individuals. The motivation is that, while the generic probabilistic model provides all the necessary statistics that can be developed and maintained by a central cancer research institute, individual women can supply the knowledge about the risk factors that are known to them, e.g., age. It is also possible to express uncertainty in having some particular risk factor.

Methodology

In order to evaluate the performance of BUNDLE , we follow the methodology of (Klinov and Parsia, 2008) where the probabilistic reasoner PRONTO is used to answer queries to increasingly complex ontologies obtained by randomly sampling axioms from the BRCA ontology. Currently the full version of BRCA ontology cannot be handled by $\mathcal{P} - \mathcal{SHIQ}^{(\mathbf{D})}$ reasoners, so in (Klinov and Parsia, 2008) the authors decided to evaluate the performance on selected fragments.

Problem instances are generated using simple random sampling: each sample is an independent probabilistic KB with the full classical part of the BRCA ontology and a subset of the PTBox constraints. The number of conditional constraints varies from 9 to 15 and, for each number, ontologies are repeatedly sampled and tested for consistency; we stop sampling when we obtain 100 consistent ontologies for each number of constraints.

In order to generate a query, an individual a is added to the ontology. a is randomly assigned to each class that appears in the sampled conditional constraints with probability 0.6. If the class is composite, as for example PostmenopausalWomanTakingTestosterone, a is assigned to the component classes rather than to the composite one. In the example above, a will be added to PostmenopausalWoman and WomanTakingTestosterone classes.

The ontologies are then translated into the DISPONTE semantics by replacing the constraint $(D|C)[l,u]$ with the axiom $u ::_x C \sqsubseteq D$. For instance, the statement that an average woman has up to 12.3% chance of developing breast cancer in her lifetime, expressed by

$$(WomanUnderAbsoluteBRCRisk|Woman)[0, 0.123]$$

is translated into

$$0.123 ::_x WomanUnderAbsoluteBRCRisk \sqsubseteq Woman$$

For each ontology the query $a : C$ is asked, where the class C is randomly selected among those that represent women under increased risk and lifetime risk, such as WomanUnderLifetimeBRCRisk and WomanUnderStronglyIncreasedBRCRisk.

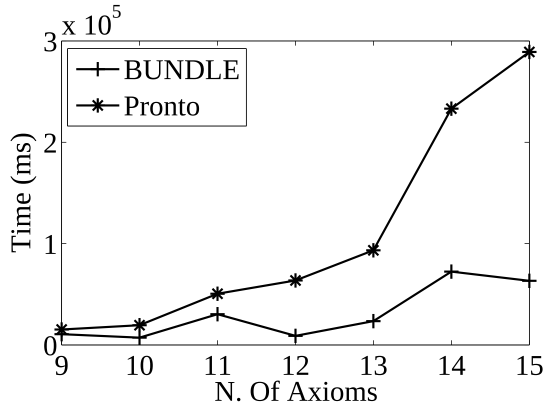
Results

We compared BUNDLE and PRONTO with regard to:

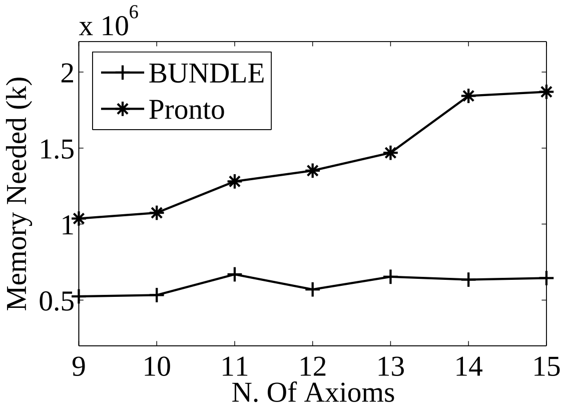
- the execution time in performing inference: Figure 17.6a shows the execution times averaged over the 100 knowledge bases as a function of the number of axioms;
- the amount of memory used, shown in Figure 17.6b, as a function of the number of axioms.

Execution times are similar for small knowledge bases, but the difference between the two reasoners rapidly increases for larger knowledge bases.
The memory usage for BUNDLE is always less than 53% with respect to PRONTO.

The results show that, despite the high worst case complexity, BUNDLE can be applied effectively to real world domains and is competitive with PRONTO.



(a) Execution times of inference (ms).



(b) Memory used (Kb).

Figure 17.6: Comparison between `BUNDLE` and `PRONTO`.

Part VI

Summary and Future Work

Chapter 18

Thesis Summary

Learning **probabilistic logic programming languages** has received an increased attention and various systems have been made available for learning the parameters or both the structure and the parameters of these languages.

The first aim of this thesis was to improve the learning algorithms for parameters and structure of directed probabilistic logic models, by employing logic programming techniques. The efficiency of these algorithms rely on inference techniques recently developed, based on Binary Decision Diagrams.

Logic Programs with Annotated Disjunctions (LPADs) have been used as a representative of the probabilistic logic programming paradigm, although this formalism can easily be translated into other languages; in fact we related this formalism to a variety of other known languages in the field of probabilistic logical learning and compared the corresponding parameter/structure learning systems. LPADs' main characteristic is to be intuitive and compact from a knowledge representation point of view. The syntax and semantics are as simple as possible to make it easy to learn the language, and provide a natural representation of relational probabilistic knowledge.

- We have presented the `EMBLEM` system, that learns probabilities in LPAD clauses using the Expectation Maximization (EM) algorithm, where the values of expectations are computed directly on BDDs. Experimental results over many real world datasets showed equal or superior performances both in terms of speed and memory usage with respect to other state-of-the-art learning systems. It is able to perform learning on larger datasets, where other systems are not able to terminate. The main issues raised by these experiments are related to datasets' size and programs' cyclicity: for large datasets it is impossible to store all BDDs in memory, and we had to set a depth bound on the query derivations and to use a "simplified" distribution semantics;

- We have presented the SLIPCASE and SLIPCOVER algorithms that learn both the structure and the parameters of LPADs, by exploiting EMBLEM. The first performs a beam search in the space of probabilistic theories using the log likelihood of the data as the guiding heuristics; the second is an evolution in the sense that uses a more complex search strategy, which first searches the space of clauses storing all the promising ones, and then performs greedy search in the space of theories. Like EMBLEM, they can be applied to all languages that are based on the distribution semantics. The experimental results show that SLIPCOVER's double search for clauses and theories separately is quite effective in achieving higher performances in most datasets tested.

The second purpose of the thesis was to propose a fresh research line in **probabilistic Description Logics**, by embedding (1) the distribution semantics for probabilistic logic languages in $\mathcal{SHOIN}^{(\mathcal{D})}$ and (2) inference techniques based on Binary Decision Diagrams.

1. The proposed semantics, called DISPONTE, differs from previous proposals because it minimally extends the description language and provides a unified framework for representing different types of probabilistic knowledge, "epistemic" and "statistical". Moreover, it allows to seamlessly represent probabilistic assertional and terminological knowledge.
   The distribution semantics allows us to define a "possible worlds" semantics over a probabilistic knowledge base, which in turn leads to reduce the inference problem of computing the probability of a query to that of finding a covering set of mutually incompatible explanations, as for the case of LPADs.

2. The inference system (BUNDLE) takes advantage of the proposed semantics for computing the probability of queries against a probabilistic ontology which follows DISPONTE semantics. Its complexity in the worst case is large since the explanations may grow exponentially and the computation of the probability through Binary Decision Diagrams has a #P-complexity in the number of explanations. Nevertheless, experiments applied on a real world dataset on breast cancer risk assessment, proved that it is able to handle domains of significant size, in less time and with less memory consumption than the inference system PRONTO for $\mathcal{P}-\mathcal{SHIQ}^{(\mathcal{D})}$.

In the future, we plan to consider the case of countably infinite covering sets of explanations and to investigate the application of BUNDLE to other real life ontologies, with particular reference to health science. Moreover, we intend to experiment with various BDD packages, in particular those employing sophisticated techniques for choosing the variable order (Grumberg et al., 2003).

Chapter 19

Future Work

In the *SRL field*, learning the structure of probabilistic logical models is a hard problem. Further steps in our work would be:

- the test of the `SLIPCOVER` system on other real world domains;
- the analysis of the effects of refining the clause heads and of background knowledge on the performance;
- the development of other search strategies (such as local search in the space of refinements).

The rising popularity of *description logics* and their use, and the need to deal with uncertainty, especially in the Semantic Web, is increasingly attracting the attention of many researchers and practitioners towards description logics able to cope with uncertainty by means of probability theory. As regards the current results, we would like to:

- test the probabilistic reasoner on other real life ontologies, with particular reference to health science;
- improve the efficiency of its inference step by experimenting with various BDD packages, in particular those employing sophisticated techniques for choosing the variable order (Grumberg et al., 2003);
- consider the case of countably infinite covering sets of explanations.

A new important path concerns the development of parameter/structure learning systems for probabilistic OWL DL ontologies under the distribution semantics.

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