Markov Logic: Theory, Algorithms and Applications

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Abstract

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AI systems need to reason about complex objects and explicitly handle uncertainty. First-order logic handles the first and probability the latter. Combining the two has been a longstanding goal of AI research. Markov logic [86] combines the power of first-order logic and Markov networks by attaching real-valued weights to formulas in first-order logic. Markov logic can be seen as defining templates for ground Markov networks.

For any representation language to be useful, it should be (a) sufficiently expressive, (b) amenable to the design of fast learning and inference algorithms and, (c) easy to use in real-world domains. In this dissertation, we address all these three aspects in the context of Markov logic.

On the theoretical front, we extend Markov logic semantics to handle infinite domains. The original formulation of Markov logic deals only with finite domains. This is a limitation on the full first-order logic semantics. Borrowing ideas from the physics literature, we generalize Markov logic to the case of infinite domains.

On the algorithmic side, we provide efficient inference and learning algorithms for Markov logic. The naive approach to inference in Markov logic is to ground out the domain theory and then apply propositional inference techniques. This leads to an explosion in time and memory. We present two algorithms: LazySAT (lazy WalkSAT) and lifted inference, which exploit the structure of the network to significantly improve the time and memory cost of inference. LazySAT, as the name suggests, grounds out the theory lazily, thereby saving very large amounts of memory without compromising speed. Lifted inference is a first-order (lifted) version of ground inference, where

inference is carried out over clusters of nodes about which we have the same information. This yields significant improvements in both time and memory. For learning the parameters (weights) of a Markov logic network, we propose a novel method based on the voted perceptron algorithm of Collins (2002).

On the application side, we demonstrate the effective use of Markov logic to two real-world problems: (a) providing a unified solution to the problem of entity resolution, and (b) identifying social relationships in image collections.

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Chapter 1
INTRODUCTION

Two key challenges in most AI applications are uncertainty and complexity. The standard framework for handling uncertainty is probability; for complexity, it is first-order logic. Thus we would like to be able to learn and perform inference in representation languages that combine the two. This is the focus of the burgeoning field of statistical relational learning [33]. Many approaches have been proposed in recent years, including stochastic logic programs [69], probabilistic relational models [27], Bayesian logic programs [46], relational dependency networks [71], and others. These approaches typically combine probabilistic graphical models with a subset of first-order logic (e.g., Horn clauses), and can be quite complex. Recently, Richardson and Domingos [86] introduced Markov logic, a language that is conceptually simple, yet provides the full expressiveness of graphical models and first-order logic in finite domains. Markov logic extends first-order logic by attaching weights to formulas. Semantically, weighted formulas are viewed as templates for constructing Markov networks. In the infinite-weight limit, Markov logic reduces to standard first-order logic. Markov logic avoids the assumption of i.i.d. (independent and identically distributed) data made by most statistical learners, by leveraging the power of first-order logic to compactly represent dependences among objects and relations.

The original formulation of Markov logic as proposed by Richardson and Domingos assumes that the domain theory is expressed using finite first-order logic. A finite set of constants is assumed. Further, functions are allowed in a very limited setting, i.e., their range is a subset of the given set of constants. This clearly is a significant limitation on the expressive power of the language. In this dissertation, we generalize Markov logic to handle functions as they are used in first-order logic. This allows us to represent potentially infinite domains. Borrowing ideas from the theory of Gibbs measures [32] in the statistical physics literature, we precisely describe conditions under which an infinite distribution in Markov logic is well defined. We describe conditions for the uniqueness of such a distribution and the properties of the set of consistent distributions in the non-unique case.

For a representation language to be of any practical use, one should be able to design efficient inference and learning algorithms for it. A straightforward approach for doing inference in Markov logic consists of first grounding out the theory and then using propositional inference techniques on the ground Markov network. Stochastic local search algorithms such as WalkSAT [45] can be used for doing MAP inference. Sampling-based methods such as MCMC [35] or belief propagation can be used for computing conditional probabilities. But the problem with this approach is that even for reasonably-sized domains, the ground network may be too large. In particular, the network size grows exponentially with highest clause arity. This leads to prohibitive costs in both time and memory. We present two solutions to this problem. The first one is called LazySAT [96] and is a lazy extension of the WalkSAT algorithm. Using the idea that most atoms are false and most clauses satisfied, we show that we only need to keep a small fraction of clauses in memory to carry out each WalkSAT step. This gives orders of magnitude performance gains in memory while keeping the time cost unchanged and giving exactly the same results. The second solution that we propose is a first-order-style lifted inference technique [98]. We provide a general framework for lifting probabilistic inference algorithms. We describe in detail how to lift a number of well-known inference algorithms, e.g., variable elimination, junction trees and belief propagation. The idea in lifting is to cluster together the set of nodes and clauses which would behave in the same way during the execution of the ground version. This lifted network can be much smaller than the original network. We show that running the algorithm (with a few small changes) on this lifted network is equivalent to running it on the ground network. Experiments on a number of datasets, using lifted belief propagation, show that lifting gives huge benefits in both time and memory.

Learning the parameters of a model involves optimizing the likelihood of the training data. Optimizing the actual log-likelihood involves doing inference at each step of learning and can be very costly. Richardson & Domingos [86] proposed using an alternative evaluation measure called pseudo-likelihood [2] which is relatively straightforward to optimize. But this gives sub-optimal results, especially when long-range dependences are present in the network. We propose a novel algorithm [93] for optimizing the actual log-likelihood. The idea is based on generalizing Collins's [12] voted perceptron algorithm for hidden Markov models (HMMs). We replace the step of finding the MAP state of the network using the Viterbi algorithm in HMMs by WalkSAT for Markov logic networks (MLNs). Experiments show that this learns much better parameters compared to optimizing pseudo-likelihood.

Taking advantage of its expressive power and the efficient learning and inference algorithms described above, Markov logic has been used for a wide variety of AI applications, including information extraction [83], link prediction [86], semantifying Wikipedia [106], robot mapping [102] and many others. In this dissertation, we will present two applications of Markov logic to real life problems, described below.

Given a set of references to some underlying objects, entity resolution is the problem of identifying which of these references correspond to the same underlying object. This is a very important problem for many applications and has been extensively studied in the literature [105]. Most of the approaches make the pairwise independence assumption [26]. Recent approaches (e.g. [63]) do take dependences into account. But most of these focus on specific aspects of the problem (e.g. transitivity) and have been developed as standalone systems. This makes it very difficult to combine useful aspects of different approaches. In this dissertation, we present a unified approach [95] to entity resolution using Markov logic. Our formulation makes it possible to express many previous approaches using at most a few formulas in Markov logic. Further, our framework allows new approaches to be incorporated in a straightforward manner.

We also present an application of Markov logic to the problem of identifying social relationships in image collections [99]. Given a user's collection of personal photos, the goal is to be able to identify various kinds of social relationships present in the collection (e.g. parent, child, friend etc.). We write a domain theory in Markov logic describing heuristic rules, e.g., parents tend to be photographed with their children, relatives and friends are clustered across images, etc. Experiments demonstrate that our approach gives significant improvements over the baseline.

The outline of this dissertation is as follows. Chapter 2 presents the necessary background on Markov networks, first-order logic and Markov logic. Chapter 3 presents the extension of Markov logic to infinite domains. Chapters 4 and 5 present the two approaches for making inference more efficient: LazySAT and lifted inference, respectively. Chapter 6 describes the voted perceptron algorithm for Markov logic. Chapters 7 and 8 present the applications to the problems of entity resolution and discovery of social relationships, respectively. Each chapter discusses the relevant related work. We conclude with a summary of the contributions of this dissertation and directions for future work.

Chapter 2
BACKGROUND

2.1 Markov Networks

A *Markov network* is a model for the joint distribution of a set of variables $\mathbf{X} = (X_1, X_2, \ldots, X_n) \in \mathcal{X}$ [77]. It is composed of an undirected graph G and a set of potential functions ϕ_k. The graph has a node for each variable, and the model has a potential function for each clique in the graph. A potential function is a non-negative real-valued function of the state of the corresponding clique. The joint distribution represented by a Markov network is given by

$$P(X = \mathbf{x}) = \frac{1}{Z} \prod_k \phi_k(\mathbf{x}) \tag{2.1}$$

where Z, known as the *partition function*, is given by $Z = \sum_{\mathbf{x}} \prod_k \phi_k(\mathbf{x})$. Markov networks are often conveniently represented as *log-linear models*, with each clique potential replaced by an exponentiated weighted sum of features of the state, leading to

$$P(\mathbf{X} = \mathbf{x}) = \frac{1}{Z} \exp\left(\sum_j w_j f_j(\mathbf{x})\right) \tag{2.2}$$

A feature may be any real-valued function of the state. In this dissertation, we will focus on binary features, $f_j(x) \in \{0, 1\}$. In the most direct translation from the potential-function form (Equation 2.1), there is one feature corresponding to each possible state of each clique, with its weight being $\log \phi_k(\mathbf{x})$. This representation is exponential in the size of the cliques. However, we are free to specify a much smaller number of features (e.g., logical functions of the state of the clique), allowing for a more compact representation than the potential-function form, particularly when large cliques are present. As we will see, Markov logic takes advantage of this.

Inference in Markov networks is #P-complete [88]. The most widely used method for approximate inference in Markov networks is Markov chain Monte Carlo (MCMC) [34], and in particular Gibbs sampling, which proceeds by sampling each variable in turn given its Markov blanket. (The

Markov blanket of a node is the minimal set of nodes that renders it independent of the remaining network; in a Markov network, this is simply the node's neighbors in the graph.) Marginal probabilities are computed by counting over these samples; conditional probabilities are computed by running the Gibbs sampler with the conditioning variables clamped to their given values. Another popular method for inference in Markov networks is belief propagation [108]. Belief propagation consists of constructing a bipartite graph of the nodes and the factors (potentials). Messages are passed from the variable nodes to the corresponding factor nodes and vice-versa. The messages represent the current approximations to node marginals. For a general Markov network, this message-passing scheme does not have any guarantees of convergence (or of giving correct marginals when it converges) but it has been shown to do very well in practice on a variety of real-world problems.

Maximum-likelihood or MAP estimates of Markov network weights cannot be computed in closed form but, because the log-likelihood is a concave function of the weights, they can be found efficiently (modulo inference) using standard gradient-based or quasi-Newton optimization methods [73]. Another alternative is iterative scaling [23]. Features can also be learned from data, for example by greedily constructing conjunctions of atomic features [23].

2.2 First-Order Logic

A *knowledge base (KB)* in propositional logic is a set of formulas over Boolean variables. Every KB can be converted to *conjunctive normal form (CNF)*: a conjunction of clauses, each clause being a disjunction of literals, each literal being a variable or its negation. *Satisfiability* is the problem of finding an assignment of truth values to the variables that satisfies all the clauses (i.e., makes them true) or determining that none exists. It is the prototypical NP-complete problem.

A *first-order knowledge base (KB)* is a set of sentences or formulas in first-order logic [30]. Formulas are constructed using four types of symbols: constants, variables, functions, and predicates. Constant symbols represent objects in the domain of interest (e.g., people: `Anna`, `Bob`, `Chris`, etc.). Variable symbols range over the objects in the domain. Function symbols (e.g., `MotherOf`) represent mappings from tuples of objects to objects. Predicate symbols represent relations among objects in the domain (e.g., `Friends`) or attributes of objects (e.g., `Smokes`). An *interpretation* specifies which objects, functions and relations in the domain are represented by which symbols.

Variables and constants may be *typed*, in which case variables range only over objects of the corresponding type, and constants can only represent objects of the corresponding type. For example, the variable `x` might range over people (e.g., Anna, Bob, etc.), and the constant `C` might represent a city (e.g, Seattle, Tokyo, etc.).

A *term* is any expression representing an object in the domain. It can be a constant, a variable, or a function applied to a tuple of terms. For example, $\mathtt{Anna}$, $\mathtt{x}$, and $\mathtt{GreatestCommonDivisor}(\mathtt{x}, \mathtt{y})$ are terms. An *atomic formula* or *atom* is a predicate symbol applied to a tuple of terms (e.g., $\mathtt{Friends}(\mathtt{x}, \mathtt{MotherOf}(\mathtt{Anna}))$). Formulas are recursively constructed from atomic formulas using logical connectives and quantifiers. If F_1 and F_2 are formulas, the following are also formulas: $\neg F_1$ (negation), which is true iff F_1 is false; $F_1 \wedge F_2$ (conjunction), which is true iff both F_1 and F_2 are true; $F_1 \vee F_2$ (disjunction), which is true iff F_1 or F_2 is true; $F_1 \Rightarrow F_2$ (implication), which is true iff F_1 is false or F_2 is true; $F_1 \Leftrightarrow F_2$ (equivalence), which is true iff F_1 and F_2 have the same truth value; $\forall \mathsf{x}\ F_1$ (universal quantification), which is true iff F_1 is true for every object `x` in the domain; and $\exists \mathsf{x}\ F_1$ (existential quantification), which is true iff F_1 is true for at least one object `x` in the domain. Parentheses may be used to enforce precedence. A *positive literal* is an atomic formula; a *negative literal* is a negated atomic formula. The formulas in a KB are implicitly conjoined, and thus a KB can be viewed as a single large formula. A *ground term* is a term containing no variables. A *ground atom* or *ground predicate* is an atomic formula all of whose arguments are ground terms. Every first-order formula can be converted into an equivalent formula in *prenex conjunctive normal form*, $Qx_1 \ldots Qx_n\, C(x_1, \ldots, x_n)$, where each Q is a quantifier, the x_i are the quantified variables, and $C(\ldots)$ is a conjunction of clauses.

The *Herbrand universe* $\mathbf{U}(\mathbf{C})$ of a set of clauses $\mathbf{C}$ is the set of all ground terms constructible from the function and constant symbols in $\mathbf{C}$ (or, if $\mathbf{C}$ contains no constants, some arbitrary constant, e.g., `A`). If $\mathbf{C}$ contains function symbols, $\mathbf{U}(\mathbf{C})$ is infinite. (For example, if $\mathbf{C}$ contains solely the function `f` and no constants, $\mathbf{U}(\mathbf{C}) = \{\mathtt{f}(\mathtt{A}), \mathtt{f}(\mathtt{f}(\mathtt{A})), \mathtt{f}(\mathtt{f}(\mathtt{f}(\mathtt{A}))), \ldots\}$.) Some authors define the *Herbrand base* $\mathbf{B}(\mathbf{C})$ of $\mathbf{C}$ as the set of all ground atoms constructible from the predicate symbols in $\mathbf{C}$ and the terms in $\mathbf{U}(\mathbf{C})$. Others define it as the set of all ground clauses constructible from the clauses in $\mathbf{C}$ and the terms in $\mathbf{U}(\mathbf{C})$. For convenience, in this thesis we will define it as the union of the two, and talk about the *atoms in* $\mathbf{B}(\mathbf{C})$ and *clauses in* $\mathbf{B}(\mathbf{C})$ as needed.

An *interpretation* is a mapping between the constant, predicate and function symbols in the language and the objects, functions and relations in the domain. In a *Herbrand interpretation* there is a one-to-one mapping between ground terms and objects (i.e., every object is represented by some ground term, and no two ground terms correspond to the same object). A *model* or *possible world* specifies which relations hold true in the domain. Together with an interpretation, it assigns a truth value to every atomic formula, and thus to every formula in the knowledge base.

A formula is *satisfiable* iff there exists at least one world in which it is true. The basic inference problem in first-order logic is to determine whether a knowledge base KB *entails* a formula F, i.e., if F is true in all worlds where KB is true (denoted by $KB \models F$). This is often done by *refutation*: KB entails F iff $KB \cup \neg F$ is unsatisfiable. (Thus, if a KB contains a contradiction, all formulas trivially follow from it, which makes painstaking knowledge engineering a necessity.) Every KB in first-order logic can be converted to clausal form using a mechanical sequence of steps. Clausal form for a first order KB is a conjunction of clauses, where each variable in the conjunction is universally quantified. [1] Clausal form is used in resolution, a sound and refutation-complete inference procedure for first-order logic [87].

Inference in first-order logic is only semidecidable. Because of this, knowledge bases are often constructed using a restricted subset of first-order logic with more desirable properties. The most widely used restriction is to *Horn clauses*, which are clauses containing at most one positive literal. The Prolog programming language is based on Horn clause logic [57]. Prolog programs can be learned from databases by searching for Horn clauses that (approximately) hold in the data; this is studied in the field of inductive logic programming (ILP) [53].

In most domains it is very difficult to come up with non-trivial formulas that are always true, and such formulas capture only a fraction of the relevant knowledge. Thus, despite its expressiveness, pure first-order logic has limited applicability to practical AI problems. Many *ad hoc* extensions to address this have been proposed. In the more limited case of propositional logic, the problem is well solved by probabilistic graphical models. The next section describes a way to generalize these models to the first-order case.

[1]This conversion includes the removal of existential quantifiers by Skolemization, which is not sound in general. However, in finite domains an existentially quantified formula can simply be replaced by a disjunction of its groundings.

Table 2.1: Example of a Markov logic network. Free variables are implicitly universally quantified.

English	First-Order Logic	Weight
Most people don't smoke.	$\neg\texttt{Smokes}(\texttt{x})$	1.4
Most people don't have cancer.	$\neg\texttt{Cancer}(\texttt{x})$	2.3
Most people aren't friends.	$\neg\texttt{Friends}(\texttt{x},\texttt{y})$	4.6
Smoking causes cancer.	$\texttt{Smokes}(\texttt{x}) \Rightarrow \texttt{Cancer}(\texttt{x})$	1.5
Friends have similar smoking habits.	$\texttt{Smokes}(\texttt{x}) \wedge \texttt{Friends}(\texttt{x},\texttt{y}) \Rightarrow \texttt{Smokes}(\texttt{y})$	1.1

2.3 Markov Logic Networks

A first-order KB can be seen as a set of hard constraints on the set of possible worlds: if a world violates even one formula, it has zero probability. The basic idea in Markov logic [86] is to soften these constraints: when a world violates one formula in the KB it is less probable, but not impossible. The fewer formulas a world violates, the more probable it is. Each formula has an associated weight (e.g., see Table 2.1) that reflects how strong a constraint it is: the higher the weight, the greater the difference in log probability between a world that satisfies the formula and one that does not, other things being equal.

Definition 1. [86] *A Markov logic network (MLN) L is a set of pairs (F_i, w_i), where F_i is a formula in first-order logic and w_i is a real number. Together with a finite set of constants $C = \{c_1, c_2, \ldots, c_{|C|}\}$, it defines a Markov network $M_{L,C}$ (Equations 2.1 and 2.2) as follows:*

1. *$M_{L,C}$ contains one binary node for each possible grounding of each atom appearing in L. The value of the node is 1 if the ground atom is true, and 0 otherwise.*

2. *$M_{L,C}$ contains one feature for each possible grounding of each formula F_i in L. The value of this feature is 1 if the ground formula is true, and 0 otherwise. The weight of the feature is the w_i associated with F_i in L.*

Thus there is an edge between two nodes of $M_{L,C}$ iff the corresponding ground atoms appear together in at least one grounding of one formula in L. For example, an MLN containing the formulas $\forall\texttt{x}\,\texttt{Smokes}(\texttt{x}) \Rightarrow \texttt{Cancer}(\texttt{x})$ (smoking causes cancer) and $\forall\texttt{x}\forall\texttt{y}\,\texttt{Smokes}(\texttt{x})\wedge\texttt{Friends}(\texttt{x},\texttt{y}) \Rightarrow$

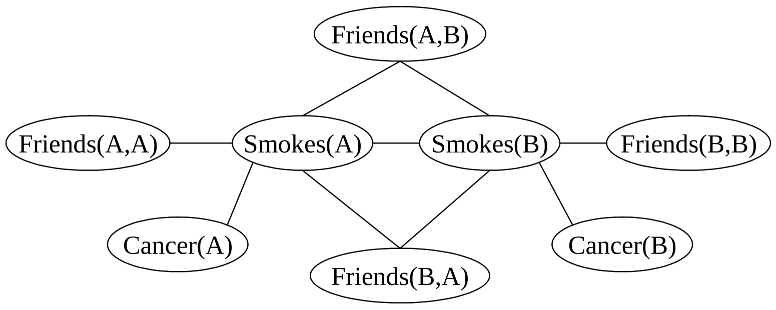


Figure 2.1: Ground Markov network obtained by applying an MLN containing the formulas $\forall \mathtt{x}\ \mathtt{Smokes}(\mathtt{x}) \Rightarrow \mathtt{Cancer}(\mathtt{x})$ and $\forall \mathtt{x} \forall \mathtt{y}\ \mathtt{Smokes}(\mathtt{x}) \wedge \mathtt{Friends}(\mathtt{x}, \mathtt{y}) \Rightarrow \mathtt{Smokes}(\mathtt{y})$ to the constants $\mathtt{Anna}$ $(\mathtt{A})$ and $\mathtt{Bob}$ $(\mathtt{B})$.

$\mathtt{Smokes}(\mathtt{y})$ (friends have similar smoking habits) applied to the constants $\mathtt{Anna}$ and $\mathtt{Bob}$ (or $\mathtt{A}$ and $\mathtt{B}$ for short) yields the ground Markov network in Figure 2.1. Its features include $\mathtt{Smokes}(\mathtt{Anna}) \Rightarrow \mathtt{Cancer}(\mathtt{Anna})$, etc. Notice that, although the two formulas above are false as universally quantified logical statements, as weighted features of an MLN they capture valid statistical regularities, and in fact represent a standard social network model [103].

An MLN can be viewed as a *template* for constructing Markov networks. From Definition 1 and Equations 2.1 and 2.2, the probability distribution over possible worlds x specified by the ground Markov network $M_{L,C}$ is given by

$$P(X = x) = \frac{1}{Z} \exp\left(\sum_i w_i f_i(x) \right) \tag{2.3}$$

where summation is over all the ground clauses, Z is the normalization constant, w_i is the weight of the ith clause, $f_i = 1$ if the ith clause is true, and $f_i = 0$ otherwise. This equation can alternately be written as

$$P(X = x) = \frac{1}{Z} \exp\left(\sum_{i=1}^{F} w_i n_i(x) \right) \tag{2.4}$$

F is the number of formulas in the MLN and $n_i(x)$ is the number of true groundings of F_i in x. As formula weights increase, an MLN increasingly resembles a purely logical KB, becoming equivalent to one in the limit of all infinite weights. When the weights are positive and finite, and all formulas are simultaneously satisfiable, the satisfying solutions are the modes of the distribution represented by the ground Markov network. Most importantly, Markov logic allows contradictions between formulas, which it resolves simply by weighing the evidence on both sides. This makes it well suited for merging multiple KBs. Markov logic also provides a natural and powerful approach to the problem of merging knowledge and data in different representations that do not align perfectly, as will be illustrated in the application section.

It is easily seen that all discrete probabilistic models expressible as products of potentials, including Markov networks and Bayesian networks, are expressible in Markov logic. In particular, many of the models frequently used in AI can be stated quite concisely as MLNs, and combined and extended simply by adding the corresponding formulas to the MLN. Most significantly, Markov logic facilitates the construction of non-i.i.d. models (i.e., models where objects are not independent and identically distributed).

When working with Markov logic, three assumptions about the logical representation are typically made: different constants refer to different objects (unique names), the only objects in the domain are those representable using the constant and function symbols (domain closure), and the value of each function for each tuple of arguments is always a known constant (known functions). These assumptions ensure that the number of possible worlds is finite and that the Markov logic network will give a well-defined probability distribution. These assumptions are quite reasonable in many practical applications, and greatly simplify the use of MLNs. Unless otherwise mentioned, we will make these assumptions in this dissertation.

There are certain cases where these assumptions have to be relaxed. The first such example is the problem of entity resolution, where we need to identify which of the constants in the language refer to the same underlying entity (or object) in the domain. Clearly, to handle this problem, the unique names assumption has to be relaxed. We will deal with this problem in detail in Chapter 7. Second, to extend the semantics of Markov logic to infinite domains and to represent them compactly we need to relax the assumption of known functions. Dealing with infinite domains is important both for theoretical reasons and because considering the infinite limit can help simplify the treatment of certain problems. The next chapter deals with this in detail. See Richardson and Domingos [86] for further details on the Markov logic representation and its relation to other statistical relational models.

Chapter 3
MARKOV LOGIC IN INFINITE DOMAINS

3.1 Introduction

One limitation of Markov logic (as proposed by Richardson and Domingos [86]) is that it is only defined for finite domains. While this is seldom a problem in practice, considering the infinite limit can simplify the treatment of some problems, and yield new insights. Study of this problem is also important to understand how far it is possible to combine the full power of first-order logic and graphical models. Thus in this chapter we extend Markov logic to infinite domains. Our treatment is based on the theory of Gibbs measures [32]. Gibbs measures are infinite-dimensional extensions of Markov networks, and have been studied extensively by statistical physicists and mathematical statisticians, due to their importance in modeling systems with phase transitions. We begin with some necessary background on Gibbs measures. We then define MLNs over infinite domains, state sufficient conditions for the existence and uniqueness of a probability measure consistent with a given MLN, and examine the important case of MLNs with non-unique measures. Next, we establish a correspondence between the problem of satisfiability in logic and the existence of MLN measures with certain properties. Finally, we discuss the relationship between infinite MLNs and previous infinite relational models.

3.2 Gibbs Measures

Gibbs measures are infinite-dimensional generalizations of Gibbs distributions. A Gibbs distribution, also known as a log-linear model or exponential model, and equivalent under mild conditions to a Markov network or Markov random field, assigns to a state $\mathbf{x}$ the probability

$$P(\mathbf{X}=\mathbf{x}) = \frac{1}{Z}\exp\left(\sum_i w_i f_i(\mathbf{x})\right) \qquad (3.1)$$

where w_i is any real number, f_i is an arbitrary function or *feature* of $\mathbf{x}$, and Z is a normalization constant. In this dissertation we will be concerned exclusively with Boolean states and functions (i.e., states are binary vectors, corresponding to possible worlds, and functions are logical formulas). Markov logic can be viewed as the use of first-order logic to compactly specify families of these functions [86]. Thus, a natural way to generalize it to infinite domains is to use the existing theory of Gibbs measures [32]. Although Gibbs measures were primarily developed to model regular lattices (e.g., ferromagnetic materials, gas/liquid phases, etc.), the theory is quite general, and applies equally well to the richer structures definable using Markov logic.

One problem with defining probability distributions over infinite domains is that the probability of most or all worlds will be zero. Measure theory allows us to overcome this problem by instead assigning probabilities to sets of worlds [6]. Let Ω denote the set of all possible worlds, and $\mathcal{E}$ denote a set of subsets of Ω. $\mathcal{E}$ must be a σ-algebra, i.e., it must be non-empty and closed under complements and countable unions. A function $\mu : \mathcal{E} \to \mathbb{R}$ is said to be a *probability measure* over $(\Omega, \mathcal{E})$ if $\mu(E) \geq 0$ for every $E \in \mathcal{E}$, $\mu(\Omega) = 1$, and $\mu(\bigcup E_i) = \sum \mu(E_i)$, where the union is taken over any countable collection of disjoint elements of $\mathcal{E}$.

A related difficulty is that in infinite domains the sum in Equation 3.1 may not exist. However, the distribution of any finite subset of the state variables conditioned on its complement is still well defined. We can thus define the infinite distribution indirectly by means of an infinite collection of finite conditional distributions. This is the basic idea in Gibbs measures.

Let us introduce some notation which will be used throughout the paper. Consider a countable set of variables $\mathbf{S} = \{X_1, X_2, \ldots\}$, where each X_i takes values in $\{0, 1\}$. Let $\mathbf{X}$ be a finite set of variables in $\mathbf{S}$, and $\mathbf{S}_{\mathbf{X}} = \mathbf{S} \setminus \mathbf{X}$. A possible world $\omega \in \Omega$ is an assignment to all the variables in $\mathbf{S}$. Let $\omega_{\mathbf{X}}$ denote the assignment to the variables in $\mathbf{X}$ under ω, and ω_{X_i} the assignment to X_i. Let $\mathcal{X}$ denote the set of all finite subsets of $\mathbf{S}$. A *basic event* $\mathbf{X} = \mathbf{x}$ is an assignment of values to a finite subset of variables $\mathbf{X} \in \mathcal{X}$, and denotes the set of possible worlds $\omega \in \Omega$ such that $w_{\mathbf{X}} = \mathbf{x}$. Let $\mathbf{E}$ be the set of all basic events, and let $\mathcal{E}$ be the σ-algebra generated by $\mathbf{E}$, i.e., the smallest σ-algebra containing $\mathbf{E}$. An element E of $\mathcal{E}$ is called an *event*, and $\mathcal{E}$ is the *event space*. The following treatment is adapted from Georgii [32].

Definition 2. *An* interaction potential *(or simply a* potential*) is a family $\Phi = (\Phi_{\mathbf{V}})_{\mathbf{V} \in \mathcal{X}}$ of functions $\Phi_{\mathbf{V}} : \mathbf{V} \to \mathbb{R}$ such that, for all $\mathbf{X} \in \mathcal{X}$ and $\omega \in \Omega$, the summation*

$$H_{\mathbf{X}}^{\Phi}(\omega) = \sum_{\mathbf{V}\in\mathcal{X},\mathbf{V}\cap\mathbf{X}\neq\emptyset} \Phi_{\mathbf{V}}(\omega_{\mathbf{V}}) \tag{3.2}$$

is finite. $H_{\mathbf{X}}^{\Phi}$ is called the Hamiltonian in $\mathbf{X}$ for Φ.

Intuitively, the Hamiltonian $H_{\mathbf{X}}^{\Phi}$ includes a contribution from all the potentials $\Phi_{\mathbf{V}}$ which share at least one variable with the set $\mathbf{X}$. Given an interaction potential Φ and a subset of variables $\mathbf{X}$, we define the conditional distribution $\gamma_{\mathbf{X}}^{\Phi}(\mathbf{X}|\mathbf{S_X})$ as[1]

$$\gamma_{\mathbf{X}}^{\Phi}(\mathbf{X}=\mathbf{x}|\mathbf{S_X}=\mathbf{y}) = \frac{\exp(H_{\mathbf{X}}^{\Phi}(\mathbf{x},\mathbf{y}))}{\sum_{\mathbf{x}\in\mathrm{Dom}(\mathbf{X})}\exp(H_{\mathbf{X}}^{\Phi}(\mathbf{x},\mathbf{y}))} \tag{3.3}$$

where the denominator is called the *partition function* in $\mathbf{X}$ for Φ and denoted by $Z_{\mathbf{X}}^{\Phi}$, and $\mathrm{Dom}(\mathbf{X})$ is the domain of $\mathbf{X}$. Equation 3.3 can be easily extended to arbitrary events $E \in \mathcal{E}$ by defining $\gamma_{\mathbf{X}}^{\Phi}(E|\mathbf{S_X})$ to be non-zero only when E is consistent with the assignment in $\mathbf{S_X}$. Details are skipped here to keep the discussion simple, and can be found in Georgii [32]. The family of conditional distributions $\gamma^{\Phi} = (\gamma_{\mathbf{X}}^{\Phi})_{\mathbf{X}\in\mathcal{X}}$ as defined above is called a *Gibbsian specification*.[2]

Given a measure μ over $(\Omega, \mathcal{E})$ and conditional probabilities $\gamma_{\mathbf{X}}^{\Phi}(E|\mathbf{S_X})$, let the composition $\mu\gamma_{\mathbf{X}}^{\Phi}$ be defined as

$$\mu\gamma_{\mathbf{X}}^{\Phi}(E) = \int_{\mathrm{Dom}(\mathbf{S_X})} \gamma_{\mathbf{X}}^{\Phi}(E|\mathbf{S_X})\,\partial\mu \tag{3.4}$$

$\mu\gamma_{\mathbf{X}}^{\Phi}(E)$ is the probability of event E according to the conditional probabilities $\gamma_{\mathbf{X}}^{\Phi}(E|\mathbf{S_X})$ and the measure μ on $\mathbf{S_X}$. We are now ready to define Gibbs measure.

Definition 3. *Let γ^{Φ} be a Gibbsian specification. Let μ be a probability measure over the measurable space $(\Omega, \mathcal{E})$ such that, for every $\mathbf{X} \in \mathcal{X}$ and $E \in \mathcal{E}$, $\mu(E) = \mu\gamma_{\mathbf{X}}^{\Phi}(E)$. Then the specification γ^{Φ} is said to admit the* Gibbs measure *μ. Further, $\mathcal{G}(\gamma^{\Phi})$ denotes the set of all such measures.*

In other words, a Gibbs measure is consistent with a Gibbsian specification if its event probabilities agree with those obtained from the specification. Given a Gibbsian specification, we can

[1]For physical reasons, this equation is usually written with a negative sign in the exponent, i.e., $\exp[-H_{\mathbf{X}}^{\Phi}(\omega)]$. Since this is not relevant in Markov logic and does not affect any of the results, we omit it.

[2]Georgii [32] defines Gibbsian specifications in terms of underlying independent specifications. For simplicity, we assume these to be equi-distributions and omit them throughout this dissertation.

ask whether there exists a Gibbs measure consistent with it ($|\mathcal{G}(\gamma^\Phi)| > 0$), and whether it is unique ($|\mathcal{G}(\gamma^\Phi)| = 1$). In the non-unique case, we can ask what the structure of $\mathcal{G}(\gamma^\Phi)$ is, and what the measures in it represent. We can also ask whether Gibbs measures with specific properties exist. The theory of Gibbs measures addresses these questions. In this paper we apply it to the case of Gibbsian specifications defined by MLNs.

3.3 Infinite MLNs

3.3.1 Definition

A Markov logic network (MLN) is a set of weighted first-order formulas. As we saw in Chapter 2, these can be converted to equivalent formulas in prenex CNF. We will assume throughout that all existentially quantified variables have finite domains, unless otherwise specified. While this is a significant restriction, it still includes essentially all previous probabilistic relational representations as special cases. Existentially quantified formulas can now be replaced by finite disjunctions. By distributing conjunctions over disjunctions, every prenex CNF can now be converted to a quantifier-free CNF, with all variables implicitly universally quantified.

The Herbrand universe $\mathbf{U}(\mathbf{L})$ of an MLN $\mathbf{L}$ is the set of all ground terms constructible from the constants and function symbols in the MLN. The Herbrand base $\mathbf{B}(\mathbf{L})$ of $\mathbf{L}$ is the set of all ground atoms and clauses constructible from the predicates in $\mathbf{L}$, the clauses in the CNF form of $\mathbf{L}$, and the terms in $\mathbf{U}(\mathbf{L})$, replacing typed variables only by terms of the corresponding type. We assume Herbrand interpretations throughout. We are now ready to formally define MLNs.

Definition 4. *A* Markov logic network (MLN) $\mathbf{L}$ *is a (finite) set of pairs* (F_i, w_i)*, where* F_i *is a formula in first-order logic and* w_i *is a real number.* $\mathbf{L}$ *defines a countable set of variables* $\mathbf{S}$ *and interaction potential* $\Phi^{\mathbf{L}} = (\Phi^{\mathbf{L}}_{\mathbf{X}})_{\mathbf{X}\in\mathcal{X}}$*,* $\mathcal{X}$ *being the set of all finite subsets of* $\mathbf{S}$*, as follows:*

1. $\mathbf{S}$ *contains a binary variable for each atom in* $\mathbf{B}(\mathbf{L})$*. The value of this variable is 1 if the atom is true, and 0 otherwise.*

2. $\Phi^{\mathbf{L}}_{\mathbf{X}}(\mathbf{x}) = \sum_j w_j f_j(\mathbf{x})$*, where the sum is over the clauses* C_j *in* $\mathbf{B}(\mathbf{L})$ *whose arguments are exactly the elements of* $\mathbf{X}$*. If* $F_{i(j)}$ *is the formula in* $\mathbf{L}$ *from which* C_j *originated, and* $F_{i(j)}$

gave rise to n clauses in the CNF form of $\mathbf{L}$, then $w_j = w_i/n$. $f_j(\mathbf{x}) = 1$ if C_j is true in world $\mathbf{x}$, and $f_j = 0$ otherwise.

For $\Phi^{\mathbf{L}}$ to correspond to a well-defined Gibbsian specification, the corresponding Hamiltonians (Equation 3.2) need to be finite. This brings us to the following definition.

Definition 5. *Let $\mathbf{C}$ be a set of first-order clauses. Given a ground atom $X \in \mathbf{B}(\mathbf{C})$, let the* neighbors $\mathbf{N}(X)$ *of X be the atoms that appear with it in some ground clause. $\mathbf{C}$ is said to be* locally finite *if each atom in the Herbrand base of $\mathbf{C}$ has a finite number of neighbors, i.e., $\forall X \in \mathbf{B}(\mathbf{C})$, $|\mathbf{N}(X)| < \infty$. An MLN (or knowledge base) is said to be locally finite if the set of its clauses is locally finite.*

It is easy to see that local finiteness is sufficient to ensure a well-defined Gibbsian specification. Given such an MLN $\mathbf{L}$, the distribution $\gamma^{\mathbf{L}}_{\mathbf{X}}$ of a set of variables $\mathbf{X} \in \mathcal{X}$ conditioned on its complement $\mathbf{S}_{\mathbf{X}}$ is given by

$$\gamma^{\mathbf{L}}_{\mathbf{X}}(\mathbf{X}{=}\mathbf{x}|\mathbf{S}_{\mathbf{X}}{=}\mathbf{y}) = \frac{\exp\left(\sum_j w_j f_j(\mathbf{x},\mathbf{y})\right)}{\sum_{\mathbf{x}'\in \mathrm{Dom}(\mathbf{X})} \exp\left(\sum_j w_j f_j(\mathbf{x}',\mathbf{y})\right)} \tag{3.5}$$

where the sum is over the clauses in $\mathbf{B}(\mathbf{L})$ that contain at least one element of $\mathbf{X}$, and $f_j(\mathbf{x},\mathbf{y}) = 1$ if clause C_j is true under the assignment $(\mathbf{x},\mathbf{y})$ and 0 otherwise. The corresponding Gibbsian specification is denoted by $\gamma^{\mathbf{L}}$.

For an MLN to be locally finite, it suffices that it be *σ-determinate*.

Definition 6. *A clause is σ-*determinate *if all the variables with infinite domains it contains appear in all literals.*[3] *A set of clauses is σ-determinate if each clause in the set is σ-determinate. An MLN is σ-determinate if the set of its clauses is σ-determinate.*

Notice that this definition does not require that all literals have the same infinite arguments; for example, the clause $\mathtt{Q}(\mathtt{x},\mathtt{y}) \Rightarrow \mathtt{R}(\mathtt{f}(\mathtt{x}),\mathtt{g}(\mathtt{x},\mathtt{y}))$ is σ-determinate. In essence, σ-determinacy requires that the neighbors of an atom be defined by functions of its arguments. Because functions can be composed indefinitely, the network can be infinite; because first-order clauses have finite length, σ-determinacy ensures that neighborhoods are still finite.

[3]This is related to the notion of a *determinate clause* in logic programming. In a determinate clause, the grounding of the variables in the head determines the grounding of all the variables in the body. In infinite MLNs, any literal in a clause can be inferred from the others, not just the head from the body, so we require that the (infinite-domain) variables in each literal determine the variables in the others.

If the MLN contains no function symbols, Definition 4 reduces to the one in Richardson and Domingos [86], with C being the constants appearing in the MLN. This can be easily seen by substituting $\mathbf{X} = \mathbf{S}$ in Equation 3.5. Notice it would be equally possible to define features for conjunctions of clauses, and this may be preferable for some applications.

3.3.2 Existence

Let $\mathbf{L}$ be a locally finite MLN. The focus of this section is to show that its specification $\gamma^{\mathbf{L}}$ always admits some measure μ. It is useful to first gain some intuition as to why this might not always be the case. Consider an MLN stating that each person is loved by exactly one person: $\forall \mathtt{x}\, \exists^! \mathtt{y}\, \mathtt{Loves}(\mathtt{y}, \mathtt{x})$. Let ω_k denote the event $\mathtt{Loves}(\mathtt{P}_k, \mathtt{Anna})$, i.e., Anna is loved by the kth person in the (countably infinite) domain. Then, in the limit of infinite weights, one would expect that $\mu(\bigcup \omega_k) = \mu(\Omega) = 1$. But in fact $\mu(\bigcup \omega_k) = \sum \mu(\omega_k) = 0$. The first equality holds because the ω_k's are disjoint, and the second one because each ω_k has zero probability of occurring by itself. There is a contradiction, and there exists no measure consistent with the MLN above.[4] The reason the MLN fails to have a measure is that the formulas are not local, in the sense that the truth value of an atom depends on the truth values of infinite others. Locality is in fact the key property for the existence of a consistent measure, and local finiteness ensures it.

Definition 7. *A function $f : \Omega \to \mathbb{R}$ is* local *if it depends only on a finite subset $\mathbf{V} \in \mathcal{X}$. A Gibbsian specification $\gamma = (\gamma_{\mathbf{X}})_{\mathbf{X} \in \mathcal{X}}$ is local if each $\gamma_{\mathbf{X}}$ is local.*

Lemma 8. *Let $\mathbf{L}$ be a locally finite MLN, and $\gamma^{\mathbf{L}}$ the corresponding specification. Then $\gamma^{\mathbf{L}}$ is local.*

Proof. Each Hamiltonian $H^{\mathbf{L}}_{\mathbf{X}}$ is local, since by local finiteness it depends only on a finite number of potentials $\phi^{\mathbf{L}}_{\mathbf{V}}$. It follows that each $\gamma^{\mathbf{L}}_{\mathbf{X}}$ is local, and hence the corresponding specification $\gamma^{\mathbf{L}}$ is also local. $\square$

We now state the theorem for the existence of a measure admitted by $\gamma^{\mathbf{L}}$.

Theorem 1. *Let $\mathbf{L}$ be a locally finite MLN, and $\gamma^{\mathbf{L}} = (\gamma^{\mathbf{L}}_{\mathbf{X}})_{\mathbf{X} \in \mathcal{X}}$ be the corresponding Gibbsian specification. Then there exists a measure μ over $(\Omega, \mathcal{E})$ admitted by $\gamma^{\mathbf{L}}$, i.e., $|\mathcal{G}(\gamma^{\mathbf{L}})| \geq 1$.*

[4] See Example 4.16 in Georgii [32] for a detailed proof.

Proof. To show the existence of a measure μ, we need to prove the following two conditions:

1. The net $(\gamma^{\mathbf{L}}_{\mathbf{X}}(\mathbf{X}|\mathbf{S}_{\mathbf{X}}))_{\mathbf{X}\in\mathcal{X}}$ has a cluster point with respect to the weak topology on $(\Omega, \mathcal{E})$.

2. Each cluster point of $(\gamma^{\mathbf{L}}_{\mathbf{X}}(\mathbf{X}|\mathbf{S}_{\mathbf{X}}))_{\mathbf{X}\in\mathcal{X}}$ belongs to $\mathcal{G}(\gamma^{\mathbf{L}})$.

It is a well known result that, if all the variables X_i have finite domains, then the net in Condition 1 has a cluster point (see Section 4.2 in Georgii [32]). Thus, since all the variables in the MLN are binary, Condition 1 holds. Further, since $\gamma^{\mathbf{L}}$ is local, every cluster point μ of the net $(\gamma^{\mathbf{L}}_{\mathbf{X}}(\mathbf{X}|\mathbf{S}_{\mathbf{X}}))_{\mathbf{X}\in\mathcal{X}}$ belongs to $\mathcal{G}(\gamma^{\mathbf{L}})$ (Comment 4.18 in Georgii [32]). Therefore, Condition 2 is also satisfied. Hence there exists a measure μ consistent with the specification $\gamma^{\mathbf{L}}$, as required. $\square$

3.3.3 Uniqueness

This section addresses the question of under what conditions an MLN admits a unique measure. Let us first gain some intuition as to why an MLN might admit more than one measure. The only condition an MLN $\mathbf{L}$ imposes on a measure is that it should be consistent with the local conditional distributions $\gamma^{\mathbf{L}}_{\mathbf{X}}$. But since these distributions are local, they do not determine the behavior of the measure at infinity. Consider, for example, a semi-infinite two-dimensional lattice, where neighboring sites are more likely to have the same truth value than not. This can be represented by formulas of the form $\forall \mathtt{x}, \mathtt{y}\ \mathtt{Q}(\mathtt{x}, \mathtt{y}) \Leftrightarrow \mathtt{Q}(\mathtt{s}(\mathtt{x}), \mathtt{y})$ and $\forall \mathtt{x}, \mathtt{y}\ \mathtt{Q}(\mathtt{x}, \mathtt{y}) \Leftrightarrow \mathtt{Q}(\mathtt{x}, \mathtt{s}(\mathtt{y}))$, with a single constant 0 to define the origin $(0, 0)$, and with $\mathtt{s}()$ being the successor function. The higher the weight w of these formulas, the more likely neighbors are to have the same value. This MLN has two extreme states: one where $\forall \mathtt{x}\ \mathtt{S}(\mathtt{x})$, and one where $\forall \mathtt{x}\ \neg\mathtt{S}(\mathtt{x})$. Let us call these states ξ and $\xi_{\neg}$, and let ξ' be a local perturbation of ξ (i.e., ξ' differs from ξ on only a finite number of sites). If we draw a contour around the sites where ξ' and ξ differ, then the log odds of ξ and ξ' increase with wd, where d is the length of the contour. Thus long contours are improbable, and there is a measure $\mu \rightarrow \delta_{\xi}$ as $w \rightarrow \infty$. Since, by the same reasoning, there is a measure $\mu_{\neg} \rightarrow \delta_{\xi_{\neg}}$ as $w \rightarrow \infty$, the MLN admits more than one measure.[5]

[5]Notice that this argument fails for a one-dimensional lattice (equivalent to a Markov chain), since in this case an arbitrarily large number of sites can be separated from the rest by a contour of length 2. Non-uniqueness (corresponding to a non-ergodic chain) can then only be obtained by making some weights infinite (corresponding to zero transition probabilities).

Let us now turn to the mathematical conditions for the existence of a unique measure for a given MLN $\mathbf{L}$. Clearly, in the limit of all non-unit clause weights going to zero, $\mathbf{L}$ defines a unique distribution. Thus, by a continuity argument, one would expect the same to be true for small enough weights. This is indeed the case. To make it precise, let us first define the notion of the oscillation of a function. Given a function $f : \mathbf{X} \to \mathbb{R}$, let the oscillation of f, $\delta(f)$, be defined as

$$\begin{aligned} \delta(f) &= \max_{\mathbf{x},\mathbf{x}' \in \mathrm{Dom}(\mathbf{X})} |f(\mathbf{x}) - f(\mathbf{x}')| \\ &= \max_{\mathbf{x}} |f(\mathbf{x})| - \min_{\mathbf{x}} |f(\mathbf{x})| \end{aligned} \tag{3.6}$$

The oscillation of a function is thus simply the difference between its extreme values. We can now state a sufficient condition for the existence of a unique measure.

Theorem 2. *Let $\mathbf{L}$ be a locally finite MLN with interaction potential Φ^L and Gibbsian specification $\gamma^{\mathbf{L}}$ such that*

$$\sup_{X_i \in \mathbf{S}} \sum_{C_j \in \mathbf{C}(X_i)} (|C_j| - 1)|w_j| < 2 \tag{3.7}$$

where $\mathbf{C}(X_i)$ is the set of ground clauses in which X_i appears, $|C_j|$ is the number of ground atoms appearing in clause C_j, and w_j is its weight. Then $\gamma^{\mathbf{L}}$ admits a unique Gibbs measure.

Proof. Based on Theorem 8.7 and Proposition 8.8 in Georgii [32], a sufficient condition for uniqueness is

$$\sup_{X_i \in \mathbf{S}} \sum_{\mathbf{V} \ni X_i} (|\mathbf{V}| - 1)\delta(\Phi^{\mathbf{L}}_{\mathbf{V}}) < 2 \tag{3.8}$$

Rewriting this condition in terms of the ground formulas in which a variable X_i appears (see Definition 4) yields the desired result. □

Note that, as alluded to before, the above condition does not depend on the weight of the unit clauses. This is because for a unit clause $|C_j| - 1 = 0$. If we define the interaction between two variables as the sum of the weights of all the ground clauses in which they appear together, then the above theorem states that the total sum of the interactions of any variable with its neighbors should be less than 2 for the measure to be unique.

Two other sufficient conditions are worth mentioning briefly. One is that, if the weights of the unit clauses are sufficiently large compared to the weights of the non-unit ones, the measure is unique. Intuitively, the unit terms “drown out” the interactions, rendering the variables approximately independent. The other condition is that, if the MLN is a one-dimensional lattice, it suffices that the total interaction between the variables to the left and right of any arc be finite. This corresponds to the ergodicity condition for a Markov chain.

3.3.4 Non-unique MLNs

At first sight, it might appear that non-uniqueness is an undesirable property, and non-unique MLNs are not an interesting object of study. However, the non-unique case is in fact quite important, because many phenomena of interest are represented by MLNs with non-unique measures (for example, very large social networks with strong word-of-mouth effects). The question of what these measures represent, and how they relate to each other, then becomes important. This is the subject of this section.

The first observation is that the set of all Gibbs measures $\mathcal{G}(\gamma^{\mathbf{L}})$ is convex. That is, if $\mu, \mu' \in \mathcal{G}(\gamma^{\mathbf{L}})$ then $\nu \in \mathcal{G}(\gamma^{L})$, where $\nu = s\mu + (1-s)\mu', s \in (0,1)$. This is easily verified by substituting ν in Equation 3.4. Hence, the non-uniqueness of a Gibbs measure implies the existence of infinitely many consistent Gibbs measures. Further, many properties of the set $\mathcal{G}(\gamma^{\mathbf{L}})$ depend on the set of extreme Gibbs measures $\operatorname{ex}\mathcal{G}(\gamma^{\mathbf{L}})$, where $\mu \in \operatorname{ex}\mathcal{G}(\gamma^{\mathbf{L}})$ if $\mu \in \mathcal{G}(\gamma^{\mathbf{L}})$ cannot be written as a linear combination of two distinct measures in $\mathcal{G}(\gamma^{\mathbf{L}})$.

An important notion to understand the properties of extreme Gibbs measures is the notion of a tail event. Consider a subset $\mathbf{S}'$ of $\mathbf{S}$. Let $\sigma(\mathbf{S}')$ denote the σ-algebra generated by the set of basic events involving only variables in $\mathbf{S}'$. Then we define the tail σ-algebra $\mathcal{T}$ as

$$\mathcal{T} = \bigcap_{\mathbf{X} \in \mathcal{X}} \sigma(\mathbf{S}_{\mathbf{X}}) \tag{3.9}$$

Any event belonging to $\mathcal{T}$ is called a tail event. $\mathcal{T}$ is precisely the set of events which do not depend on the value of any finite set of variables, but rather only on the behavior at infinity. For example, in the infinite tosses of a coin, the event that ten consecutive heads come out infinitely many times is a tail event. Similarly, in the lattice example in the previous section, the event that a finite number of variables have the value 1 is a tail event. Events in $\mathcal{T}$ can be thought of as representing macroscopic properties of the system being modeled.

Definition 9. *A measure μ is trivial on a σ-algebra $\mathcal{E}$ if $\mu(E) = 0$ or 1 for all $E \in \mathcal{E}$.*

The following theorem (adapted from Theorem 7.8 in Georgii [32]) describes the relationship between the extreme Gibbs measures and the tail σ-algebra.

Theorem 3. *Let $\mathbf{L}$ be a locally finite MLN, and $\gamma^{\mathbf{L}}$ denote the corresponding Gibbsian specification. Then the following results hold:*

1. *A measure $\mu \in \operatorname{ex} \mathcal{G}(\gamma^{\mathbf{L}})$ iff it is trivial on the tail σ-algebra $\mathcal{T}$.*
2. *Each measure μ is uniquely determined by its behavior on the tail σ-algebra, i.e., if $\mu_1 = \mu_2$ on $\mathcal{T}$ then $\mu_1 = \mu_2$.*

It is easy to see that each extreme measure corresponds to some particular value for all the macroscopic properties of the network. In physical systems, extreme measures correspond to phases of the system (e.g., liquid vs. gas, or different directions of magnetization), and non-extreme measures correspond to probability distributions over phases. Uncertainty over phases arises when our knowledge of a system is not sufficient to determine its macroscopic state. Clearly, the study of non-unique MLNs beyond the highly regular ones statistical physicists have focused on promises to be quite interesting. In the next section we take a step in this direction by considering the problem of satisfiability in the context of MLN measures.

3.4 Satisfiability and Entailment

Richardson and Domingos [86] showed that, in finite domains, first-order logic can be viewed as the limiting case of Markov logic when all weights tend to infinity, in the following sense. If we convert a satisfiable knowledge base $\mathbf{K}$ into an MLN $\mathbf{L}_{\mathbf{K}}$ by assigning the same weight $w \to \infty$ to all clauses, then $\mathbf{L}_{\mathbf{K}}$ defines a uniform distribution over the worlds satisfying $\mathbf{K}$. Further, $\mathbf{K}$ entails a formula α iff $\mathbf{L}_{\mathbf{K}}$ assigns probability 1 to the set of worlds satisfying α (Proposition 4.3). In this section we extend this result to infinite domains.

Consider an MLN $\mathbf{L}$ such that each clause in its CNF form has the same weight w. In the limit $w \to \infty$, $\mathbf{L}$ does not correspond to a valid Gibbsian specification, since the Hamiltonians defined in Equation 3.2 are no longer finite. Revisiting Equation 3.5 in the limit of all equal infinite clause weights, the limiting conditional distribution is equi-distribution over those configurations $\mathbf{X}$

which satisfy the maximum number of clauses given $\mathbf{S_X} = \mathbf{y}$. It turns out we can still talk about the existence of a measure consistent with these conditional distributions, because they constitute a valid specification (though not Gibbsian) under the same conditions as in the finite weight case. We omit the details and proofs for lack of space; they can be found in Singla and Domingos [97]. Existence of a measure follows as in the case of finite weights because of the locality of conditional distributions. We now define the notion of a *satisfying measure*, which is central to the results presented in this section.

Definition 10. *Let $\mathbf{L}$ be a locally finite MLN. Given a clause $C_i \in \mathbf{B}(\mathbf{L})$, let $\mathbf{V}_i$ denote the set of Boolean variables appearing in C_i. A measure $\mu \in \mathcal{G}(\gamma^{\mathbf{L}})$ is said to be a* satisfying measure *for $\mathbf{L}$ if, for every ground clause $C_i \in \mathbf{B}(\mathbf{L})$, μ assigns non-zero probability only to the satisfying assignments of the variables in C_i, i.e., $\mu(\mathbf{V}_i = \mathbf{v}_i) > 0$ implies that $\mathbf{V}_i = \mathbf{v}_i$ is a satisfying assignment for C_i. $\mathcal{S}(\gamma^{\mathbf{L}})$ denotes the set of all satisfying measures for $\mathbf{L}$.*

Informally, a satisfying measure assigns non-zero probability only to those worlds which are consistent with all the formulas in $\mathbf{L}$. Intuitively, existence of a satisfying measure for $\mathbf{L}$ should be in some way related to the existence of a satisfying assignment for the corresponding knowledge base. Our next theorem formalizes this intuition.

Theorem 4. *Let $\mathbf{K}$ be a locally finite knowledge base, and let $\mathbf{L}_\infty$ be the MLN obtained by assigning weight $w \to \infty$ to all the clauses in $\mathbf{K}$. Then there exists a satisfying measure for $\mathbf{L}_\infty$ iff $\mathbf{K}$ is satisfiable. Mathematically,*

$$|\mathcal{S}(\gamma^{\mathbf{L}_\infty})| > 0 \;\Leftrightarrow\; \mathit{Satisfiable}(\mathbf{K}) \tag{3.10}$$

Proof. Let us first prove that existence of a satisfying measure implies satisfiability of $\mathbf{K}$. This is equivalent to proving that unsatisfiability of $\mathbf{K}$ implies non-existence of a satisfying measure. Let $\mathbf{K}$ be unsatisfiable. Equivalently, $\mathbf{B}(\mathbf{K})$, the Herbrand base of $\mathbf{K}$, is unsatisfiable. By Herbrand's theorem, there exists a finite set of ground clauses $\mathbf{C} \subseteq \mathbf{B}(\mathbf{K})$ that is unsatisfiable. Let $\mathbf{V}$ denote the set of variables appearing in $\mathbf{C}$. Then every assignment $\mathbf{v}$ to the variables in $\mathbf{V}$ violates some clause in $\mathbf{C}$. Let μ denote a measure for $\mathbf{L}_\infty$. Since μ is a probability measure, $\sum_{\mathbf{v} \in \mathrm{Dom}(\mathbf{V})} \mu(\mathbf{V} = \mathbf{v}) = 1$. Further, since $\mathbf{V}$ is finite, there exists some $\mathbf{v} \in \mathrm{Dom}(\mathbf{V})$ such that $\mu(\mathbf{V} = \mathbf{v}) > 0$. Let $C_i \in \mathbf{C}$ be some clause violated by the assignment $\mathbf{v}$ (every assignment violates some clause). Let $\mathbf{V}_i$ denote the set of variables in C_i and $\mathbf{v}_i$ be the restriction of assignment $\mathbf{v}$ to the variables in $\mathbf{V}_i$. Then $\mathbf{v}_i$ is an unsatisfying assignment for C_i. Further, $\mu(\mathbf{V}_i = \mathbf{v}_i) \geq \mu(\mathbf{V} = \mathbf{v}) > 0$. Hence μ cannot be a satisfying measure for $\mathbf{L}_\infty$. Since the above argument holds for any $\mu \in \mathcal{G}(\gamma^{\mathbf{L}_\infty})$, there does not exist a satisfying measure for $\mathbf{L}_\infty$ when $\mathbf{K}$ is unsatisfiable.

Next, we need to prove that satisfiability of $\mathbf{K}$ implies existence of a satisfying measure. We will only give a proof sketch here; the full proof can be found in Singla and Domingos [97]. Let $\mathbf{K}$ be satisfiable. Now, consider a finite subset $\mathbf{X}$ of the variables defined by $\mathbf{L}_\infty$. Given $\mathbf{X}$, let $\Delta_{\mathbf{X}}$ denote the set of those probability distributions over $\mathbf{X}$ which assign non-zero probability only to the configurations which are partial satisfying assignments of $\mathbf{K}$. We will call $\Delta_{\mathbf{X}}$ the set of satisfying distributions over $\mathbf{X}$. $\Delta_{\mathbf{X}}$ is a compact set. Let $\mathbf{Y}$ denote the set of neighbors of the variables in $\mathbf{X}$. We define $F_{\mathbf{X}} : \Delta_{\mathbf{Y}} \rightarrow \Delta_{\mathbf{X}}$ to be the function which maps a satisfying distribution over $\mathbf{Y}$ to a satisfying distribution over $\mathbf{X}$ given the conditional distribution $\gamma_{\mathbf{X}}^{\mathbf{L}_\infty}(\mathbf{X}|\mathbf{S}_{\mathbf{X}})$. The mapping results in a satisfying distribution over $\mathbf{X}$ because, in the limit of all equal infinite weights, the conditional distribution over $\mathbf{X}$ is non-zero only for the satisfying assignments of $\mathbf{X}$. Since $\Delta_{\mathbf{Y}}$ is compact, its image under the continuous function $F_{\mathbf{X}}$ is also compact.

Given $\mathbf{X}_i \subset \mathbf{X}_j$ and their neighbors, $\mathbf{Y}_i$ and $\mathbf{Y}_j$ respectively, we show that if $\pi_{\mathbf{X}_j} \in \Delta_{\mathbf{X}_j}$ is in the image of $\Delta_{\mathbf{Y}_j}$ under $F_{\mathbf{X}_j}$, then $\pi_{\mathbf{X}_i} = \sum_{\mathbf{X}_j - \mathbf{X}_i} \pi_{\mathbf{X}_j}$ is in the image of Δ_{X_i} under $F_{\mathbf{X}_i}$. This process can then be repeated for ever-increasing sets $\mathbf{X}_k \supset \mathbf{X}_i$. This defines a sequence $(\mathbf{T}_i^j)_{j=i}^{j=\infty}$ of non-empty subsets of satisfying distributions over $\mathbf{X_i}$. Further, it is easy to show that $\forall k\ \mathbf{T}_i^{k+1} \subseteq \mathbf{T}_i^k$. Since each $\mathbf{T}_i^k$ is compact and non-empty, from the theory of compact sets we obtain that the countably infinite intersection $\mathbf{T}_i = \bigcap_{j=i}^{j=\infty} \mathbf{T}_i^j$ is also non-empty.

Let $(X_1, X_2, \ldots, X_k, \ldots)$ be some ordering of the variables defined by $\mathbf{L}_\infty$, and let $\mathbf{X}_k = \{X_1, X_2, \ldots X_k\}$. We now define a satisfying measure μ as follows. We define $\mu(\mathbf{X_1})$ to be some element of $\mathbf{T}_1$. Given $\mu(\mathbf{X}_k)$, we define $\mu(\mathbf{X}_{k+1})$ to be that element of $\mathbf{T}_{k+1}$ whose marginal is $\mu(\mathbf{X}_k)$ (such an element always exists, by construction). For an arbitrary set of variables $\mathbf{X}$, let k be the smallest index such that $\mathbf{X} \subseteq \mathbf{X}_k$, and define $\mu(\mathbf{X}) = \sum_{\mathbf{X_k} \setminus \mathbf{X}} \mu(\mathbf{X_k})$. We show that μ defined in such a way satisfies the properties of a probability measure (see Section 3.2). Finally, μ is a satisfying measure because $\forall k\ \mu(\mathbf{X_k}) \in \mathbf{T}_k$ and each $\mathbf{T}_k$ is a set of satisfying distributions over $\mathbf{X}_k$. $\square$

Corollary 11. *Let $\mathbf{K}$ be a locally finite knowledge base. Let α be a first-order formula, and $\mathbf{L}_\infty^\alpha$ be the MLN obtained by assigning weight $w \to \infty$ to all clauses in $\mathbf{K} \cup \{\neg\alpha\}$. Then $\mathbf{K}$ entails α iff $\mathbf{L}_\infty^\alpha$ has no satisfying measure. Mathematically,*

$$\mathbf{K} \models \alpha \;\Leftrightarrow\; |\mathcal{S}(\gamma^{\mathbf{L}_\infty^\alpha})| = 0 \tag{3.11}$$

Thus, for locally finite knowledge bases with Herbrand interpretations, first-order logic can be viewed as the limiting case of Markov logic when all weights tend to infinity. Whether these conditions can be relaxed is a question for future work.

3.5 Relation to Other Approaches

A number of relational representations capable of handling infinite domains have been proposed in recent years. Generally, they rely on strong restrictions to make this possible. To our knowledge, Markov logic is the most flexible language for modeling infinite relational domains to date. In this section we briefly review the main approaches.

Stochastic logic programs [69] are generalizations of probabilistic context-free grammars. PCFGs allow for infinite derivations but as a result do not always represent valid distributions [8]. In SLPs these issues are avoided by explicitly assigning zero probability to infinite derivations. Similar remarks apply to related languages like independent choice logic [80] and PRISM [90].

Many approaches combine logic programming and Bayesian networks. The most advanced one is arguably Bayesian logic programs [46]. Kersting and De Raedt show that, if all nodes have a finite number of ancestors, a BLP represents a unique distribution. This is a stronger restriction than finite neighborhoods. Richardson and Domingos [86] showed how BLPs can be converted into Markov logic without loss of representational efficiency.

Jaeger [41] shows that probabilistic queries are decidable for a very restricted language where a ground atom cannot depend on other groundings of the same predicate. Jaeger shows that if this restriction is removed queries become undecidable.

Recursive probability models are a combination of Bayesian networks and description logics [78]. Like Markov logic, RPMs require finite neighborhoods, and in fact existence for RPMs can be proved succinctly by converting them to Markov logic and applying Theorem 1. Pfeffer and Koller show that RPMs do not always represent unique distributions, but do not study conditions for uniqueness. Description logics are a restricted subset of first-order logic, and thus MLNs are considerably more flexible than RPMs.

Contingent Bayesian networks [65] allow infinite ancestors, but require that, for each variable with infinite ancestors, there exist a set of mutually exclusive and exhaustive contexts (assignments to finite sets of variables) such that in every context only a finite number of ancestors affect the probability of the variable. This is a strong restriction, excluding even simple infinite models like backward Markov chains [78].

Multi-entity Bayesian networks are another relational extension of Bayesian networks [52]. Laskey and Costa claim that MEBNs allow infinite parents and arbitrary first-order formulas, but the definition of MEBN explicitly requires that, for each atom X and increasing sequence of substates $S_1 \subset S_2 \subset \ldots$, there exist a finite N such that $P(X|S_k) = P(X|S_N)$ for $k > N$. This assumption necessarily excludes many dependencies expressible in first-order logic (e.g., $\forall \mathtt{x}\ \exists^! \mathtt{y}\ \mathtt{Loves}(\mathtt{y}, \mathtt{x})$). Further, unlike in Markov logic, first-order formulas in MEBNs must be hard (and consistent). Laskey and Costa do not specify a language for specifying conditional distributions; they simply assume that a terminating algorithm for computing them exists. Thus the question of what infinite distributions can be specified by MEBNs remains open.

3.6 Conclusion

In this chapter, we extended the semantics of Markov logic to infinite domains using the theory of Gibbs measures. We gave sufficient conditions for the existence and uniqueness of a measure consistent with the local potentials defined by an MLN. We also described the structure of the set of consistent measures when it is not a singleton, and showed how the problem of satisfiability can be cast in terms of MLN measures.

Chapter 4
LAZY INFERENCE

4.1 Introduction

Statistical relational models are defined over objects and relations in the domain of interest, and hence have to support inference over them. We will refer to such domains as relational domains. A straightforward approach to inference in relational domains is to first propositionalize the theory, followed by satisfiability testing. As we will show, MAP/MPE inference in these domains can be reduced to the problem of weighted satisfiability testing. The theory is first propositionalized (e.g., the ground Markov network is created, in the case of Markov logic) and then standard SAT solvers are used over the propositionalized theory. This approach has been given impetus by the development of very fast solvers like WalkSAT [91] and zChaff [68]. Despite its successes, the applicability of this approach to complex relational problems is still severely limited by at least one key factor: the exponential memory cost of propositionalization. To apply a satisfiability solver, we need to create a Boolean variable for every possible grounding of every predicate in the domain, and a propositional clause for every grounding of every first-order clause. If n is the number of objects in the domain and r is the highest clause arity, this requires memory on the order of n^r. Clearly, even domains of moderate size are potentially problematic, and large ones are completely infeasible. This becomes an even bigger problem in the context of learning, where inference has to be performed over and over again. We will revisit this issue in Chapter 6.

In this dissertation, we propose two ways to overcome the problem described above. The first one, described in this chapter, can be characterized as lazy inference. The basic idea in lazy inference is to ground out the theory lazily, creating only those clauses and atoms which are actually considered at the time of the inference. The next chapter will present another technique called lifted inference, which is conceptually similar to the idea of resolution in first-order logic. The key idea in lifted inference is to perform inference together for a set (cluster) of nodes about which we have the same information.

Our approach for lazy inference is based on a property that seems to characterize almost all relational domains: their extreme sparseness. The vast majority of predicate groundings are false, and as a result the vast majority of clauses (all clauses that have at least one false precondition) are trivially satisfied. For example, in the domain of scientific research, most groundings of the predicate $\texttt{Author}(\texttt{person}, \texttt{paper})$ are false, and most groundings of the clause $\texttt{Author}(\texttt{person1}, \texttt{paper}) \wedge \texttt{Author}(\texttt{person2}, \texttt{paper}) \Rightarrow \texttt{Coauthor}(\texttt{person1}, \texttt{person2})$ are satisfied. Our approach is embodied in LazySAT, a variant of WalkSAT that reduces memory while producing the same results. In LazySAT, the memory cost does not scale with the number of possible clause groundings, but only with the number of groundings that are potentially unsatisfied at some point in the search. Clauses that are never considered for flipping literals are never grounded. Experiments on entity resolution and planning problems show that this can yield very large memory reductions, and these reductions increase with domain size. For domains whose full instantiations fit in memory, running time is comparable; as problems become larger, full instantiation for WalkSAT becomes impossible.

Though we describe the lazy inference in the context of purely relational domains and for MAP/MPE inference (using WalkSAT) in statistical relational domains, the technique of lazy inference has been extended to other inference problems, including computing conditional probabilities. See Poon *et al.* [84] for details. We begin the chapter by briefly reviewing some necessary background. We then describe LazySAT in detail, and report on our experiments.

4.2 Relational Inference Using Satisfiability

Satisfiability is the problem of finding an assignment of truth values to the variables that satisfies all the formulas in a knowledge base expressed in CNF (see Chapter 2 for details). The last decade and a half has seen tremendous progress in the development of highly efficient satisfiability solvers. One of the most efficient approaches is stochastic local search, exemplified by the WalkSAT solver [91]. Starting from a random initial state, WalkSAT repeatedly flips (changes the truth value of) a variable in a random unsatisfied clause. With probability p, WalkSAT chooses the variable that minimizes a cost function (such as the number of currently satisfied clauses that become unsatisfied, or the total number of unsatisfied clauses; see Gent & Walsh [31] for discussion), and with probability $1 - p$ it chooses a random variable. WalkSAT keeps going even if it finds a local maximum, and after n

flips restarts from a new random state. The whole procedure is repeated m times. WalkSAT can solve random problems with hundreds of thousands of variables in a fraction of a second, and hard ones in minutes. However, it cannot distinguish between an unsatisfiable CNF and one that takes too long to solve.

The MaxWalkSAT [44] algorithm extends WalkSAT to the weighted satisfiability problem, where each clause has a weight and the goal is to maximize the sum of the weights of satisfied clauses. (Systematic solvers have also been extended to weighted satisfiability, but tend to work less well.) Park [75] showed how the problem of finding the most likely state of a Bayesian network given some evidence can be efficiently solved by reduction to weighted satisfiability. WalkSAT is essentially the special case of MaxWalkSAT obtained by giving all clauses the same weight. For simplicity, in this dissertation we will just treat them as one algorithm, called WalkSAT, with the sum of the weights of *unsatisfied* clauses as the cost function that we seek to minimize. Algorithm 1 gives pseudo-code for WalkSAT. DeltaCost(*v*) computes the change in the sum of weights of unsatisfied clauses that results from flipping variable *v* in the current solution. Uniform(0,1) returns a uniform deviate from the interval $[0, 1]$.

First-order logic (FOL) allows us to explicitly represent a domain's relational structure (see Chapter 2). Objects are represented by constants, and the relations among them by predicates. As mentioned earlier, we make the assumptions of unique names, domain closure and known functions. A predicate or formula is *grounded* by replacing all its variables by constants. *Propositionalization* is the process of replacing a first-order KB by an equivalent propositional one. In finite domains, this can be done by replacing each universally (existentially) quantified formula with a conjunction (disjunction) of all its groundings. A first-order KB is satisfiable iff the equivalent propositional KB is satisfiable. Hence, inference over a first-order KB can be performed by propositionalization followed by satisfiability testing.

Turning now to the problem of inference in statistical relational domains, let us revisit Equation 2.3, which gives the distribution defined by a Markov logic network. The probability of a state x in a ground Markov network can be written as $P(x) = (1/Z) \exp\left(\sum_i w_i f_i(x)\right)$, where Z is the normalization constant, w_i is the weight of the ith clause, $f_i = 1$ if the ith clause is true, and $f_i = 0$ otherwise. Finding the most probable state of a grounded MLN given some evidence is thus an instance of weighted satisfiability.

Algorithm 1 **WalkSAT**(*weighted_clauses*, *max_flips*, *max_tries*, *target*, *p*)

```
vars ← variables in weighted_clauses
for i ← 1 to max_tries do
    soln ← a random truth assignment to vars
    cost ← sum of weights of unsatisfied clauses in soln
    for i ← 1 to max_flips do
        if cost $\leq$ target then
            return “Success, solution is”, soln
        end if
        c ← a randomly chosen unsatisfied clause
        if Uniform(0,1) $<$ p then
            $v_f$ ← a randomly chosen variable from c
        else
            for each variable v in c do
                compute DeltaCost(v)
            end for
            $v_f$ ← v with lowest DeltaCost(v)
        end if
        soln ← soln with $v_f$ flipped
        cost ← cost + DeltaCost($v_f$)
    end for
end for
return “Failure, best assignment is”, best soln found
```

The LazySAT algorithm we develop in this dissertation can be used to scale relational inference to much larger domains than standard WalkSAT. As mentioned earlier, the ideas in LazySAT are also directly applicable to scaling up the computation of marginal and conditional probabilities in statistical relational domains, using Markov chain Monte Carlo algorithms [84].

4.3 Memory-Efficient Inference

The LazySAT algorithm reduces the memory required by satisfiability testing in relational domains by taking advantage of their sparseness. Because the great majority of ground atoms are false, most clauses are satisfied throughout the search, and never need to be considered. LazySAT grounds clauses lazily, at each step in the search adding only the clauses that could become unsatisfied. In contrast, WalkSAT grounds all possible clauses at the outset, consuming time and memory exponential in their arity.

Algorithm 2 gives pseudo-code for LazySAT, highlighting the places where it differs from WalkSAT. LazySAT inputs an MLN (or a pure first-order KB, in which case all clauses are assigned weight 1) and a database (DB). A database is a set of ground atoms. (For example, in planning problems the database is the set of ground atoms describing the initial and goal states. In probabilistic inference, the database is the evidence we condition on.) An *evidence atom* is either a ground atom in the database, or a ground atom that is false by the closed world assumption (i.e., it is a grounding of an evidence predicate, and does not appear in the database). The truth values of evidence atoms are fixed throughout the search, and ground clauses are simplified by removing the evidence atoms. LazySAT maintains a set of *active atoms* and a set of *active clauses*. A clause is active if it can be made unsatisfied by flipping zero or more of its active atoms. (Thus, by definition, an unsatisfied clause is always active.) An atom is active if it is in the initial set of active atoms, or if it was flipped at some point in the search. The initial active atoms are all those appearing in clauses that are unsatisfied if only the atoms in the database are true, and all others are false. We use dynamic arrays to store the active clauses and the atoms in them. The unsatisfied clauses are obtained by simply going through each possible grounding of all the first-order clauses and materializing the groundings that are unsatisfied; search is pruned as soon the partial grounding of a clause is satisfied. Given the initial active atoms, the definition of active clause requires that some clauses become active, and these are found using a similar process (with the difference that, instead of checking whether a ground clause is unsatisfied, we check whether it should be active).[1] Each run of LazySAT is initialized by assigning random truth values to the active atoms. This differs from WalkSAT, which assigns random values to all atoms. However, the LazySAT initialization is a valid WalkSAT initialization, and we have verified experimentally that the two give very similar results. Given the same initialization, the two algorithms will produce exactly the same results.

At each step in the search, the variable that is flipped is activated, as are any clauses that by definition should become active as a result. When evaluating the effect on cost of flipping a variable v, if v is active then all of the relevant clauses are already active, and DeltaCost(v) can be computed as in WalkSAT. If v is inactive, DeltaCost(v) needs to be computed using the knowledge base. (In principle, repeated calculation of this kind can be avoided by activating a variable (and its clauses) when it is first encountered, but we found the time savings from this to be outweighed by the added memory cost.) This is done by retrieving from the KB all first-order clauses containing the predicate that v is a grounding of, and grounding each such clause with the constants in v and all possible groundings of the remaining variables. As before, we prune search as soon as a partial grounding is satisfied, and add the appropriate multiple of the clause weight to DeltaCost(v). (A similar process is used to activate clauses.) While this process is costlier than using pre-grounded clauses, it is amortized over many tests of active variables. In typical satisfiability problems, a small core of "problem" clauses is repeatedly tested, and when this is the case LazySAT will be quite efficient.

At each step, LazySAT flips the same variable that WalkSAT would, and hence the result of the search is the same. The memory cost of LazySAT is on the order of the maximum number of clauses active at the end of a run of flips. (The memory required to store the active atoms is dominated by the memory required to store the active clauses, since each active atom appears in at least one active clause.) In the current version of LazySAT, clauses and atoms are never deactivated, but this could easily be changed to save memory without affecting the output by periodically reinitializing the active sets (using the current truth values of all non-evidence atoms, instead of all false). In our experiments this was not necessary, but it could be quite useful in very long searches.

[1] Although for simplicity the pseudo-code does not show this, the initial set of active clauses and active atoms can be saved and reused for each restart, saving time.

4.4 Experiments

We performed experiments on two entity resolution domains and a planning domain to compare the memory usage and running time of LazySAT and WalkSAT. We implemented LazySAT as an extension of the Alchemy system [48], and used Kautz *et al.*'s (1997) implementation of MaxWalk-SAT, included in Alchemy. When propositionalizing a problem for WalkSAT, we did not ground clauses that are always true given the evidence, and this saved a significant amount of memory. Since the two algorithms can be guaranteed to produce the same results by using the same random initialization for both, we do not report solution quality. In all the experiments we ran WalkSAT and LazySAT for a million flips, with no restarts. The experiments were run on a cluster of nodes, each node having 3.46 GB of RAM and two processors running at 3 GHz. All results reported are averages over five random problem instances.

4.4.1 Entity Resolution

In many domains, the entities of interest are not uniquely identified, and we need to determine which observations correspond to the same entity. For example, when merging databases we need to determine which records are duplicates. This problem is of crucial importance to many large scientific projects, businesses, and government agencies, and has received increasing attention in the AI community in recent years. We will talk about this problem in detail in Chapter 7. We used two publicly available citation databases in our experiments: McCallum's Cora database as segmented by Bilenko and Mooney [4]. This dataset contains 1295 citations and is extracted from the original Cora database of over 50,000 citations. We further cleaned this dataset to fill in some missing values and correct some labels. The cleaned version contained references to 132 distinct research papers and is publicly available on the Alchemy [48] website. Bibserv dataset is available from BibServ.org, which combines CiteSeer, DBLP, and user-donated databases. BibServ contains approximately half a million citations. We used the user-donated subset of BibServ, with 21,805 citations. The inference task was to de-duplicate citations, authors and venues (i.e., to determine which pairs of citations refer to the same underlying paper, and similarly for author fields and venue fields). We used the Markov logic network constructed by Singla and Domingos [93], ignoring clauses with negative weight. Clauses weights were learnt on the Cora dataset using their algorithm and used on both Cora and Bibserv. (We could not learn weights on BibServ because the data is not labeled.)

This contains 33 first-order clauses stating regularities such as: if two fields have high TF-IDF similarity, they are (probably) the same; if two records are the same, their fields are the same, and vice-versa; etc. Crucially, we added the transitivity rule with a very high weight: $\forall x, y, z$ $x = y \wedge y = z \Rightarrow x = z$. This rule is used in an *ad hoc* way in most entity resolution systems, and greatly complicates inference. The highest clause arity, after conditioning on evidence, was three.

We varied the number of records from 50 to 500 in intervals of 50, generating five random subsets of the data for each number of records. We ensured that each real cluster in the data was either completely included in a subset or completely excluded, with the exception of the last one to be added, which had to be truncated to ensure the required number of records. Figure 4.1 shows how the total number of clauses grounded by LazySAT and WalkSAT varies with the number of records. The RAM usage in bytes correlates closely with the number of groundings (e.g., for 250 records WalkSAT uses 2.1 GB, and LazySAT 288 MB). The memory reduction obtained by LazySAT increases rapidly with the number of records. At 250 records, it is about an order of magnitude. Beyond this point, WalkSAT runs out of memory. To extrapolate beyond it, we fitted the function $f(x) = ax^b$ to both curves, obtaining $a = 1.19$, $b = 2.97$ (with $R^2 = 0.99$) for WalkSAT and $a = 6.02$, $b = 2.34$ (with $R^2 = 0.98$) for LazySAT. Using these, on the full Cora database LazySAT would reduce memory usage by a factor of over 300.

Figure 4.2 compares the speed of the two algorithms in average flips per second (i.e., total number of flips over total running time). LazySAT is somewhat faster than WalkSAT for low numbers of records, but by 250 records this advantage has disappeared. Recall that total running time has two main components: initialization, where LazySAT has the advantage, and variable flipping, where WalkSAT does. The relative contribution of the two depends on the problem size and total number of flips. WalkSAT flips variables at a constant rate throughout the search. LazySAT initially flips them slower, on average, but as more clauses become active its flipping rate increases and converges to WalkSAT's.

On BibServ, we formed random subsets of size 50 to 500 records using the same approach as in Cora, except that instead of using the (unknown) real clusters we formed clusters using the canopy approach of McCallum *et al.* [61]. Figure 4.3 shows the number of clause groundings as a function

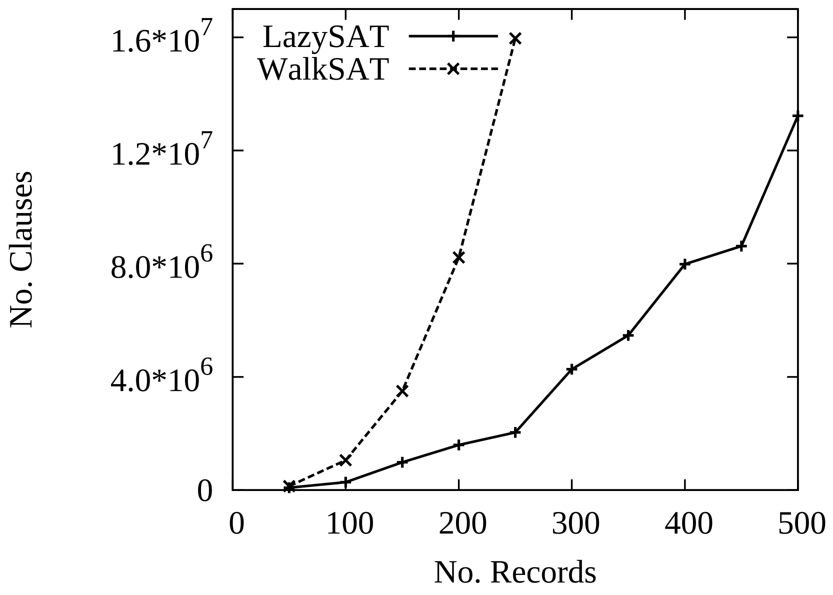


Figure 4.1: Experimental results on Cora: memory as a function of the number of records

of the number of records. RAM usage behaved similarly, being 1.9 GB for WalkSAT and 78 MB for LazySAT at 250 records. As before, WalkSAT runs out of memory at 250 records. LazySAT's memory requirements increase at a much lower rate on this database, giving it a very large advantage over WalkSAT. Fitting the function $f(x) = ax^b$ to the two curves, we obtained $a = 1.02$, $b = 2.98$ (with $R^2 = 0.99$) for WalkSAT and $a = 28.15$, $b = 1.75$ (with $R^2 = 0.98$) for LazySAT. Extrapolating these, on the full BibServ database LazySAT would reduce memory compared to WalkSAT by a factor of over 400,000. The greater advantage of LazySAT on BibServ is directly attributable to its larger size and consequent greater sparseness, and we expect the advantage to be even greater for larger databases. (To see why larger size leads to greater sparseness, consider for example the predicate $\texttt{Author}(\texttt{person}, \texttt{paper})$. When the number of papers and authors increases, its number of true groundings increases only approximately proportionally to the number of papers, while the number of possible groundings increases proportionally to its product by the number of authors. On a database with thousands of authors, the resulting difference can be quite large.)

Figure 4.4 compares the speeds of the two algorithms. They are similar, with LazySAT being slightly faster below 100 objects and WalkSAT slightly faster above.

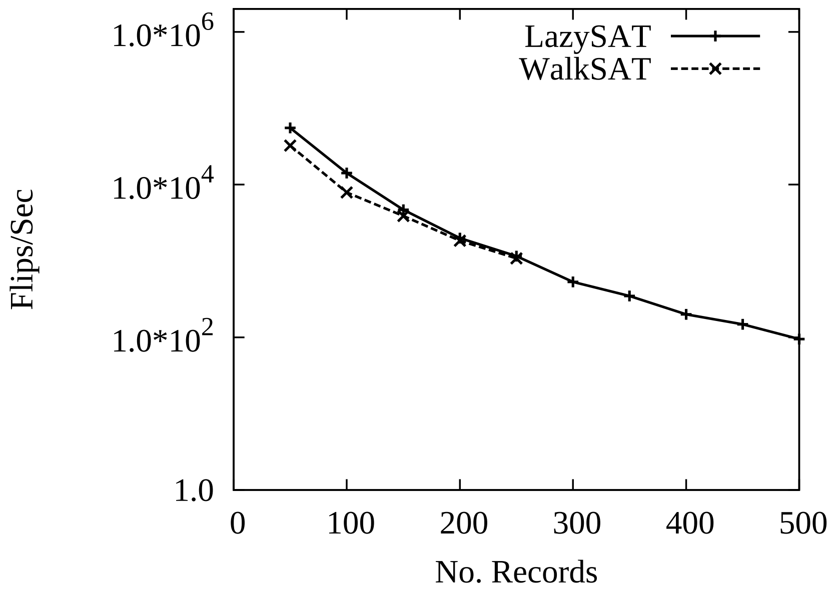


Figure 4.2: Experimental results on Cora: speed as a function of the number of records

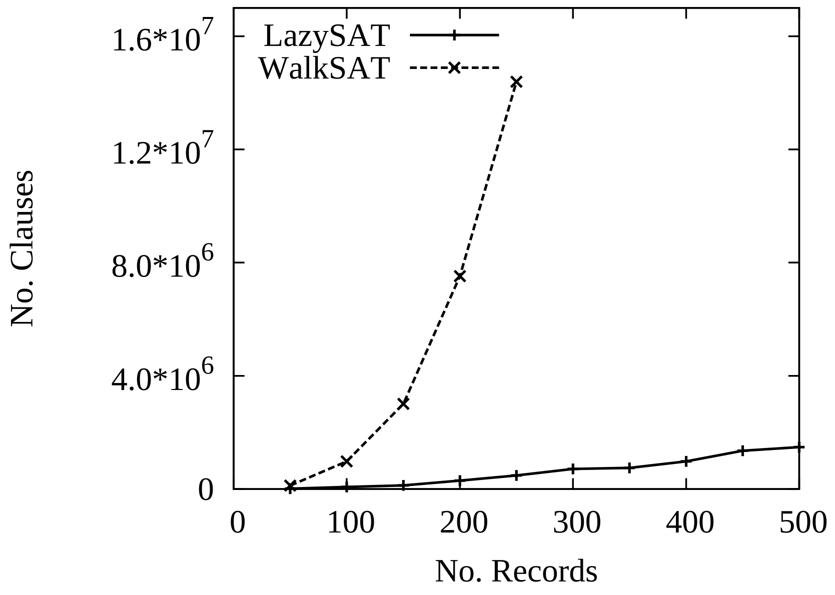


Figure 4.3: Experimental results on Bibserv: memory as a function of the number of records

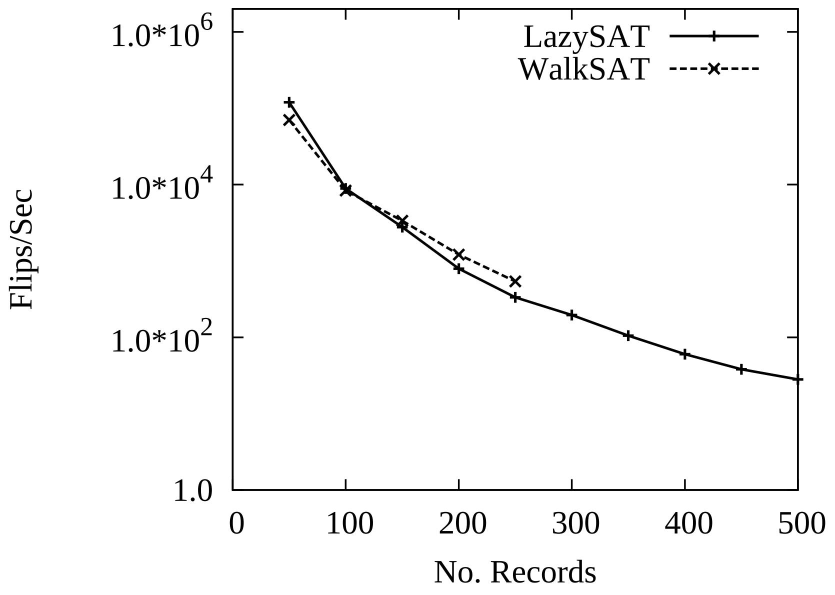


Figure 4.4: Experimental results on Bibserv: speed as a function of the number of records

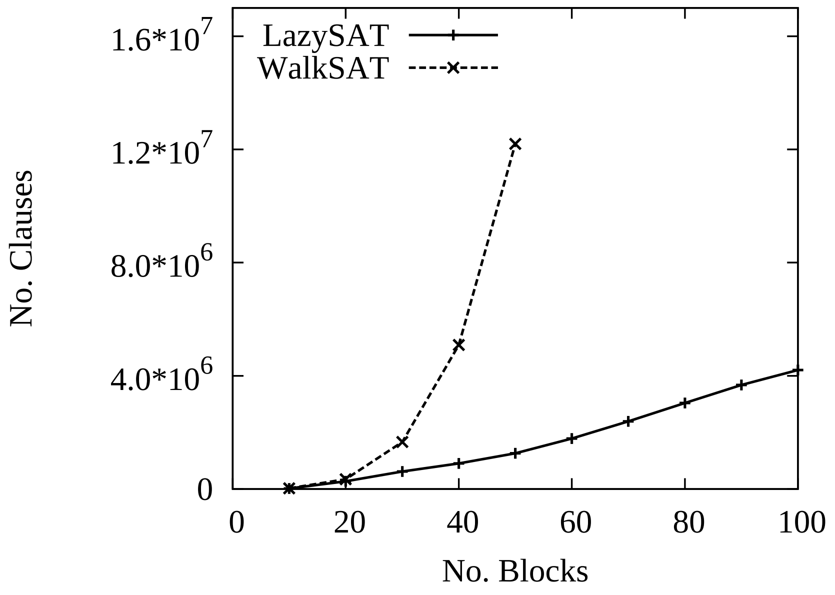


Figure 4.5: Experimental results on blocks world: memory as a function of the number of records

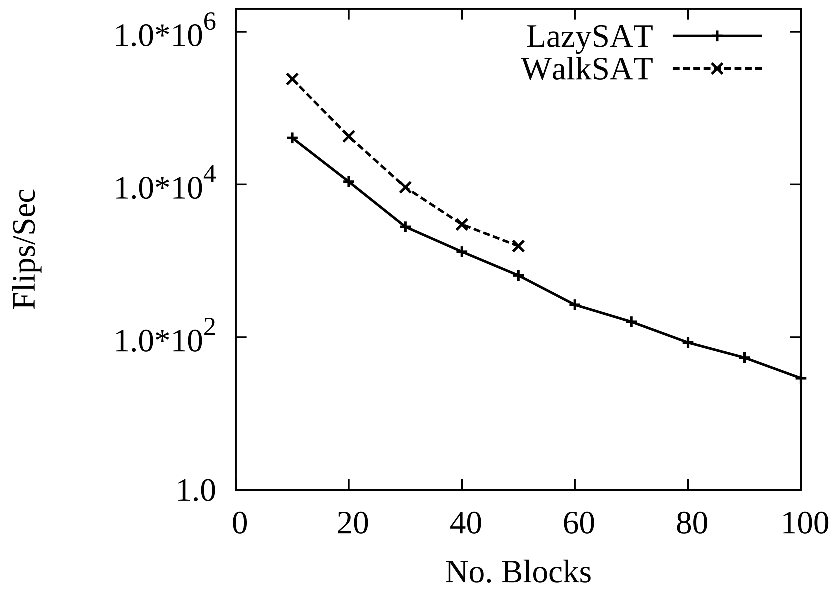


Figure 4.6: Experimental results on blocks world: speed as a function of the number of records

4.4.2 Planning

To compare LazySAT and WalkSAT on a pure (unweighted) satisfiability problem, we experimented on the classical blocks world planning domain, where the goal is to find a sequence of block moves that transforms the initial stacking of blocks into the goal stacking. Kautz & Selman [43] showed how to encode planning problems as instances of satisfiability, by writing formulas that specify action definitions, frame axioms, etc., and using a database of ground atoms to specify the initial state and goal state. We used the formulas they wrote for the blocks world domain (publicly available at http://www.cs.washington.edu/homes/kautz/satplan/blackbox/satplan_dist_2001.tar.Z). The maximum clause arity was four. All the clauses were assigned unit weight. Given a number of blocks, we generated random problem instances as follows. We set the number of stacks in both the initial and goal state to the square root of the number of blocks (truncated to the nearest integer). The stacks were then populated by randomly assigning blocks to them. The number of allowed moves was liberally set to the length of the trivial solution (unstacking and restacking all the blocks). We added rules to allow null moves, making it possible for the algorithms to find shorter plans. We varied the number of blocks from 10 to 100 in increments of 10, and generated five random instances for each.

Figure 4.5 shows how the number of clauses grounded by the two algorithms varies with the number of blocks. LazySAT once again obtains very large reductions. RAM usage closely paralleled the number of clauses, being 1.6 GB for WalkSAT and 203 MB for LazySAT at 50 blocks. WalkSAT is only able to go up 50 blocks, and LazySAT's gain at this size is about an order of magnitude. Fitting the function $f(x) = ax^b$ to the two curves, we obtained $a = 2.79$, $b = 3.90$ (with $R^2 = 0.99$) for WalkSAT, and $a = 1869.58$, $b = 1.68$ (with $R^2 = 0.99$) for LazySAT. The difference in the asymptotic behavior is even more prominent here than in the entity resolution domains.

Figure 4.6 compares the speed of the two algorithms. WalkSAT is somewhat faster, but the difference decreases gradually with the number of blocks.

In all domains, LazySAT reduced memory by an order of magnitude or more at the point that WalkSAT exceeded available RAM. Most importantly, LazySAT makes it feasible to solve much larger problems than before.

4.5 Conclusion

Satisfiability testing is very effective for inference in relational domains, but is limited by the exponential memory cost of propositionalization. The LazySAT algorithm overcomes this problem by exploiting the sparseness of relational domains. Experiments on entity resolution and planning problems show that it greatly reduces memory requirements compared to WalkSAT, without sacrificing speed or solution quality.

Algorithm 2 **LazySAT**(*weighted_KB*, *DB*, *max_flips*, *max_tries*, *target*, *p*)

```
for $i \leftarrow 1$ to $max\_tries$ do
  $active\_atoms \leftarrow$ atoms in clauses not satisfied by $DB$
  $active\_clauses \leftarrow$ clauses activated by $active\_atoms$
  $soln \leftarrow$ a random truth assignment to $active\_atoms$
  $cost \leftarrow$ sum of weights of unsatisfied clauses in $soln$
  for $i \leftarrow 1$ to $max\_flips$ do
    if $cost \leq target$ then
      return "Success, solution is", $soln$
    end if
    $c \leftarrow$ a randomly chosen unsatisfied clause
    if Uniform(0,1) $< p$ then
      $v_f \leftarrow$ a randomly chosen variable from $c$
    else
      for each variable $v$ in $c$ do
        compute DeltaCost($v$), using $weighted\_KB$ if $v \notin active\_atoms$
      end for
      $v_f \leftarrow v$ with lowest DeltaCost($v$)
    end if
    if $v_f \notin active\_atoms$ then
      add $v_f$ to $active\_atoms$
      add clauses activated by $v_f$ to $active\_clauses$
    end if
    $soln \leftarrow soln$ with $v_f$ flipped
    $cost \leftarrow cost +$ DeltaCost($v_f$)
  end for
end for
return "Failure, best assignment is", best $soln$ found
```

Chapter 5
LIFTED INFERENCE

5.1 Introduction

In the last chapter, we talked about lazy inference as a way to avoid fully grounding out the network during inference. But lazy inference still works at the propositional level, in the sense that the units of operation during inference are ground clauses. In contrast, a key property of first-order logic is that it allows *lifted* inference, where queries are answered without materializing all the objects in the domain (e.g., resolution [87]). Lifted inference is potentially much more efficient than propositionalized inference (or for that matter even lazy inference), and extending it to probabilistic logical languages is a desirable goal.

The only approach to lifted probabilistic inference to date was developed by Poole [81] and extended by de S. Braz *et al.* ([20], [21]). (Limited lifted aspects are present in some earlier systems, like Pfeffer *et al.*'s [79] SPOOK.) Poole and Braz *et al.* introduced a lifted version of variable elimination, the simplest algorithm for inference in probabilistic graphical models. Unfortunately, variable elimination has exponential cost in the treewidth of the graph, making it infeasible for most real-world applications. Scalable approximate algorithms for probabilistic inference fall into three main classes: loopy belief propagation (BP), Monte Carlo methods, and variational methods. Jaimovich *et al.* [42] pointed out that, if there is no evidence, BP in probabilistic logical models can be trivially lifted, because all groundings of the same first-order predicates and features become indistinguishable.

In this chapter we develop a general framework for lifting a number of probabilistic inference algorithms including variable elimination and belief propagation. Our approach proceeds by identifying the subsets of nodes and features (groundings of the first-order predicates and features, respectively) that remain indistinguishable even after evidence is taken into account. We call them them *supernodes* and *superfeatures*. The key operations involved in constructing the supernodes and superfeatures are *join* and *project* as defined in the database literature. Supernodes at a given step are joined together to obtain the next round of superfeatures which in turn are projected back to obtain the new supernodes. The algorithm now operates on these constructs rather than the ground nodes and features, thereby saving a large number of repeated calculations. Execution of the inference algorithm may necessitate further splitting of the supernodes and superfeatures, which is done as the execution proceeds.

We first provide the general framework for lifting and then apply it to specific algorithms: bucket elimination [22], which generalizes many inference algorithms, including variable elimination and then to belief propagation and junction tree algorithm. We prove the correctness of our algorithm, showing that it gives exactly the same results as the ground version. In the case of BP, we show that there is a unique minimal lifted network (on which lifted BP can be run) for every inference problem, and that our algorithm returns it. We then extend our algorithm for approximate lifting, which can provide further gains in time and memory efficiency trading off some accuracy. The key idea in approximate lifting is to merge the nodes (features) which are approximately similar to each other. We formalize this notion approximate similarity and describe two ways of constructing the approximate network.

Our method is applicable to essentially any probabilistic logical language, including approaches based on Bayesian networks and Markov networks. We will use Markov logic as a concrete example [86]. Our algorithm is also much simpler than the algorithms of Poole and Braz *et al.* We present the first experimental results for lifted probabilistic inference on a number of real domains. These, and systematic experiments on synthetic problems, show that lifted probabilistic inference can greatly outperform the standard propositionalized version.

5.2 Background

As discussed in Chapter 2, *Graphical models* compactly represent the joint distribution of a set of variables $\mathbf{X} = (X_1, X_2, \ldots, X_n) \in \mathcal{X}$ as a product of factors [77]: $P(\mathbf{X}=\mathbf{x}) = \frac{1}{Z}\prod_k g_k(\mathbf{x}_k)$, where each factor g_k is a non-negative function of a subset of the variables $\mathbf{x}_k$, and Z is a normalization constant. Under appropriate restrictions, the model is a *Bayesian network* and $Z = 1$. The main inference task in graphical models is to compute the conditional probability of some variables (the query) given the values of some others (the evidence), by summing out the remaining variables.

This problem is #P-complete, but becomes tractable if the graph is a tree. A number of inference algorithms (exact as well as approximate) have been proposed in the literature for carrying out inference in graphical models. Next, we will present a few of the important inference algorithms which will become the candidates for our lifting framework in the later part of the chapter.

5.2.1 Bucket Elimination

Bucket elimination [22] is a unifying framework for a variety of inference algorithms. Given a distribution defined over the set of variables $\mathbf{X}$ using a set of factors $\mathbf{g}$, the algorithm proceeds by operating on buckets, where each bucket represents the calculation corresponding to elimination of a variable in set $\mathbf{X}$. In the beginning, we create $n = |V|$ buckets, one for each variable. Some ordering $b_1, b_2, \ldots, b_n$ of the buckets is chosen. The query variable is placed in the lowest bucket, i.e., b_1. Given a factor g, it is placed in the bucket with the highest index such that the corresponding variable appears in g. Bucket elimination now proceeds by eliminating the highest indexed bucket in turn. All the factors in the bucket being eliminated are multiplied to obtain a single factor. Then the variable being eliminated is summed out. The resulting factor is placed in the bucket with the highest index (among the remaining buckets) whose variable appears in the factor. The evidence is handled slightly differently. In the case of evidence variables, there is no need to multiply and sum out. The evidence value is substituted into each factor in the bucket, and the factor simplified. The simplified factor is then placed in the appropriate bucket down the line. The process continues until only the query bucket remains. At this point, all the factors can be multiplied together and the bucket contains the unnormalized probability of the query. The pseudo-code is given in Tables 5.1 and 5.2. Function "AddToBucket" puts the input feature (first argument) into the input bucket (second argument). Function "ElimNode" performs a pointwise multiplication of the potentials represented by the input features, sums the input node (variable) out and returns the resulting feature.

In addition to the problem of estimating probabilities, the bucket elimination framework as described above can be used for various other inference tasks such as MPE estimation, MAP estimation and MEU estimation. This is done by replacing the summation operation in the "ElimNode" function by a maximization operation (MPE), a combination of summation and maximization (MAP) or some other such variant (e.g., MEU). A number of algorithms such as directional resolution for propositional satisfiability, adaptive consistency for constraint satisfaction, Fourier and Gaussian elimination for linear equalities and inequalities, dynamic programming for combinatorial optimization, and Pearl's poly-tree algorithm (when the graph is a tree) turn out to be a special case of bucket elimination. See Dechter [22] for details. Therefore, in lifting bucket elimination, we essentially present a method for lifting all these different inference tasks and algorithms which are expressible in the bucket elimination framework.

5.2.2 *Belief Propagation*

Graphical models can be represented as *factor graphs* [49]. A factor graph is a bipartite graph with a node for each variable and factor in the model. (For convenience, we will consider one factor $g_i(\mathbf{x}) = \exp(w_i f_i(\mathbf{x}))$ per feature $f_i(\mathbf{x})$, i.e., we will not aggregate features over the same variables into a single factor.) Variables and the factors they appear in are connected by undirected edges.

When the graph is a tree, the marginal probabilities of the query variables can be computed in polynomial time by *belief propagation*, which consists of passing messages from variable nodes to the corresponding factor nodes and vice-versa. The message from a variable x to a factor g is

$$\mu_{x \to g}(x) = \prod_{h \in nb(x) \setminus \{g\}} \mu_{h \to x}(x) \tag{5.1}$$

where $nb(x)$ is the set of factors x appears in. The message from a factor to a variable is

$$\mu_{g \to x}(x) = \sum_{\sim\{x\}} \left(g(\mathbf{x}) \prod_{y \in nb(g) \setminus \{x\}} \mu_{y \to g}(y) \right) \tag{5.2}$$

where $nb(g)$ are the arguments of g, and the sum is over all of these except x. The messages from leaf variables are initialized to 1, and a pass from the leaves to the root and back to the leaves suffices. The (unnormalized) marginal of each variable x is then given by $\prod_{h \in nb(x)} \mu_{h \to x}(x)$. Evidence is incorporated by setting $g(\mathbf{x}) = 0$ for states $\mathbf{x}$ that are incompatible with it. This very closely matches with the variable elimination, where each variable being eliminated can be seen as passing a message on the upward link, the root of the tree being the query variable. (Note that no new factors are introduced during variable elimination on trees.) In belief propagation, the algorithm computes the marginal probability of each variable (as opposed to computing the probability of the query only in variable elimination), which is done by sending the messages from the root back to the leaf nodes. This algorithm can still be applied when the graph has loops, repeating the message-passing until convergence. Although this *loopy* belief propagation has no guarantees of convergence or of giving the correct result, in practice it often does, and can be much more efficient than other methods. Different schedules may be used for message-passing. Here we assume *flooding*, the most widely used and generally best-performing method, in which messages are passed from each variable to each corresponding factor and back at each step (after initializing all variable messages to 1).

5.2.3 Junction Tree Algorithm

Belief propagation can also be used for exact inference in arbitrary graphs, by combining nodes until a tree is obtained. Although this suffers from the same combinatorial explosion as variable elimination, it is the basis of the most widely used exact inference algorithm: the junction tree algorithm. In this algorithm, a tree data structure called the junction tree is first constructed [77]. Each node of the junction tree represents a set of nodes in the original graph. A junction tree is characterized by the running intersection property i.e. given two nodes v and w in the junction tree, each node on the unique path between v and w contains the intersection of the nodes represented by v and w. To construct a junction tree, the original graph is first converted into a chordal graph. A chordal graph is a graph containing no chordless cycles. The nodes in the junction tree are simply the maximal cliques in the chordal graph. The construction of the junction tree is analogous to the variable elimination process. Each variable and all its neighbors form a clique, and each maximal clique is connected to a parent clique, typically the one with which it shares the largest number of variables [22]. Each potential is assigned to a node (maximal clique) containing the clique it is over. Each edge (separator) of the junction tree represents the intersection of the two clique nodes it connects. Given a junction tree, the marginals of all the nodes can be now computed using a message passing scheme analogous to the one described in the previous section. Messages are passed from a clique to its neighbor by first summing out the variables not in the separator and then multiplying the new separator marginal into the neighbor's distribution.

5.3 A General Framework for Lifting

We begin with some necessary definitions and theorems. These assume the existence of an MLN $\mathbf{M}$, set of constants $\mathbf{C}$, and evidence database $\mathbf{E}$ (set of ground literals). Given an algorithm $\mathbf{A}$ for manipulating the variables, features and probabilities associated with them, we define the following constructs.

Definition 12. A *supernode* is a set of groundings of a predicate that can be treated as indistinguishable from each other during the execution of algorithm $\mathbf{A}$, given $\mathbf{M}$, $\mathbf{C}$ and $\mathbf{E}$. We say two groundings n_1 and n_2 are indistinguishable if the calculations involved in processing n_1 are identical to the those involved in processing n_2. The supernodes of a predicate form a partition of its groundings.

A *superfeature* is a set of groundings of a clause that all can be treated as indistinguishable from each other during the execution of $\mathbf{A}$, given $\mathbf{M}$, $\mathbf{C}$ and $\mathbf{E}$, where indistinguishable groundings are as defined before. The superfeatures of a clause form a partition of its groundings.

Note that a supernode (superfeature) can be thought of as defining a relation over the domains of the variables appearing in the corresponding predicate (clause). For simplicity, our definitions and explanation of the algorithm will assume that each predicate appears at most once in any given MLN clause. We will then describe how to handle multiple occurrences of a predicate in a clause.

The basis of our lifting framework will be to identify all the nodes which have the same marginal probability. This brings us to the notion of probability equivalence.

Definition 13. *Two ground atoms (nodes) are* probability equivalent *if they have the same marginal probabilities. A supernode N is said to be probability equivalent if each pair of ground atoms in it is probability equivalent.*

The process of lifting in our framework essentially corresponds to starting with a coarse set of supernodes and superfeatures, and then iteratively refining them, so as to separate out the nodes which are not probability equivalent. Lifting allows us to treat all the nodes which can be processed in a similar manner (at any given step of the algorithm) as a group, thereby reducing (as in some cases completely eliminating) the amount of redundant calculation. At the end of the lifting process, we will obtain a set of supernodes which are probability equivalent modulo the inference algorithm, i.e., each ground node in a supernode will have the same probability under the given inference algorithm. To manipulate the supernodes and superfeatures as described above, we will need to define the following basic constructs.

Definition 14. *Given a set of supernodes $\{N_1, N_2, \ldots, N_k\}$ respectively belonging to the set of predicates $\{P_1, P_2, \ \ldots, P_k\}$,* join$(N_1, N_2, \ldots, N_k)$ *returns a relation defined over the domains $D_1, D_2, \ldots, D_l$, where each D_i represents the domain of a variable in the set of unique variables appearing in the predicates $P_1, P_2, \ldots, P_k$. The relation is obtained by forming a cartesian product of the relations defined by the supernodes $N_1, N_2, \ldots, N_k$, and selecting the tuples in which the corresponding arguments agree with each other.*

Definition 15. *Let F be a superfeature and C be the corresponding clause. Given a predicate P appearing in C,* project(F,P) *returns a relation defined over the domains $D_1, D_2, \ldots, D_k$ where D_i's are the domains of the variables appearing in P. The relation is obtained by restricting the tuples in F onto the variables in P. Given a ground atom n_1 corresponding to predicate P, the* projection count *of F onto n_1 is defined as the number of F tuples that results in n_1 when the operation project(F,P) is applied.*

Next, we will define the notion of a stable configuration among a set of supernodes and superfeatures, which will be central to our description of the lifting framework. Intuitively, a set of supernodes and superfeatures are in a stable configuration if (a) the superfeatures can be constructed by joining the supernodes and (b) each ground predicate in a supernode is involved in the same number of the same kind of superfeatures. Formalizing this notion, we give the following definition.

Definition 16. *Let $\mathbf{N}$ be some set of supernodes and $\mathbf{F}$ be the set of superfeatures. We say that $\mathbf{N}$ and $\mathbf{F}$ are in a* stable configuration *with respect to each other if the following conditions are satisfied.*

- *Given a superfeature $F \in \mathbf{F}$, F can be obtained by a join of the supernodes in the set $\{N_1, N_2, \ldots, N_k\}$, where each $N_i \in \mathbf{N}$.*

- *Given any two ground atoms n_1, n_2 belonging to a supernode $N \in \mathbf{N}$, n_1 and n_2 have the same projection counts for every superfeature $F \in \mathbf{F}$.*

To handle clauses with multiple occurrences of a predicate, when projecting superfeatures onto supernodes, a separate count is maintained for each occurrence and the counts have to match up for each occurrence. We are now ready to describe the process of constructing a network of supernodes and superfeatures which are in a stable configuration. Initially, the groundings of each predicate fall into three groups: known true, known false and unknown. (One or two of these may be empty.) Each such group constitutes an initial supernode. All groundings of a clause whose atoms have the same combination of truth values (true, false or unknown) now can be thought of as forming a superfeature. In turn, all ground atoms that appear in the same number of same kind of superfeatures form a supernode. As the effect of the evidence propagates through the network, finer and finer supernodes and superfeatures are created. Thus, the creation of supernodes and superfeatures proceeds by alternating between two steps:

1. Form superfeatures by doing joins of the supernodes.

2. Form supernodes by projecting superfeatures down to their predicates, and merging atoms with the same projection counts.

The first step corresponds to a *join* operation. It takes as input the current set of superfeatures and supernodes and returns the finer set of superfeatures. Each superfeature F is split into finer superfeatures by doing a join over the current set of supernodes. Figure 5.3 presents the pseudo-code. The second step corresponds to the *project* operation. It takes as input the current set superfeatures and returns the finer set of supernodes. For each predicate P, the finer supernodes are obtained by projecting every superfeature in $F \in \mathbf{F}$ onto P and merging those tuples with have the same counts from every superfeature F. Figure 5.4 presents the pseudo-code. Once a stable configuration of supernodes and superfeatures is reached, we perform one step of the original algorithm, i.e., eliminating a variable (a supernode) in case of variable elimination (VE) or passing a message in the case of belief propagation (BP). This advances the algorithm by one step, where is performed at the level of supernodes/superfeatures, thereby saving a large number of repeated calculations. This step in some cases may result in creation of newer supernodes/superfeatures, therefore we may now have to again refine the supernodes and superfeatures to reach a stable configuration. The above two steps of first creating a stable state of supernodes and superfeatures and then advancing the algorithm by one step are thus repeated until the run of the algorithm is complete. We will see the specifics as we describe the details of each algorithm.

In a nutshell, the method for lifting probabilistic inference can be described as consisting of the following steps.

1. **Initialize** the supernodes: For each predicate, create three supernodes, corresponding to the true, false and unknown groundings. Perform other initializations specific to algorithm.

2. **Repeat** the following until convergence. Convergence is declared when the set of superfeatures do not change from the previous iteration.

   - **Join** the supernodes to obtain the refined superfeatures.
   - **Project** the superfeatures to obtain the refined supernodes. (Each refined supernode is such that the ground atoms in it have the same projection counts from each superfeature.)

3. **Advance** the algorithm by one step (e.g., pass the messages in BP, or eliminate one supernode in VE).

4. **Project** the new superfeatures obtained (if any) onto the ground atoms to obtain finer supernodes. Return to step 2 to further refine the supernodes/superfeatures.

Next, we will show how this general framework can be applied to lift some of the very basic algorithms for probabilistic inference, namely variable elimination, belief propagation and junction tree algorithm. But before doing so, we will prove a theorem about obtaining probability equivalent nodes under certain conditions imposed on the tuples on which superfeatures in an MLN are defined. The intuition behind the theorem is that if the supernodes and superfeatures are sufficiently refined, and have a specific structure, wherein the bindings of a variable in a supernode (or a superfeature) take values independent of other variables, then the supernodes provide a probability equivalent decomposition of the ground atoms. (This may not always be the best decomposition, i.e., the one with minimum number of supernodes.)

Definition 17. *Given an MLN M, let F be a superfeature in M and $X_1, X_2, \ldots X_k$ be the variables appearing in F. Let $D_1, D_2 \ldots D_k$ be the corresponding domains. Let $\mathbf{T}_F$ be the set of tuples over* *which F is defined. Given $t = \{x_1, x_2 \ldots x_k\} \in \mathbf{T}_F$, we define t to be a duplicate argument tuple with respect to F if there exists i, j such that $x_i = x_j$ and there is a predicate P in F which has as its arguments both X_i and X_j.*

Theorem 5. *Let M be an MLN in which the supernodes and superfeatures are in a stable configuration. Given a superfeature F in M, let $X_1, X_2, \ldots, X_k$ be the variables appearing in it. Let $D_1, D_2, \ldots, D_k$ be their domains. Let $\mathbf{T}_F$ denote the set of tuples, $\mathbf{T}_F \subseteq D_1 \times D_2 \times \ldots \times D_k$, over which F is defined. Let $\mathbf{T}_F$ be such that it can be expressed as a product of sub-domains of D_1, $D_2 \ldots, D_k$ minus the duplicate argument tuples. If every superfeature in M can be expressed in this form of product of sub-domains minus duplicate argument tuples, then all the supernodes in M are probability equivalent.*

Proof. Let P be a predicate and N be one of its supernodes. Let $F_1, F_2, \ldots, F_n$ be the set of all superfeatures. For clarity of presentation, let us assume that P is binary and let us denote it by $P(X_i, X_j)$. The argument is the same for non-binary predicates as well for the predicates where some of the arguments are repeated, e.g., $P(X, X)$. Let $n_1, n_2 \in N$ be two ground atoms. Without loss of generality, let $n_1 = P(a, b), a \neq b$ and $n_2 = P(c, d), c \neq d$ where a, b, c, d are some constants. Now, the marginal probability of n_1 (or n_2) is calculated by multiplying out the ground features represented by the features $F_1, F_2, \ldots, F_n$ and then summing out everything except n_1 (or n_2). Let us consider the ground feature F_G obtained by multiplying out all the feature instances. Now, since each variable takes values independent of others in each of the superfeatures (since they come from a product of sub-domains) and n_1 and n_2 come from the same supernode, they participate in exactly the same way in the ground feature F_G. Pairs (a, b) and (c, d) can be simply treated as place holders and hence, will eventually result in the same marginal table when summed out. Hence, they have the same marginal probability and hence, are probability equivalent. Since the predicate P and its groundings n_1 and n_2 were chosen arbitrarily, the argument holds for any pair of ground nodes in any supernode. Hence, all the supernodes in M are probability equivalent. $\square$

5.4 Lifted Bucket Elimination

We will now present the lifted version of the bucket elimination algorithm based on our description in Section 5.3. A *supernode* is a set of groundings of a predicate that are placed in one elimination bucket and can be eliminated in one step of the algorithm. A *superfeature* is the set of clauses which together compactly represent the subset of features associated with a particular elimination bucket.

The algorithm for lifted bucket elimination works by maintaining a set of supernodes and superfeatures such that all the atoms in a supernode can be eliminated in one step. As described in the general framework, the initial supernodes consist of three groups for each predicate: known true, known false and unknown. We also create a separate supernode for the query predicate. The supernodes and superfeatures are then iteratively refined to reach a stable configuration. Once a stable configuration of supernodes and superfeatures is reached, we create one bucket for each supernode. We decide an elimination ordering for the buckets. Each superfeature is put in the bucket highest in the order that contains some supernode appearing in the superfeature. We are now ready to eliminate one bucket (and hence the corresponding supernode). We consider two cases. If the supernode is evidence, we do not explicitly need to multiply out the superfeatures in the bucket. We simplify each one of them independently by setting the supernode to the evidence value and simplifying. When the supernode to be eliminated is not evidence, we need to multiply out the factors and sum out the variables being eliminated. We use the machinery developed by de S. Braz [19] do perform this step. In particular, we use inversion elimination, counting elimination or propositionalization as the case may be [19] (Section 3.3).

Inversion elimination works by realizing that there is one to one correspondence between the logical variables in the supernode being eliminated and the variables in the rest of the superfeature. In such cases, the product and the sum operations can be inverted, carrying out the sum first, as if each variable in the superfeature represents a constant (example below). The summation (which is the costly operation) can now be done in time independent of the size of the underlying domain. When inversion elimination is not applicable, counting elimination can be used which works by identifying repeated summations and applying a counting argument over them, instead of carrying them out over and over again. This operation typically depends on the size of the domain but can still exponentially speed up the computation. Counting elimination is applicable when logical variables in different supernodes take values independent of each other. When none of inversion or counting elimination is applicable, standard propositionalization is used.

In both the evidence and no-evidence cases, the new superfeatures replace the old ones in the bucket. Since new superfeatures may now have disturbed the balance of supernodes and superfeatures, we again need to iteratively refine them until convergence. Note that when the underlying graph is a tree (example follows), there is a one-to-one correspondence between the variables in the supernode being eliminated and the superfeature(s). Hence, inversion elimination is applicable. In this case, even after eliminating a supernode, the supernodes and superfeatures are already in a stable configuration and no new supernodes need to be created.

The above two steps of first creating a stable state of supernodes and superfeatures and then eliminating a supernode are repeated in turn (creating new buckets if needed) and eliminating each bucket in turn. The algorithm terminates when we are left with the bucket for the query predicate. The probabilities can be read by multiplying out the superfeatures in the bucket and normalizing. Pseudo-code for the algorithm is shown in Tables 5.5 and 5.6. The function "ElimSuperNode" eliminates a supernode using one of the schemes described above.

Before going any further, let us have a look at an example. Let us say we have an MLN with two rules:

$\texttt{Intelligent}(\texttt{x}) \wedge \texttt{HardWork}(\texttt{x}) \Rightarrow \texttt{GoodPubRecord}(\texttt{x})$

$\texttt{GoodPubRecord}(\texttt{x}) \Rightarrow \texttt{GoodResearch}$

The first rule is saying that if someone is intelligent and if they work hard, then they have a good publication record. Second rule says that if of all people in the domain someone has a good publication record, then good research is happening. For simplicity of notation, we will represent the two rules as, $\texttt{I}(\texttt{x}) \wedge \texttt{H}(\texttt{x}) \Rightarrow \texttt{P}(\texttt{x})$ and $\texttt{P}(\texttt{x}) \Rightarrow \texttt{R}$. Now, let us say that $\texttt{I}(\texttt{x})$ and $\texttt{H}(\texttt{x})$ are evidence and $\texttt{P}(\texttt{x})$ is unknown. We are interested in finding the probability of R being true. Also, let us assume that there 100 people in the domain, represented by the set of constants $\{P_1, P_2 \ldots P_{100}\}$. The first fifty are intelligent and all those with odd indices are hard working (i.e., $P_1, P_3 \ldots P_{99}$). Then the constants corresponding to initial supernodes are: $I^T = \{P_1, P_2, \ldots P_{49}\}$, $I^F = \{P_{50}, P_{51}, \ldots P_{100}\}$, $H^T = \{P_1, P_3, \ldots P_{99}\}$, $H^F = \{P_2, P_4, \ldots P_{100}\}$, $P^U = \{P_1, P_2, \ldots P_{100}\}$, where the letter denotes the predicate name and the superscript denotes the truth value, i.e., true(T), false(F) or unknown(U). R is the query predicate and is unknown. Now, we need to join the supernodes to obtain the superfeatures and then project them back to obtain the finer supernodes. It is easy to see that in a stable configuration the set of supernodes correspond to a four way partition of the set of constants: $S_1 = \{P_1, P_3, \ldots P_{49}\}$ ($\texttt{I}(\texttt{x}) = \texttt{True}, \texttt{H}(\texttt{x}) = \texttt{True}$), $S_2 = \{P_2, P_4, \ldots P_{50}\}$ ($\texttt{I}(\texttt{x}) = \texttt{True}, \texttt{H}(\texttt{x}) = \texttt{False}$), $S_3 = \{P_{51}, P_{53}, \ldots P_{99}\}$ ($\texttt{I}(\texttt{x}) = \texttt{False}, \texttt{H}(\texttt{x}) = \texttt{True}$) and $S_4 = \{P_{50}, P_{52}, \ldots P_{100}\}$ ($\texttt{I}(\texttt{x}) = \texttt{False}, \texttt{H}(\texttt{x}) = \texttt{False}$). Hence there are four supernodes for each of the predicates I, H and P. There is one supernode for the query predicate R. We construct a bucket for each of them. Now, let us choose an ordering such that we eliminate the false supernodes first. The only feature which appears in these buckets is $\texttt{I}(\texttt{x}) \wedge \texttt{H}(\texttt{x}) \Rightarrow \texttt{P}(\texttt{x})$. Whenever any one of the arguments in the antecedents is false, the feature is trivially satisfied and can be ignored. Thus, the buckets corresponding to false nodes can simply be eliminated. Next, let us eliminate the bucket where $\texttt{I}(\texttt{x})$ is true. Simplifying the clause, we obtain $H(x) \Rightarrow P(x)$. This is now added to the bucket for $\texttt{H}(\texttt{x})$ being true. This bucket is eliminated in turn, giving rise to the simplified feature $\texttt{P}(\texttt{x})$. This is now added to the bucket for the supernode $\texttt{P}(\texttt{x})$ defined over the constant set S_1. To recap, we now have four buckets corresponding to the four supernodes for the predicate $\texttt{P}(\texttt{x})$. For three of these (for the sets S_2, S_3 and S_4) the only feature appearing in the bucket is $\texttt{P}(\texttt{x}) \Rightarrow \texttt{R}$. These can be eliminated using inversion elimination [19]. The resulting superfeature is stable with the given set of supernodes and hence no further splitting needs to be done. The resulting feature is now added to the query bucket. The last $\texttt{P}(\texttt{x})$ bucket (for the set S_1) has two features, one from earlier buckets, i.e., $\texttt{P}(\texttt{x})$ and the second one being $\texttt{P}(\texttt{x}) \Rightarrow \texttt{R}$. These can be multiplied together and again inversion elimination can be applied. In this case also, no further splitting of supernodes is needed. In the end, we are left with the query bucket with a set of features which can now be multiplied to give the unnormalized probability of R.

Our approach for doing lifted variable elimination has a number of advantages over the one described in de S. Braz [19]. The first and the key one is that we present our approach in the framework of bucket elimination which is a generalizing framework for many different inference algorithms (see background section). On the other hand, de S. Braz [19] presents its own framework which is quite complicated and hard to follow. Second, shattering is presented as a stand-alone preprocessing step which splits the superfeatures and supernodes (in their terminology parfactors and c-atoms, respectively) into a state where various kinds of inversions can be applied. In contrast, we believe that this refinement is central to the whole lifting process and therefore needs to be closely integrated into the lifting framework. This is reflected in our approach. Lastly, its treatment of the evidence atoms is inadequate. de S. Braz [19] simply says that they can be handled by creating additional parfactors for them. It is not clear whether a separate c-atom is created for each evidence (which can be very costly) or if they are represented using a single (or a few) c-atoms. Also, how these interplay with the rest of the algorithm seems to be missing from the explanation. Our approach clearly describes how evidence is handled.

Theorem 6. Given an MLN $\mathbf{M}$, set of constants $\mathbf{C}$, set of ground literals $\mathbf{E}$ and a query atom $\mathbf{Q}$, the lifted variable elimination algorithm computes the same probability for $\mathbf{Q}$ as the ground variable elimination run on the ground Markov network generated by $\mathbf{M}$ and $\mathbf{C}$.

Proof. It is easy to see that the algorithm for lifted bucket elimination emulates ground bucket elimination except for one key difference: the bucket being eliminated now corresponds to a set of variables rather than a single variable. The algorithm ensures that supernodes and superfeatures are in a stable configuration before each elimination. This guarantees that each superfeature belongs to a well-defined bucket before elimination, namely, the bucket with the highest index whose supernode appears in the superfeature being considered. In terms of the ground version, a supernode bucket can be simply seen as merging together all the buckets for the ground nodes which constitute the supernode. All the corresponding features are also put in the merged bucket. Instead of eliminating all the individual buckets one by one, lifted bucket elimination does that in one step by eliminating the merged bucket (function “ElimSuperNode”). For performing this step, we borrow the machinery of de S. Braz [19] and hence, the correctness of this step follows from the correctness of their algorithm. The resulting supernodes and superfeatures are then split again until a stable configuration is reached. This again guarantees the unique correspondence between a superfeature and the bucket to which it belongs. In turn, each bucket is eliminated in a similar fashion, imitating a series of eliminations in the ground version. After all the buckets except the query are eliminated, the query bucket contains the desired unnormalized probabilities as in the ground version. $\square$

5.5 Lifted Belief Propagation

Now, we will present the lifted version of the belief propagation algorithm. A *supernode* is a set of groundings of a predicate that all send and receive the same messages at each step of belief propagation. A *superfeature* is a set of groundings of a clause that all send and receive the same messages at each step of belief propagation. As in case of lifted VE, our definitions and explanation of the algorithm will assume that each predicate appears at most once in any given MLN clause. We will then describe how to handle multiple occurrences of a predicate in a clause.

It is easy to see that for BP, once the supernodes and superfeatures reach a stable configuration, the message passing step does not change them (as opposed to lifted VE where new superfeatures are created at every elimination step). So, lifted BP can be simply described as consisting of two separate steps. The first step of lifted BP is to construct the minimal lifted network. The second step is to pass messages on the lifted network with few modifications. First, let us describe the construction of the lifted network.

Definition 18. A *lifted BP network* is a factor graph composed of supernodes and superfeatures. The factor corresponding to a superfeature $f(\mathbf{x})$ is $\exp(wf(\mathbf{x}))$, where w is the weight of the corresponding first-order clause. A supernode and a superfeature have an edge between them iff some ground atom in the supernode appears in some ground clause in the superfeature. Each edge has a positive integer weight. A *minimal lifted network* is a lifted network with the smallest possible number of supernodes and superfeatures.

The size of this network is $O(nm)$, where n is the number of supernodes and m the number of superfeatures. In the best case, the lifted network has the same size as the MLN; in the worst case, as the ground Markov network. The second step in lifted BP is to apply standard BP to the lifted network, with two changes:

1. The message from supernode x to superfeature f becomes $\mu_{f\to x}^{n(f,x)-1} \prod_{h\in nb(x)\setminus\{f\}} \mu_{h\to x}(x)^{n(h,x)}$, where $n(h,x)$ is the weight of the edge between h and x.

2. The (unnormalized) marginal of each supernode (and therefore of each ground atom in it) is given by $\prod_{h\in nb(x)} \mu_{h\to x}^{n(h,x)}(x)$.

The weight of an edge is the number of identical messages that would be sent from the ground clauses in the superfeature to each ground atom in the supernode if BP was carried out on the ground network. The $n(f,x)-1$ exponent reflects the fact that a variable's message to a factor excludes the factor's message to the variable.

The lifted network is constructed by (essentially) simulating BP and keeping track of which ground atoms and clauses send the same messages. Pseudo-code for the algorithm is shown in

Table 5.7. The projection counts at convergence are the weights associated with the corresponding edges.

To handle clauses with multiple occurrences of a predicate, we keep a tuple of edge weights, one for each occurrence of the predicate in the clause. A message is passed for each occurrence of the predicate, with the corresponding edge weight. As in case of lifted VE, when projecting superfeatures into supernodes, a separate count is maintained for each occurrence, and only tuples with the same counts for all occurrences are merged.

Theorem 7. Given an MLN $\mathbf{M}$, set of constants $\mathbf{C}$ and set of ground literals $\mathbf{E}$, there exists a unique minimal lifted network $\mathbf{L}^*$, and algorithm LNC($\mathbf{M}$, $\mathbf{C}$, $\mathbf{E}$) returns it. Belief propagation applied to $\mathbf{L}^*$ produces the same results as belief propagation applied to the ground Markov network generated by $\mathbf{M}$ and $\mathbf{C}$.

Proof. We prove each part in turn.

The uniqueness of $\mathbf{L}^*$ is proved by contradiction. Suppose there are two minimal lifted networks $\mathbf{L}_1$ and $\mathbf{L}_2$. Then there exists a ground atom a that is in supernode N_1 in $\mathbf{L}_1$ and in supernode N_2 in $\mathbf{L}_2$, and $N_1 \neq N_2$; or similarly for some superfeature c. Then, by Definition 12, all nodes in N_1 send the same messages as a and so do all nodes in N_2, and therefore $N_1 = N_2$, resulting in a contradiction. A similar argument applies to c. Therefore there is a unique minimal lifted network $\mathbf{L}^*$.

We now show that LNC returns $\mathbf{L}^*$ in two subparts:

1. The network $\mathbf{L}_i$ obtained by LNC at any iteration i is no finer than $\mathbf{L}^*$ in the sense that, if two ground atoms are in different supernodes in $\mathbf{L}_i$, they are in different supernodes in $\mathbf{L}^*$, and similarly for ground clauses.

2. LNC converges in a finite number of iterations to a network $\mathbf{L}$ where all ground atoms (ground clauses) in a supernode (superfeature) receive the same messages during ground BP.

The claim follows immediately from these two statements, since if $\mathbf{L}$ is no finer than $\mathbf{L}^*$ and no coarser, it must be $\mathbf{L}^*$.

For subpart 1, it is easy to see that if it is satisfied by the atoms at the ith iteration, then it is also satisfied by the clauses at the ith iteration. Now, we will prove subpart 1 by induction. Clearly, it is true at the start of the first iteration. Suppose that a supernode N splits into N_1 and N_2 at the ith iteration. Let $a_1 \in N_1$ and $a_2 \in N_2$. Then there must be a superfeature F in the ith iteration such that $T(a_1, F) \neq T(a_2, F)$. Since $\mathbf{L}_i$ is no finer than $\mathbf{L}^*$, there exist superfeatures F_j in $\mathbf{L}^*$ such that $F = \bigcup_j F_j$. Since $T(a_1, F) \neq T(a_2, F)$, $\exists j\ T(a_1, F_j) \neq T(a_2, F_j)$, and therefore a_1 and a_2 are in different supernodes in $\mathbf{L}^*$. Hence $\mathbf{L}_{i+1}$ is no finer than $\mathbf{L}^*$, and by induction this is true at every iteration.

We prove subpart 2 as follows. In the first iteration each supernode either remains unchanged or splits into finer supernodes, because each initial supernode is as large as possible. In any iteration, if each supernode remains unchanged or splits into finer supernodes, each superfeature also remains unchanged or splits into finer superfeatures, because splitting a supernode that is joined into a superfeature necessarily causes the superfeature to be split as well. Similarly, if each superfeature remains unchanged or splits into finer superfeatures, each supernode also remains unchanged or splits into finer supernodes, because (a) if two nodes are in different supernodes they must have different counts from at least one superfeature, and (b) if two nodes have different counts from a superfeature, they must have different counts from at least one of the finer superfeatures that it splits into, and therefore must be assigned to different supernodes.

Therefore, throughout the algorithm supernodes and superfeatures can only remain unchanged or split into finer ones. Because there is a maximum possible number of supernodes and superfeatures, this also implies that the algorithm converges in a finite number of iterations. Further, no splits occur iff all atoms in each supernode have the same counts as in the previous iteration, which implies they receive the same messages at every iteration, and so do all clauses in each corresponding superfeature.

The proof that BP applied to $\mathbf{L}$ gives the same results as BP applied to the ground network follows from Definitions 12 and 18, the previous parts of the theorem, modifications 1 and 2 to the BP algorithm, and the fact that the number of identical messages sent from the ground atoms in a superfeature to each ground atom in a supernode is the cardinality of the projection of the superfeature onto the supernode. $\square$

Clauses involving evidence atoms can be simplified (false literals and clauses containing true literals can be deleted). As a result, duplicate groundings may appear. These are merged with each other while maintaining a count of the duplicates. During the creation of supernodes, $T(s, F)$ is now the number of F tuples projecting into s multiplied by the corresponding duplicate count. This can greatly reduce the size of the lifted network. When no evidence is present, our algorithm reduces to the one proposed by Jaimovich *et al.* [42].

5.6 Lifted Junction Tree Algorithm

The junction tree algorithm consists of two stages, the first one being the construction of the junction tree and the second running message passing on it. The first stage very much resembles the variable elimination algorithm (see background section for details). Hence, the same lifting procedure can be applied. Supernodes and superfeatures are defined in a similar manner. There is no specific query variable, so the query supernode is treated as empty. Further, no evidence is incorporated at this stage of the algorithm. In the step where we advance the variable elimination step by eliminating a supernode, now we also need to construct the corresponding clique of supernodes. This is simply all the neighbors of the supernode being eliminated. The superfeature for a clique node is obtained by point-wise multiplication of potentials represented by the superfeatures in the bucket. For doing this operation efficiently, ideas similar to ones applicable in inversion elimination or counting elimination can be used. As in the ground version, each maximal clique of supernodes is connected to a parent clique node with which it has the maximum intersection. This process will give us a junction tree over the supernodes. Since no evidence has been incorporated yet, each supernode corresponds to the unknown truth value.

Once the junction tree has been constructed, the lifting process for message passing follows the lifted belief propagation algorithm described in Section 5.5. To incorporate the evidence, each supernode obtained during the construction of the junction tree is further split into three bins, based on the truth value. This corresponds to the initialization step. The resulting supernodes are then joined to obtain the new superfeatures. The new superfeatures are then projected back to obtain the refined supernodes. This process is repeated until convergence. One detail that needs to be taken care of is how to assign the refined supernodes and superfeatures to the clique nodes in the junction tree. At each step of refinement, the refined supernodes and superfeatures are simply assigned to the nodes their parents came from. Since we know the initial assignment, this process is well defined.

The messages are then passed over this refined (lifted) junction tree.

Passing messages from the clique (super)nodes in a lifted junction tree to the separator (super)nodes involves summing out certain (super)nodes. Function "ElimSuperNode" can be used to carry out this operation. Elimination of certain supernodes may now result in new superfeatures being constructed. These (and the corresponding supernodes) are refined further until convergence. The refined supernodes and superfeatures are then assigned to the junction tree nodes from which their parents came from. The message passing is then resumed. The process is run until convergence at which point the (super)nodes contain the correct marginals.

5.7 Representation

An important question remains: how to represent supernodes and superfeatures. Although this does not affect the space or time cost of inference on the lifted network (where each supernode and superfeature is represented by a single symbol), it can greatly affect the cost of constructing the lifted network. In general, finding the most compact representation for supernodes and superfeatures is an intractable problem. Here we will describe a few possible approaches.

5.7.1 Extensional Representation

The simplest option is to represent each supernode or superfeature *extensionally* as a set of tuples (i.e., a relation), in which case joins and projections can implemented as standard database operations. However, in this case the cost of constructing the lifted network is similar to the cost of constructing the full ground network, and can easily become the bottleneck. Next, we will describe two approaches which ameliorate this problem.

5.7.2 Resolution-like Representation

A better option is to use a more compact *resolution-like* representation. A ground atom can be viewed as a first-order atom with all variables constrained to be equal to constants, and similarly for ground clauses. (For example, $\mathtt{R}(\mathtt{A},\mathtt{B})$ is $\mathtt{R}(\mathtt{x},\mathtt{y})$ with $\mathtt{x} = \mathtt{A}$ and $\mathtt{y} = \mathtt{B}$.) We represent supernodes by sets of (α, γ) pairs, where α is a first-order atom and γ is a set of constraints, and similarly for superfeatures. Constraints are of the form $x = y$ or $x \neq y$, where x is an argument of the atom and y is either a constant or another argument. For example, $(\mathtt{S}(\mathtt{v},\mathtt{w},\mathtt{x},\mathtt{y},\mathtt{z}),\{\mathtt{w}=\mathtt{x},\mathtt{y}=\mathtt{A},\mathtt{z}\neq\mathtt{B},\mathtt{z}\neq\mathtt{C}\})$ compactly represents all groundings of $\mathtt{S}(\mathtt{v},\mathtt{w},\mathtt{x},\mathtt{y},\mathtt{z})$ compatible with the constraints. Notice that variables may be left unconstrained, and that infinite sets of atoms can be finitely represented in this way.

Let the *default value* of a predicate R be its most frequent value given the evidence (true, false or unknown). Let $\mathbf{S}_{\mathtt{R},i}$ be the set of constants that appear as the ith argument of R only in groundings with the default value. Supernodes not involving any members of $\mathbf{S}_{\mathtt{R},i}$ for any argument i are represented extensionally (i.e. with pairs (α,γ) where γ contains a constraint of the form $\mathtt{x}=\mathtt{A}$, where A is a constant, for each argument x). Initially, supernodes involving members of $\mathbf{S}_{\mathtt{R},i}$ are represented using (α,γ) pairs containing constraints of the form $\mathtt{x}\neq\mathtt{A}$ for each $\mathtt{A}\in\mathbf{C}\setminus\mathbf{S}_{\mathtt{R},i}$.[1] When two or more supernodes are joined to form a superfeature F, if the kth argument of F's clause is the $i(j)$th argument of its jth literal, $\mathbf{S}_k=\bigcap_j \mathbf{S}_{r(j),i}$, where $r(j)$ is the predicate symbol in the jth literal. F is now represented analogously to the supernodes, according to whether or not it involves elements of $\mathbf{S}_k$. If F is represented using resolution-like representation, each (α,γ) pair is divided into one pair for each possible combination of equality/inequality constraints among the clause's arguments, which are added to γ. When forming a supernode from superfeatures, the constraints in each (α,γ) pair in the supernode are the union of (a) the corresponding constraints in the superfeatures on the variables included in the supernode, and (b) the constraints induced by the excluded variables on the included ones.

5.7.3 Hypercube Representation

A third, even more compact option is to use a *hypercube* representation. Each supernode/superfeature is represented be a union of disjoint hypercubes, where each hypercube is simply a cross product of sub-domains of the variables appearing in the supernode/superfeature. Initially, for each supernode (true, false and unknown for each predicate), hypercubes are created by subdividing the tuple set into a union of hypercubes. For example, given a tuple set $\{(\mathtt{X1},\mathtt{Y1}),(\mathtt{X1},\mathtt{Y2}),(\mathtt{X1},\mathtt{Y3}),(\mathtt{X2},\mathtt{Y4}),(\mathtt{X2},\mathtt{Y5})\}$, it can be represented as a union of two hypercubes: $\{\mathtt{X1}\}\times\{\mathtt{Y1},\mathtt{Y2},\mathtt{Y3}\}$ and $\{\mathtt{X2}\}\times\{\mathtt{Y4},\mathtt{Y5}\}$. Notice that this representation can be exponentially more compact than both the exten-

[1]In practice, variables are typed, and $\mathbf{C}$ is replaced by the domain of the argument; and the set of constraints is only stored once, and pointed to as needed.

sional and resolution-like representations. In general, there can be more than one minimal decomposition (one having minimal number) of hypercubes into a set of hypercubes, and finding the best one is an intractable problem. A simple approach to constructing the hypercubes is to proceed bottom-up: start with hypercubes for individual tuples and then repeatedly merge pairs of hypercubes that differ from each other only in one argument. The process stops when no such pair can be found. This process is guaranteed to find some locally minimal decomposition. If the decomposition is not minimal then there is a pair of hypercubes that can be merged and hence the bottom-up merging process has not finished yet. When there is a large number of tuples, this can be very slow. An alternate way is to proceed top-down. First, a bounding hypercube is constructed, i.e., one which includes all the tuples in the set. For example, given the previous example, a choice for bounding hypercube would be $\{\mathtt{X1}, \mathtt{X2}\} \times \{\mathtt{Y1}, \mathtt{Y2}, \mathtt{Y3}, \mathtt{Y4}, \mathtt{Y5}\}$. This is a crude approximation to the set of tuples which need to be represented. The hypercube is then recursively sub-divided so as to split apart tuples from non-tuples. If r_h denotes the ratio of tuples to non-tuples in hypercube h, then the hypercube is divided into two hypercubes h_1 and h_2 such that r_{h_1} and r_{h_2} are as far apart as possible from the original ratio r_h (note that one will be greater and the other will be less that r_h). This is similar to splitting at a node in decision trees, and a similar information gain criterion can be used. The process is continued recursively until we obtain pure hypercubes, i.e., each hypercube either contains all valid tuples or none (in which case it is discarded). The top down process does not guarantee a minimal splitting (since hypercubes from two different branches could potentially be merged). Therefore, once the final set of hypercubes is obtained, we run the bottom-up approach on these to obtain a minimal set.

The join operation is now defined in terms of the hypercubes. When joining two supernodes, we join each possible hypercube pair (each element of the pair coming from the respective supernode). Joining a pair of hypercubes simply corresponds to taking an intersection of the common variables and keeping the remaining remaining ones as is. For example, given $\mathtt{P}(\mathtt{X}, \mathtt{Y})$ and $\mathtt{Q}(\mathtt{Y}, \mathtt{Z})$ defined over the singleton hypercube sets $\{\{\mathtt{X1}, \mathtt{X2}\} \times \{\mathtt{Y1}, \mathtt{Y2}\}\}$ and $\{\{\mathtt{Y1}, \mathtt{Y3}\} \times \{\mathtt{Z1}, \mathtt{Z2}\}\}$, respectively, the joined hypercube set is $\{\{\mathtt{X1}, \mathtt{X2}\} \times \{\mathtt{Y1}\} \times \{\mathtt{Z1}, \mathtt{Z2}\}\}$. Instead of joining each possible pair of hypercubes, an index can be maintained which tells which pairs will have a non-zero intersection.

The project operation projects each of the superfeature hypercube onto the hypercube variables which appear in the predicate being projected on. During the project operation, the counts are now maintained for the set of predicates represented by each hypercube. This presents a problem because different superfeatures may now project onto hypercubes which are neither disjoint nor identical. For example, let us say we have superfeatures $\mathtt{P}(\mathtt{X},\mathtt{Y}) \vee \mathtt{Q}(\mathtt{Y},\mathtt{Z})$ and $\mathtt{P}(\mathtt{X},\mathtt{Y}) \vee \mathtt{R}(\mathtt{Y},\mathtt{Z})$ defined over the hypercube sets $\{\{\mathtt{X1},\mathtt{X2}\} \times \{\mathtt{Y1}\} \times \{\mathtt{Z1},\mathtt{Z2}\}\}$ and $\{\{\mathtt{X1},\mathtt{X2}\} \times \{\mathtt{Y1},\mathtt{Y2}\} \times \{\mathtt{Z1},\mathtt{Z2}\}\}$, respectively. Projecting on the predicate $\mathtt{P}(\mathtt{X},\mathtt{Y})$, the resulting hypercube sets are $\{\{\mathtt{X1},\mathtt{X2}\} \times \{\mathtt{Y1}\}\}$ and $\{\{\mathtt{X1},\mathtt{X2}\} \times \{\mathtt{Y1},\mathtt{Y2}\}\}$, which are neither disjoint nor identical. Therefore, the hypercubes resulting from the project operation have to be split into finer hypercubes such that each pair of resulting hypercubes is either identical with each other or disjoint. This can be done by choosing each intersecting (non-disjoint) pair of hypercubes in turn and splitting them into the intersection, and remaining components. The process continues until each pair of hypercubes is disjoint. In the above example, the finer set of hypercubes to split into would be $\{\{\mathtt{X1},\mathtt{X2}\} \times \{\mathtt{Y1}\}, \{\mathtt{X1},\mathtt{X2}\} \times \{\mathtt{Y2}\}\}$.

5.8 Approximate Lifting

For many applications, refining the supernodes and superfeatures exactly may be too costly in both time and memory. (We will see a few such examples in the experiments section.) In such cases, we can resort to approximate lifting, in which we approximate the construction of supernodes and superfeatures, often trading off some accuracy for time and memory gain. As we will see, these gains come without any loss in accuracy. Here we describe two such approximation schemes.

5.8.1 Early Stopping

During the project and join operations while refining the supernodes and superfeatures, we can stop the refinement process after a certain number of iterations instead of running it until convergence. During the last project operation, no new supernodes are created. We simply adjust the superfeature counts for each supernode as the average of the counts of the ground predicates in them (note that since the refinement process has not converged, the counts will be different in general). Next step of the algorithm is run on these approximate supernodes and superfeatures.

Early stopping is quite useful for domains where the effect of a small amount of evidence propagates through the network rendering each node different from others, while for all practical purposes most of them can be treated as similar to each other. For example, consider a semi-infinite linear chain with evidence at the first node. At iteration i of the refinement process, the i^{th} node falls into a supernode of its own. Nodes at distances greater than i are still in one supernode. Continuing this process until convergence, each node falls into a supernode of its own. However, we know that for all practical probability calculations, nodes a distance greater than n (n being some positive number) can be treated as the same because the stationary distribution is reached. This is due to the fact that effect of evidence dies down as one moves farther away from it. Early stopping makes this approximation possible by stopping the refinement at iteration n. Notice that running exact ground BP in this case would not even terminate constructing the network (since the chain is infinite), whereas lifted BP combined with early stopping gives the desired results after a few iterations. In the experiment section, we will see another example where early stopping can be very useful (denoising a binary image).

5.8.2 Introducing Noise Tolerance During Hypercube Formation

This approximation can be used when the hypercube representation is used for supernodes and superfeatures. During the top-down construction of hypercubes, instead of refining the hypercubes until the end, we stop the process on the way allowing for atmost a certain maximum amount of noise in each hypercube. The goal is to obtain largest possible hypercubes while staying within the noise tolerance threshold. Different measures of noise tolerance can be used. One such measure which is simple to use and does well in practice is the number of tuples not sharing the majority truth value (true/false/unknown) in the hypercube. Depending on the application, other measures can be used.

The above scheme allows for a more compact representation of supernodes (and superfeatures). This potentially leads to gains in both memory and time. The representation is more compact (saving memory) and hence operations can be run faster (saving time). In addition to yielding a more compact representation within each supernode, this approximation also allows the construction of larger supernodes, by virtue of making certain ground predicates probability equivalent which were earlier in different supernodes. These gains come at the cost of some loss in accuracy due to the approximations introduced by noise tolerance. However, as we will see in the experiment section, many a times the loss in accuracy is offset by the gains in both time and memory.

5.9 Experiments

We compared the performance of lifted BP (exact and approximate) with the ground version on five real domains and one artificial domain. We implemented lifted BP as an extension of the open-source Alchemy system [48]. Our algorithm (in the exact case) is guaranteed to produce the same results as the ground version. We report accuracy comparisons for the approximate versions. We used the trained models available from previous research wherever applicable. In other cases, the models were trained using L-BFGS to optimize the pseudo-likelihood of the training data [2], which is quite fast. More complex learning algorithms (like voted perceptron [93]) were used when the simple approach of optimizing pseudo-likelihood did not give good results. In all these cases, exactly the same model was used for testing all the algorithms on any given dataset. Diagnosing the convergence of BP is a difficult problem; we ran it for 1000 steps for all algorithms in all experiments. BP did not always converge. Either way, in the worst case, it was marginally less accurate than Gibbs sampling. The experiments were run on a cluster of nodes, each node having 16 GB of RAM and eight processors running at 2.33 GHz.

5.9.1 Datasets

Entity Resolution

Entity resolution is the problem of determining which observations (e.g., records in a database) correspond to the same objects. This problem is of crucial importance to many large scientific projects, businesses, and government agencies, and has received increasing attention in the AI community in recent years. We used the version of McCallum's Cora database available on the Alchemy website [48]. The dataset contains 1295 citations to 132 different research papers. The inference task was to de-duplicate citations, authors, titles and venues (i.e., to determine which pairs of citations refer to the same underlying paper, and similarly for author, title and venue fields). A TF-IDF-based model was used, as described by Singla and Domingos [93]. This contains 46 first-order clauses stating regularities such as: if two fields have high TF-IDF similarity, they are (probably) the same; if two records are the same, their fields are the same, and vice-versa; etc. The data was divided into 5 splits for cross validation. Voted perceptron (with $\eta = 10^{-5}$ and a Gaussian prior) was used for training the model[2]. Canopies were used to eliminate obvious non-matches [61]

Advising Relationships

We experimented on three different link prediction tasks. Link prediction is an important problem with many applications: social network analysis, law enforcement, bibliometrics, identifying metabolic networks in cells, etc. The first one was to predict the advising relationships between students and professors (task as described in Richardson and Domingos [86]), using the UW-CSE database and MLN publicly available from the Alchemy website [48] [3]. The database is divided into five areas (AI, graphics, etc.). The database contains a total of 2678 groundings of predicates describing whether someone is a student or professor, who has teaches which class, who published which papers, etc. The MLN includes 94 formulas stating regularities like: each student has at most one advisor; if a student is an author of a paper, so is her advisor; etc. The task is to predict who is whose advisor, i.e., the $\mathtt{AdvisedBy}(\mathtt{x},\mathtt{y})$ predicate, from information about paper authorships, classes taught, etc. The model was trained using L-BFGS to optimize pseudo-likelihood; the default parameter settings in Alchemy were used.

Protein Interactions

The second link prediction task was to predict interactions among a set of proteins. The data for the Yeast Protein task come from the MIPS (Munich Information Center for Protein Sequence) Comprehensive Yeast Genome Database as of February 2005 [64]. The data set, originally used in Davis *et al.* [15], includes information on protein location, function, phenotype, class, and enzymes. It also includes information about protein-protein interactions and protein complexes.

The original data contains information about approximately 4500 proteins and their interactions. We used the processed version this dataset as described by Davis and Domingos [16]. This consists of four disjoint subsamples of the original data, each containing around 450 proteins. To create each subsample, starting with a randomly selected seed set of proteins, all previously unselected proteins that appeared within two links (via the interaction predicate) of the seed set were included. The goal

[2]For our experiments, we used the parameters learned on one of the train/test split.

[3]We removed the clauses containing existential qualifiers.

was predict the interaction relation. We used the MLN learned by the Refine algorithm described in Davis and Domingos [16]. In addition to the singleton rule for predicting the interaction relationship, i.e., the $\texttt{Interacts}(\texttt{x}, \texttt{y})$ predicate, the model has three other rules describing how protein functions relate to interactions between them, e.g., two interacting proteins tend to have similar functions.

Hyperlink Analysis

The third and the final link prediction task came from a Web domain where the goal was to predict which Web pages point to each other, given their topics. We used the WebKB data set, which consists of labeled Web pages from the computer science departments of four universities. We used the relational version of the data set from Craven and Slattery [13]. We used only those Web pages for which we had page class information. This contained 1208 Web pages and 10063 Web links. Each Web page is marked with some subset of the following categories: person, student, faculty, department, research project, and course.

A very simple MLN was used with one rule for each ordered pair of classes. The rule states that if a page is of the first class and links to another page, then the linked page is likely to have the second class. An additional rule for stating reflexivity (if A links to B, then B is also likely to link to A) was also incorporated. The model was trained by optimizing pseudo-likelihood using L-BFGS. Default parameter settings in Alchemy (with no prior on weights) were used.

Image Denoising

Image denoising is an important vision problem. This is the problem of removing noise from an image where some of the pixel values have been corrupted. We experimented on a very simple example of a binary image, with some text in the foreground and a given background. We used the image in Bishop ([7], Section 8.3.3), down-sampled to a size of 400 by 400 pixels. We randomly introduced noise in each of the pixels with 10% probability (i.e. noisy pixels were flipped from being in the background to foreground and vice-versa). The MLN consisted of four rules. The first pair of rules stated that the actual value of a pixel is likely to be same as the observed value. The second pairs of rules stated that neighbors are likely to have the same pixel value. As suggested in Bishop [7], the first two rules were given a weight of 2.1 and the last two were given a weight of

1.0. We will refer to it as the Denoise dataset.

Social Networks

We also experimented with the example “Friends and Smokers” MLN in Table **??**. The goal here was to examine how the relative performance of lifted BP and ground BP varies with the number of objects in the domain and the fraction of objects we have evidence about. We varied the number of people from 250 to 2500 in increments of 250, and the fraction of known people KF from 0 to 1. A KF of r means that we know for a randomly chosen r fraction of all people (a) whether they smoke or not and (b) who 10 of their friends are (other friendship relations are still assumed to be unknown). $\texttt{Cancer}(\texttt{x})$ is unknown for all $\texttt{x}$. The people with known information were randomly chosen. The whole domain was divided into a set of friendship clusters of size 50 each. For each known person, we randomly chose each friend with equal probability of being inside or outside their friendship cluster. All unknown atoms were queried. For brevity, we will refer to this domain as FS (short for Friends & Smokers).

5.9.2 Algorithms and Metrics

We compared the performance of the following algorithms on all the datasets.[4] The last two algorithms below implement approximate versions of lifted BP.

- **Ground:** Plain ground version of BP.
- **Extensional:** Lifted BP using explicit representation of supernodes and superfeatures.
- **Resolution:** Lifted BP using resolution-like representation of supernodes and superfeatures.
- **Hypercube:** Lifted BP using the hypercube representation of supernodes and superfeatures.
- **Early Stop:** Lifted BP using the early stopping approximation. Three iterations were used. Unless otherwise mentioned, this is used with the hypercube representation.

[4]For certain datasets, not all the algorithms were compared. These cases will be mentioned specifically in the results section.

- **Noise-Tolerant:** Lifted BP with noise tolerance during the hypercube construction phase. The metric used is the number of tuples that do not have the majority truth value. We used a tolerance level of one.

The above algorithms were compared on the following metrics.

- **Time:** Running time for the algorithm in seconds. Three different times were compared.
  - **Construct:** Time taken to construct the BP network.
  - **BP:** Time taken by the actual run of the BP message passing algorithm.
  - **Total:** Total time taken (sum of the construction and BP running times).
- **Memory:** Memory usage for the algorithm. The following three metrics were used.
  - **Physical:** Actual physical memory used (in megabytes).
  - **Features:** Number of (super)features constructed by the algorithm.
  - **Tuples:** Total number of explicit tuples (or hypercubes) constructed by the algorithm. Note that one superfeature will typically consists of many tuples (or hypercubes).
- **Accuracy:** In the exact case, ground BP and lifted BP are guaranteed to give the same results. Accuracy numbers are a measure of how well BP does on each of the domains. This is also useful for comparing the approximate versions with the exact ones.
  - **CLL:** The conditional log-likelihood (CLL) of a set of predicates is the average over all their groundings of the ground atom's log-probability given the evidence. The advantage of CLL is that it directly measures the quality of the probability estimates produced.
  - **AUC:** The AUC is the area under the precision-recall curve for the query predicates. The advantage of AUC is that it is insensitive to the large number of true negatives (i.e., ground atoms that are false and predicted to be false), that is characteristic of most relational domains.

5.9.3 Results

For each dataset, we present a table of results comparing time, memory and accuracy for the various algorithms described above. For all the datasets, the reported results are the average over the respective splits described in the datasets section. Tables 5.8, 5.9, 5.10, 5.11, 5.12 and 5.13 present the results for the Cora, UW-CSE, Yeast, WebKB, Denoise and FS datasets, respectively. For Denoise, the hypercube representation results in degenerate hypercubes, therefore we simply run the algorithm with single atom hypercubes, which is equivalent to the extensional representation[5]. For FS, we do not report accuracy results, as we did not have the ground truth.

On most datasets, LNC is slower than grounding the full network. WebKB with hypercube representation is an exception where LNC is much faster than grounding out the network. This is due to the structure of the network, where ground predicates can be compactly described (in the beginning of the algorithm) using about a hundred hypercubes, roughly corresponding to each ordered pair of Web page topics. LNC runs over these compact clusters and is thereby much faster. Introducing noise tolerance helps LNC run faster on all domains (outperforming the ground version on Cora and FS). This comes at the cost of some loss in accuracy, as discussed below. All versions of BP are much faster on the lifted network, resulting in better overall times in all domains. On Yeast, the gain is of an order of magnitude, on FS two orders of magnitude, and on WebKB three orders of magnitude. An exception to this is the Denoise dataset. Here running LNC to the end does not give any benefit and degenerates into the ground network. Hence, BP running times are almost the same. But stopping LNC early on Denoise is highly beneficial. This results in order-of-magnitude improvements in running times, with negligible loss in AUC.

On all the datasets, lifted BP has a much smaller number of (super)features. The gain on Cora, UW-CSE and Yeast is five times or more. On UW-CSE, early stopping helps achieve some of this gain, without any compromise in accuracy. On WebKB, the gain is three orders of magnitude, and on FS five orders of magnitude. On Denoise, exact lifting does not give any benefits, as discussed earlier. Early stopping results in a gain more than three orders of magnitude. The reduction in number of superfeatures does not fully translate into reduction in actual memory requirements. The reason is that each superfeature also needs to store the ground tuples inside it, which can be

[5]Owing to this, no separate results are reported for the hypercube representation for Denoise.

degenerate in the worst case. Among the lifted versions of BP, the hypercube version is able to save the most memory (except in Denoise, where early stopping gives good results), using only 50 to 80 percent of the memory used by the ground version. On WebKB, the gain is about 5 times. Introducing noise tolerance helps reduce the memory requirements further, at the cost of some accuracy.

Accuracies for the ground and lifted versions of exact BP are the same. Interestingly, early stopping does not affect the accuracy at all. Denoise is an exception, where CLL is affected, and also AUC to a very small extent. Introducing noise tolerance does result in some loss of accuracy (AUC and/or CLL), but it yields large improvements in time and memory.

We also wanted to analyze how time, memory and accuracy change with varying criteria for early stopping and noise tolerance. To save space, we present these results only for two datasets, one for each of early stopping and noise tolerance. Figures 5.1 and 5.2 show the variations in time and memory, respectively, on Denoise as the number of iterations of LNC is varied from 1 to 10 (10 represents the case of running LNC until convergence). Time increases monotonically with increasing number of iterations. Memory usage is almost constant until six iterations, after which it increases monotonically. The almost constant behavior is due to the fact that very few extra superfeatures are created in the first few iterations. Looking at Figures 5.3 and 5.4, which give the variations in CLL and AUC, we see that both of them converge to the optimum after four iterations. Note that at four iterations, the time and memory requirements of the algorithm are still very small compared to running LNC until the end. Intuitively, this behavior corresponds to how the effect of evidence propagates in the denoising case. Since noise is random, each ground predicate is different from the others in terms of how far it is from various noise pixels and the boundary. So, running LNC until end results in the full ground network. But the actual effect of evidence can be realized in only three to four iterations, at which point most of the nodes can be clustered together, resulting into a much smaller network and a much more efficient denoising algorithm.

Figures 5.5 and 5.6 show the variations in time and memory, respectively, on Yeast as the noise tolerance is varied from zero to five (zero being the exact case). Both decrease monotonically with increasing noise tolerance, as expected. Figures 5.7 and 5.8 show the variations in CLL and AUC, respectively. Increasing noise tolerance does not seem to have any effect on CLL, which stays constant. AUC decreases monotonically, as expected.

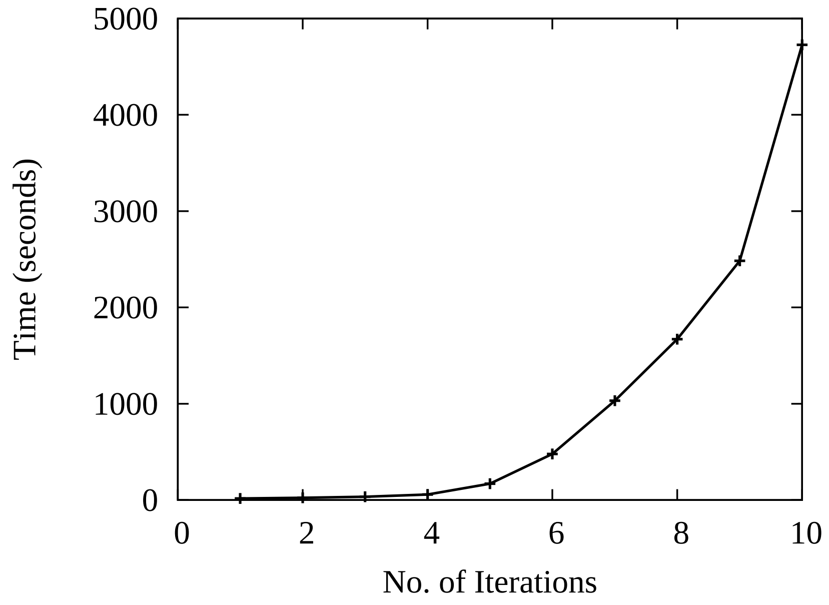


Figure 5.1: Time vs. number of iterations for early stopping on Denoise.

We also conducted experiments on the FS domain varying the number of objects in the domain and the amount of evidence. Figure 5.9 shows how network size varies with the number of people in the FS domain, for $KF = 0.1$. The lifted network is always much smaller, and the difference increases markedly with the number of objects (note the logarithmic scale on the Y axis). The ground version ran out of memory for more than 1250 people. Figure 5.10 shows how the network size varies as we vary KF. (Again, the Y axis is on a logarithmic scale.) The ground network size stays almost the constant, while the lifted network size varies with KF. At very low and very high values of KF, the network is smaller compared to the mid-range values, where the size stays almost constant. This reflects the fact that, at extreme values, many nodes fall into the same supernode (unknown at low values of KF and true/false at high values of KF). The lifted network is always smaller than the ground one by at least four orders of magnitude, rising to five for extreme values of KF.

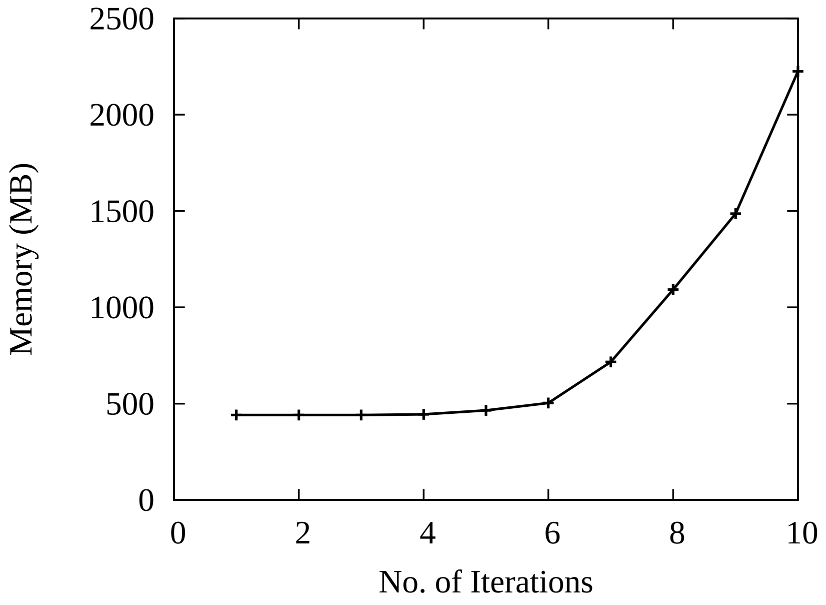


Figure 5.2: Memory vs. number of iterations for early stopping on Denoise.

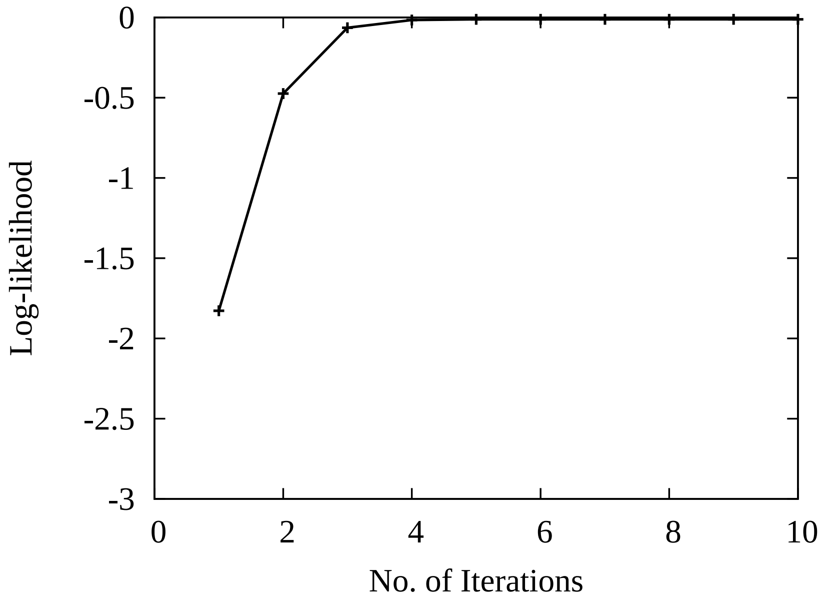


Figure 5.3: Log-likelihood vs. number of iterations for early stopping on Denoise.

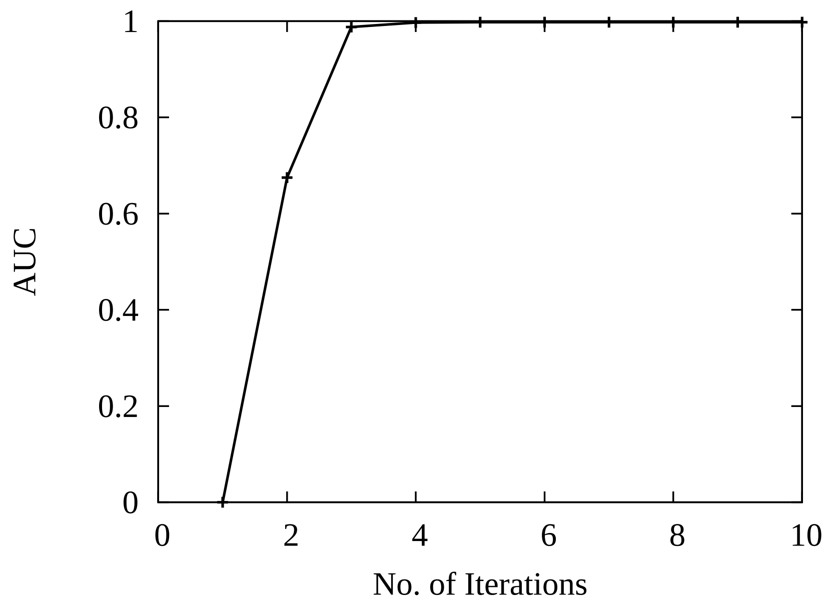


Figure 5.4: AUC vs. number of iterations for early stopping on Denoise.

Table 5.1: Bucket elimination.

```
**function** BE($\mathbf{M}$, $\mathbf{E}$, $Q$)
  **inputs:** $\mathbf{M}$, a Markov network
           $\mathbf{E}$, a set of true/false nodes
           $Q$, query variable
  **output:** $p(\mathbf{Q})$, probability distribution of the query variable
Create a bucket $b_i$ for each node $n_i$
Query $Q$ is put in bucket $b_1$
$\mathbf{f}$ will denote the set of factors and $\mathbf{n}$ the set of variables in $\mathbf{M}$
Choose an ordering $b_2, \ldots, b_k$ for the buckets
Let $B(f)$ be the bucket with highest index among the buckets whose node appears in $f$
**while(**$|B| > 1$**)**
  **for each** factor $f$
    AddToBucket($f$, $B(f)$)
  $n_k$ = supernode in bucket $n_k$ ($k$ being the highest indexed bucket)
  $\mathbf{f_k}$ = superfeatures appearing in bucket $b_k$
  $\mathbf{f}$ = $\mathbf{f} \setminus \mathbf{f_k}$
  $\mathbf{f_k^{new}}$ = $\{\}$
```

Table 5.2: Bucket elimination (contd.).

```
 if $n_k$ is evidence
   for each superfeature $f$ in $\mathbf{f_k}$
     $f \leftarrow$ substitute the evidence value for $n_k$ in $f$ & simplify
     $\mathbf{f_k^{new}} = \mathbf{f_k^{new}} \cup \{f\}$
 else
   $\mathbf{f_k^{new}}$ = ElimNode($\mathbf{f_k}$, $n_k$)
 $\mathbf{f} = \mathbf{f} \cup \mathbf{f_k^{new}}$
done
Multiply out the superfeatures in the query bucket and normalize
return the probability table in query bucket
```

Table 5.3: Join operation

```
function Join($\mathbf{F}$, $\mathbf{N}$)
  inputs: $\mathbf{F}$, a set superfeatures
          $\mathbf{N}$, a set of supernodes
  output: $\mathbf{F^{new}}$, new refined set of superfeatures
$\mathbf{F^{new}}$ = $\{\}$
for each superfeature $F$ involving predicates $P_1, \ldots, P_k$
  $N_1^F, \ldots, N_k^F \leftarrow$ projections of $F$ onto the respective predicates
  for each tuple of supernodes $(N_1, \ldots, N_k)$, where $N_i$ is a $P_i$ supernode and $N_i \subseteq N_i^F$
    form a new superfeature $F^{new}$ by joining $N_1, \ldots, N_k$
    $\mathbf{F^{new}}$ = $\mathbf{F^{new}} \cup F^{new}$
return $\mathbf{F^{new}}$
```

Table 5.4: Project operation

```
**function** Project(**F**)
  **inputs:** **F**, a set superfeatures
  **output:** **N**, new refined set of supernodes
**N** = {}
**for each** predicate $P$
  **for each** superfeature $F$ it appears in
    $S(P, F) \leftarrow$ projection of the tuples in $F$ down to the variables in $P$
    **for each** tuple $s$ in $S(P, F)$
      $T(s, F) \leftarrow$ number of $F$'s tuples that were projected into $s$
  $S(P) \leftarrow \bigcup_F S(P, F)$
  form a new supernode $N$ from each set of tuples in $S(P)$ with the same $T(s, F)$ counts for all $F$
  **N** = **N** $\cup N$
**return** **N**
```

Table 5.5: Lifted bucket elimination.

```
function LBE($\mathbf{M}$, $\mathbf{C}$, $\mathbf{E}$, $Q$)
  inputs: $\mathbf{M}$, a Markov logic network
          $\mathbf{C}$, a set of constants
          $\mathbf{E}$, a set of ground literals
          $Q$, a ground query atom
  output: $\mathbf{P}(Q)$, probability distribution of the query predicate
Create one superfeature $F$ for each clause $C$ containing all the clause groundings
for each predicate $P$
  for each truth value $t$ in $\{$true, false, unknown$\}$
    form a supernode containing all groundings of $P$ with truth value $t$
    create a bucket $b_i$ for the supernode $N_i$
Let $b_1$ be the bucket containing the query node
F will denote the set of superfeatures and N the set of supernodes
while($|B| > 1$)
  repeat
    F = Join(F, N)
    N = Project(F)
  until convergence
  Create a bucket $b_i$ for each supernode $N_i$
  Choose an ordering $b_2, \ldots, b_k$ for the buckets
  Let $B(F)$ be the bucket with highest index among the buckets whose supernode appears in $F$
```

Table 5.6: Lifted bucket elimination (contd.).

```
    for each superfeature $F$
        AddToBucket($F$, $B(F)$)
    $N_k$ = supernode in bucket $b_k$
    $\mathbf{F_k}$ = superfeatures appearing in bucket $b_k$
    $\mathbf{F} = \mathbf{F} \setminus \mathbf{F_k}$
    $\mathbf{F_k^{new}} = \{\}$
    if $N_k$ is evidence
        for each superfeature $F$ in $\mathbf{F_k}$
            $F \leftarrow$ substitute the evidence value for $N_k$ in $F$ and simplify
            $\mathbf{F_k^{new}} = \mathbf{F_k^{new}} \cup \{F\}$
    else
        $\mathbf{F_k^{new}}$ = ElimSuperNode($\mathbf{F_k}$, $N_k$)
    $\mathbf{F} = \mathbf{F} \cup \mathbf{F_k^{new}}$
    $\mathbf{N}$ = Project($\mathbf{M}$,$\mathbf{F}$)
done
Multiply out the superfeatures in the query bucket and normalize
return the probability table in the query bucket
```

Table 5.7: Lifted network construction.

```
function LNC(M, C, E)
  inputs: M, a Markov logic network
          C, a set of constants
          E, a set of ground literals
  output: L, a lifted network
for each predicate $P$
  for each truth value $t$ in {true, false, unknown}
    form a supernode containing all groundings of $P$
      with truth value $t$
repeat
  F = Join(F, N)
  N = Project(F)
until convergence
add all current supernodes and superfeatures to L
for each supernode $N$ and superfeature $F$ in L
  add to L an edge between $N$ and $F$ with weight $T(s, F)$
return L
```

Table 5.8: Results on Cora

Algorithm	**Time (in seconds)**			**Memory**			**Accuracy**	
	Const.	BP	Total	Memory (MB)	Features (1000's)	Tuples (1000's)	CLL	AUC
Ground	10.9	299.3	310.2	138	110.3	110.3	-0.531	0.935
Extensional	14.8	49.0	63.8	137	15.4	110.3	-0.531	0.935
Resolution	15.0	49.1	64.1	138	15.4	110.3	-0.531	0.935
Hypercube	7.4	46.4	53.8	110	15.4	38.3	-0.531	0.935
Early Stop	5.0	30.3	35.4	108	14.4	38.3	-0.531	0.935
Noise-Tol.	5.4	32.3	37.8	102	13.4	20.0	-1.624	0.914

Table 5.9: Results on UW-CSE

Algorithm	**Time (in seconds)**			**Memory**			**Accuracy**	
	Const.	BP	Total	Memory (MB)	Features (1000's)	Tuples (1000's)	CLL	AUC
Ground	1.6	502.0	503.7	101	227.3	227.3	-0.022	0.338
Extensional	7.9	215.7	223.6	193	92.1	227.3	-0.022	0.338
Resolution	8.0	214.8	222.9	193	92.1	227.3	-0.022	0.338
Hypercube	19.2	232.9	252.1	180	92.1	92.4	-0.022	0.338
Early Stop	4.1	100.5	104.6	80	47.6	86.1	-0.022	0.338
Noise-Tol.	8.1	91.6	99.8	76	37.0	37.4	-0.024	0.224

Table 5.10: Results on Yeast

Algorithm	**Time (in seconds)**			**Memory**			**Accuracy**	
	Const.	BP	Total	Memory (MB)	Features (1000's)	Tuples (1000's)	CLL	AUC
Ground	34.8	1743.0	1777.9	426	639.5	639.5	-0.033	0.043
Extensional	75.4	5.9	81.3	443	142.4	639.5	-0.033	0.043
Resolution	77.9	6.1	84.0	443	142.4	639.5	-0.033	0.043
Hypercube	206.8	1.9	208.7	354	142.4	146.4	-0.033	0.043
Early Stop	207.4	1.9	209.3	354	142.4	146.4	-0.033	0.043
Noise-Tol.	97.7	1.3	99.0	304	107.8	100.1	-0.033	0.043

Table 5.11: Results on WebKB

Algorithm	**Time (in seconds)**			**Memory**			**Accuracy**	
	Const.	BP	Total	Memory (MB)	Features (1000's)	Tuples (1000's)	CLL	AUC
Ground	13.3	1333.0	1346.3	393	997.8	997.8	-0.036	0.016
Extensional	26.9	0.8	27.8	285	0.9	997.8	-0.036	0.016
Resolution	27.1	0.8	27.9	287	0.9	997.8	-0.036	0.016
Hypercube	0.1	0.6	0.8	94	0.9	1.0	-0.036	0.016
Early Stop	0.1	0.6	0.8	94	0.9	1.0	-0.036	0.016
Noise-Tol.	0.1	0.6	0.8	94	0.9	1.0	-0.036	0.016

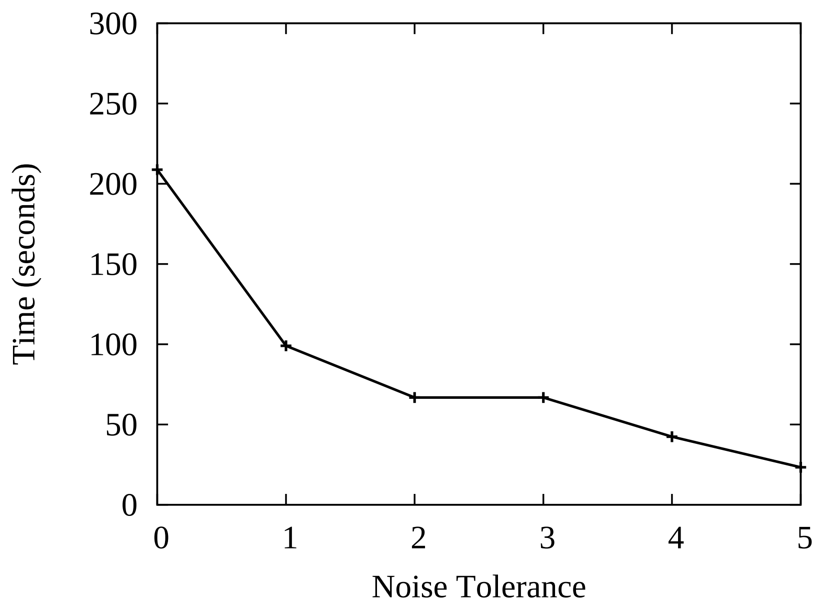
Table 5.12: Results on Denoise

Algorithm	**Time (in seconds)**			**Memory**			**Accuracy**	
	Const.	BP	Total	Memory (MB)	Features (1000's)	Tuples (1000's)	CLL	AUC
Ground	16.7	4389.8	4406.6	748	1269.3	1269.3	-0.011	0.997
Extensional	211.6	4313.6	4525.3	2202	1269.3	1269.3	-0.011	0.997
Resolution	342.1	4289.7	4631.9	2247	1269.3	1269.3	-0.011	0.997
Early Stop	32.7	1.2	34.0	440	0.6	1269.3	-0.064	0.987

Table 5.13: Results on Friends and Smokers

Algorithm	**Time (in seconds)**			**Memory**		
	Const.	BP	Total	Memory (MB)	Features (1000's)	Tuples (1000's)
Ground	22.8	5919.4	5942.2	1873	1093.40	1093.4
Extensional	163.6	0.1	163.7	2074	0.06	1093.4
Resolution	45.2	0.1	45.3	1423	0.06	823.3
Hypercube	52.0	0.1	52.1	1127	0.06	21.0
Early Stop	51.6	0.1	51.7	1127	0.06	21.0
Noise-Tol.	3.0	0.1	3.1	1123	0.04	4.6

Figure 5.5: Time vs. noise tolerance on Yeast.



5.9.4 *Summary*

Lifted BP gives very large gains on a number of real and artificial datasets in terms of total BP running times over the ground version. This is by virtue of constructing a lifted network which is much smaller than the ground network. This also results in substantial gains in memory usage. Stopping early can be quite helpful on some of the domains, without compromising accuracy. Introducing noise tolerance in the hypercube formation phase also helps reduce the time and memory requirements of lifted BP, at the cost of some loss in accuracy.

5.10 Conclusion

We presented a unified framework for lifting probabilistic inference algorithms, and the first application of these to real-world domains. Our method works on supernodes and superfeatures, corresponding to sets of nodes and features that are indistinguishable given the evidence, and applies the underlying probabilistic inference algorithms to them, with few changes to the original algorithm. Our experiments using lifted belief propagation on a number of domains illustrate the efficiency gains obtainable by this method.

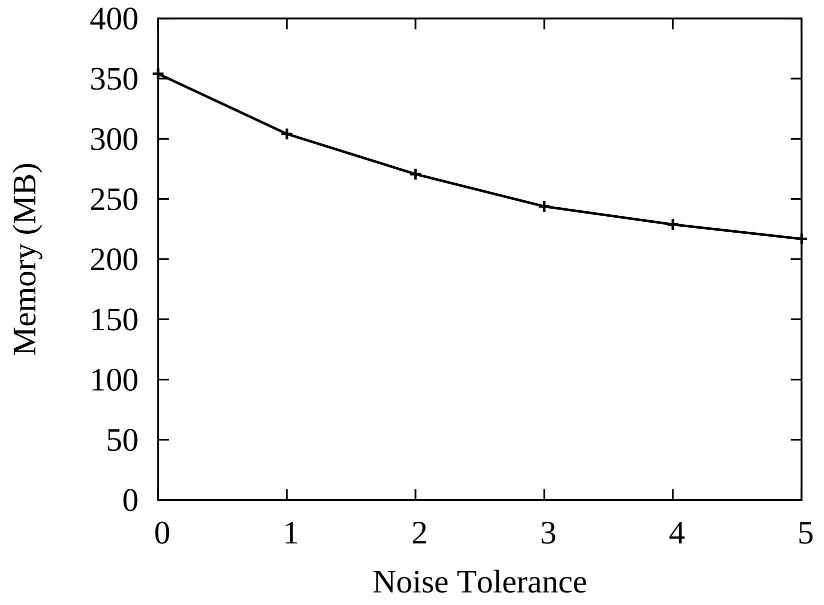


Figure 5.6: Memory vs. noise tolerance on Yeast.

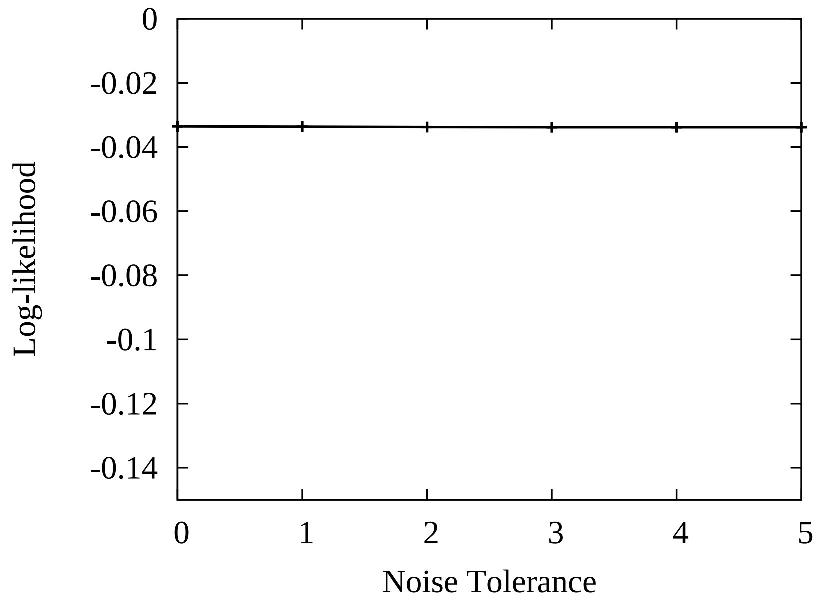
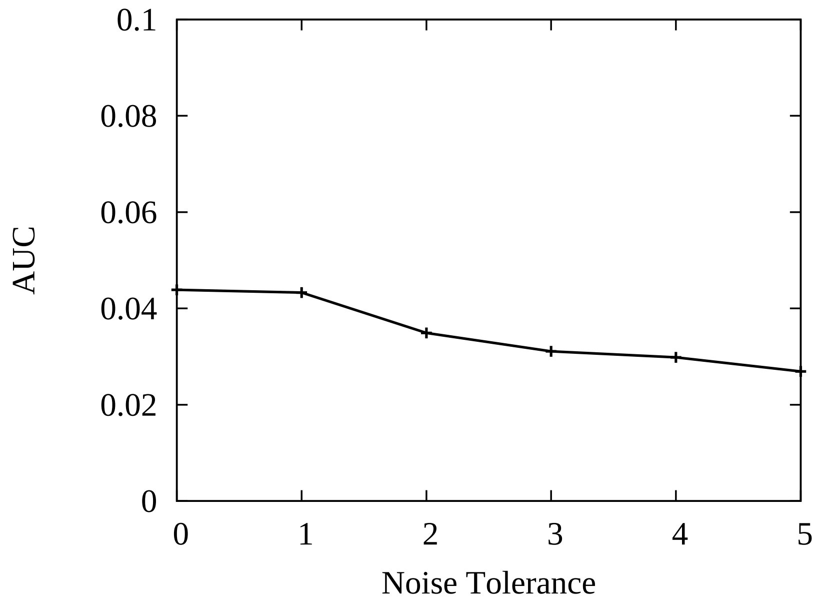


Figure 5.7: Log-likelihood vs. noise tolerance on Yeast.

Figure 5.8: AUC vs. noise tolerance on Yeast.



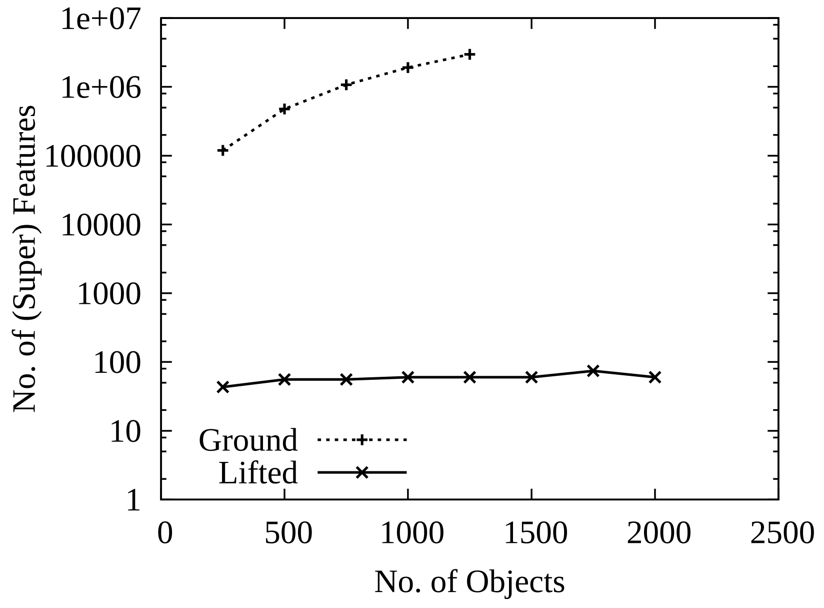


Figure 5.9: Growth of network size on Friends & Smokers domain.

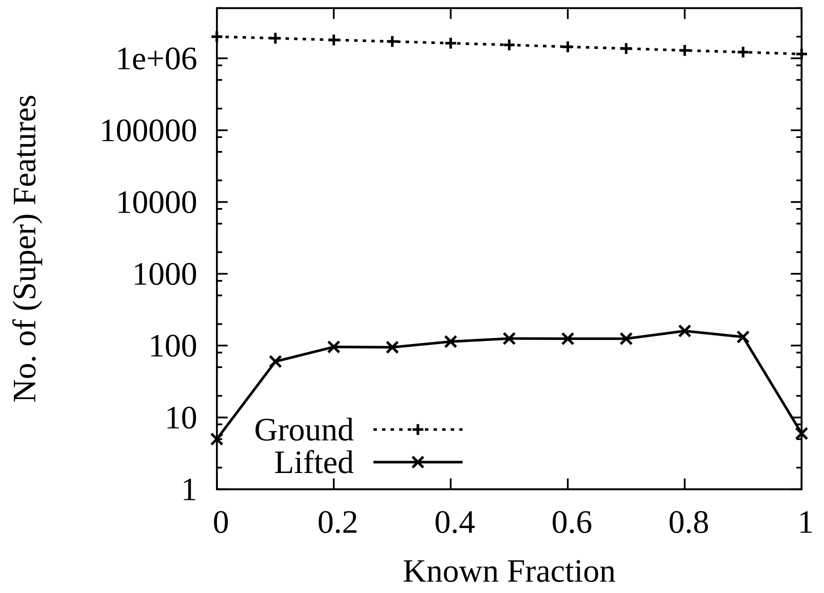


Figure 5.10: Change in known fraction parameter on Friends & Smokers domain.

Chapter 6
PARAMETER LEARNING

6.1 Introduction

Learning the parameters of a Markov logic network involves finding the weights that optimize a likelihood function given the training data. This is a difficult task because computing the likelihood and its gradient requires performing inference, which has worst-case exponential cost. An oft-used alternative is to optimize instead a pseudo-likelihood measure, which involves only each variable's probability given its Markov blanket (graph neighbors) in the data [2]. This is the approach used by Richardson and Domingos [86]. However, the pseudo-likelihood ignores non-local interactions between variables, and may underperform when these need to be taken into account at inference time.

Both likelihood and pseudo-likelihood are generative learning approaches in the sense that they attempt to optimize the joint distribution of all variables. In contrast, discriminative approaches maximize the conditional likelihood of a set of outputs given a set of inputs (e.g., Lafferty *et al.* [50]). This often produces better results, because no effort is spent modeling dependencies between inputs. The voted perceptron is a discriminative algorithm for labeling sequence data, a special case in which tractable inference is possible using the Viterbi algorithm [12]. In this chapter we generalize the voted perceptron to arbitrary Markov logic networks, by replacing the Viterbi algorithm with a weighted satisfiability solver. Experiments in two real-world domains show the promise of this approach.

We should point out that since the time of the research described in this chapter, more sophisticated algorithms (some of them based on second-order methods) for discriminatively learning MLN weights have been proposed. See Lowd and Domingos [59] for details.

We first describe the generative training method. We then describe our algorithm for discriminative learning of MLNs. Finally, we report our experiments.

6.2 Generative Training

MLN weights can be learned generatively by maximizing the likelihood of a relational database (Equation 2.4). (A closed-world assumption is made, whereby all ground atoms not in the database are assumed false.) The gradient of the log-likelihood with respect to the weights is

$$\frac{\partial}{\partial w_i} \log P_w(X = x) = n_i(x) - \sum_{x'} P_w(X = x')\, n_i(x') \tag{6.1}$$

where the sum is over all possible databases x', and $P_w(X = x')$ is $P(X = x')$ computed using the current weight vector $w = (w_1, \ldots, w_i, \ldots)$. In other words, the ith component of the gradient is simply the difference between the number of true groundings of the ith formula in the data and its expectation according to the current model. Unfortunately, computing these expectations requires inference over the model, which can be very expensive. Most fast numeric optimization methods (e.g., conjugate gradient with line search, L-BFGS) also require computing the likelihood itself and hence the partition function Z, which is also intractable. Although inference can be done approximately using Markov chain Monte Carlo, Richardson and Domingos [86] found this to be too slow. Instead, they maximized the pseudo-likelihood of the data, an alternative measure widely used in areas like spatial statistics, social networks and natural language [2]. If x is a possible world (relational database) and x_l is the lth ground atom's truth value, the pseudo-log-likelihood of x given weights w is

$$\log P^*_w(X = x) = \sum_{l=1}^{n} \log P_w(X_l = x_l | MB_x(X_l)) \tag{6.2}$$

where $MB_x(X_l)$ is the state of X_l's Markov blanket in the data (i.e., the truth values of the ground atoms it appears in some ground formula with). Computing the pseudo-likelihood and its gradient does not require inference, and is therefore much faster. However, the pseudo-likelihood parameters may lead to poor results when inference across non-neighboring variables is required.

6.3 Discriminative Training

In many applications, we know *a priori* which predicates will be evidence and which ones will be queried, and the goal is to correctly predict the latter given the former. If we partition the ground atoms in the domain into a set of evidence atoms X and a set of query atoms Y, the *conditional likelihood* of Y given X is

$$\begin{aligned} P(y|x) &= \frac{1}{Z_x} \exp\left(\sum_{i \in F_Y} w_i n_i(x,y) \right) \\ &= \frac{1}{Z_x} \exp\left(\sum_{j \in G_Y} w_j g_j(x,y) \right) \end{aligned} \tag{6.3}$$

where F_Y is the set of all MLN clauses with at least one grounding involving a query atom, $n_i(x,y)$ is the number of true groundings of the ith clause involving query atoms, G_Y is the set of ground clauses in $M_{L,C}$ involving query atoms, and $g_j(x,y) = 1$ if the jth ground clause is true in the data and 0 otherwise. When some variables are "hidden" (i.e., neither query nor evidence) the conditional likelihood should be computed by summing them out, but for simplicity we treat all non-evidence variables as query variables. The gradient of the conditional log-likelihood (CLL) is

$$\begin{aligned} \frac{\partial}{\partial w_i} \log P_w(y|x) &= n_i(x,y) - \sum_{y'} P_w(y'|x) n_i(x,y') \\ &= n_i(x,y) - E_w[n_i(x,y)] \end{aligned} \tag{6.4}$$

As before, computing the expected counts $E_w[n_i(x,y)]$ is intractable. However, they can be approximated by the counts $n_i(x, y_w^*)$ in the MAP state $y_w^*(x)$. This will be a good approximation if most of the probability mass of $P_w(y|x)$ is concentrated around $y_w^*(x)$. Computing the gradient of the CLL now requires only MAP inference to find $y_w^*(x)$, which is much faster than the full conditional inference for $E_w[n_i(x,y)]$. (If the training database is broken up into separate examples, an MAP inference per example is performed.) This approach was used successfully by Collins (2002) in the special case of a Markov network (and hence of an MLN) where the query nodes form a linear chain. In this case, the MAP state can be found in polynomial time using the Viterbi algorithm, a form of dynamic programming [85]. Collins's *voted perceptron* algorithm initializes all weights to zero, performs T iterations of gradient ascent using the approximation above, and returns the parameters averaged over all iterations, $w_i = \sum_{t=1}^{T} w_{i,t}/T$. The parameter averaging helps to combat overfitting. T is chosen using a validation subset of the training data.

Generalizing this solution to arbitrary MLNs requires replacing the Viterbi algorithm with a general-purpose algorithm for MAP inference in MLNs. The form of Equation 6.3 suggests a solution. Since $y^*_w(x)$ is the state that maximizes the sum of the weights of the satisfied ground clauses, it can be found using the MaxWalkSat solver (see the section on logic). Given an MLN and set of evidence atoms, the KB to be passed to MaxWalkSat is formed by constructing all groundings of clauses in the MLN involving query atoms, replacing the evidence atoms in those groundings by their truth values, and simplifying. When hidden variables are present, the algorithm of Richardson and Domingos (2006, Table III) is used. (In practice, it is often convenient to make a closed world assumption on the evidence predicates, whereby all ground predicates not explicitly listed in the evidence database are assumed false.)

Unlike the Viterbi algorithm, MaxWalkSat is not guaranteed to find the global MAP state. This is a potential additional source of error in the weight estimates produced. The quality of the estimates can be improved by running a Gibbs sampler starting at the state returned by MaxWalkSat, and averaging counts over the samples. If the $P_w(y|x)$ distribution has more than one mode, doing multiple runs of MaxWalkSat followed by Gibbs sampling may also be useful. In the limit, this is equivalent to computing the expected counts exactly, which gives us a straightforward way of trading off computational cost and accuracy of estimates.

MaxWalkSat assumes that all weights are positive, while learning can produce negative weights. However, it is easily shown that a formula with a negative weight in a grounded MLN is equivalent to its negation with the symmetric weight. We thus perform this conversion, if necessary, before passing a ground network to MaxWalkSat. The negation of a clause $\bigvee_{i=1}^{n} L_i$, where L_i is a literal, is $\bigwedge_{i=1}^{n} \neg L_i$, a conjunction of n unit clauses. If the original clause's weight is w, we assign a weight of $-w/n$ to each of these unit clauses.

A step of gradient ascent consists of setting $w_{i,t} = w_{i,t-1} + \eta \frac{\partial}{\partial w_i} \log P_w(y|x)|_{w_{t-1}}$. The original voted perceptron algorithm uses a learning rate of $\eta = 1$. In the generalized version, we have found it useful to set this value using a validation set, as is typically done. Weights are initialized to the corresponding clauses' log odds of being true in the data; this tends to produce faster convergence. (Because the optimization problem is convex, the initial state does not affect the solution found.)

6.4 Experiments

6.4.1 Databases

We carried out experiments on two publicly-available databases: the UW-CSE database used by Richardson and Domingos [86], and McCallum's Cora database of computer science citations.

The UW-CSE database describes the relationships between professors, students, courses, publications etc. in the UW computer science department. The dataset has already been described in detail in Chapter 5. We used the hand-coded knowledge base provided with it, which includes 94 formulas stating various regularities. The query atoms are all groundings of $\texttt{AdvisedBy}(\texttt{person1}, \texttt{person2})$, and the evidence atoms are all groundings of all other predicates except $\texttt{Student}(\texttt{person})$ and $\texttt{Professor}(\texttt{person})$, corresponding to the "Partial Information" scenario in Richardson and Domingos [86].

The Cora database is a collection of 1295 different citations to computer science research papers. The details of the dataset have already been described in Chapter 4. We used the hand-coded KB available with the dataset, consisting of 46 clauses stating various regularities.

6.4.2 Systems

We compared three versions of MLN weight learning, applied to the formulas in the hand-coded KB: the voted perceptron algorithm with MaxWalkSat inference, as described in the previous section (MLN(VP)); maximum likelihood using MC-MLE, as described in Richardson and Domingos [86] (MLN(ML)); and pseudo-likelihood, as described in Richardson and Domingos [86] (MLN(PL)). In addition, we compared MLN learning with a pure ILP approach (CLAUDIEN [18] (CL)), a pure knowledge-based approach (the hand-coded KB (KB)), and two pure probabilistic approaches: naive Bayes (NB) [24] and Bayesian networks (BN) [37].

In MLN(VP) training, we used a single run of MaxWalkSat during each learning iteration. In the UW-CSE domain we used $\eta = 0.001$ and $T = 200$. In Cora we used $\eta = 5 \times 10^{-7}$ and $T = 100$. (Cora has a much larger number of query predicates than UW-CSE, necessitating the use of a much smaller learning rate.) Following Richardson and Domingos [86], we trained MLN(PL) and MLN(ML) using L-BFGS with a zero-centered Gaussian prior. We used Gibbs sampling to approximate the function value and gradient for MLN(ML). Running it to convergence was found to be too slow for the learning to complete in any practical amount of time. A single inference did not satisfy the convergence criteria even when run for more than 24 hours. To obtain the estimates in a reasonable time, we limited each Gibbs sampling inference to at most 50,000 passes for burn-in and 500,000 passes for mixing. The total learning time was limited to a maximum of three days. For inference in all the MLN systems, we used a single run of MaxWalkSat to compute the MAP truth values of non-evidence atoms, followed by Gibbs sampling to compute their conditional probabilities given the evidence.

We used the same settings for CLAUDIEN as Richardson and Domingos, and let CLAUDIEN run for 24 hours on a Sun Blade 1000 workstation.[1]

In the UW-CSE domain, we used the algorithm of Richardson and Domingos [86] to construct attributes for the naive Bayes and Bayesian network learners. Following Richardson and Domingos, we tried using order-1 and order-1+2 attributes, and report the best results. In the Cora domain, we used the evidence predicates as attributes (i.e., we predicted whether two fields values are the same from their TF-IDF similarity scores; for the citations, evidence values from all the corresponding fields were used as attributes.).

6.4.3 Methodology

In the UW-CSE domain, we used the same leave-one-area-out methodology as Richardson and Domingos [86]. In the Cora domain, we performed eight-fold cross-validation, ensuring that no true set of matching records was split between folds, to avoid train-test set contamination. For each system on each test set, we measured the conditional log-likelihood (CLL) and area under the precision-recall curve (AUC) for the query predicate. The advantage of the CLL is that it directly measures the quality of the probability estimates produced. The advantage of the AUC is that it is insensitive to the large number of true negatives (i.e., ground atoms that are false and predicted to be false). The CLL of a query predicate is the average over all its groundings of the ground atom's log-probability given the evidence. The precision-recall curve for a predicate is computed by varying the threshold CLL above which a ground atom is predicted to be true. We computed the standard deviations of the AUCs using the method of Richardson and Domingos [86]. To obtain probabilities

[1]CLAUDIEN only runs on Solaris machines.

Table 6.1: Experimental results on the UW-CSE database.

System	CLL	AUC
MLN(VP)	-0.033 ± 0.003	0.295 ± 0.022
MLN(ML)	-0.063 ± 0.004	0.077 ± 0.011
MLN(PL)	-0.034 ± 0.003	0.232 ± 0.024
KB	-0.053 ± 0.004	0.114 ± 0.004
CL	-0.693 ± 0.000	0.006 ± 0.000
NB	-1.237 ± 0.035	0.065 ± 0.000
BN	-0.046 ± 0.002	0.020 ± 0.000

from CL and KB (required to compute CLLs and AUCs) we treated CLAUDIEN's output and the hand-coded KBs as MLNs with all equal infinite weights. We smoothed all probabilities for all systems as in Richardson and Domingos [86].

6.4.4 Results

The results on the UW-CSE domain are shown in Table 6.1. MLNs with discriminative training clearly outperform all the other approaches. The poor results of MLN(ML) are attributable to the fact that learning using non-converged chains of Gibbs sampling produces parameters which are far from optimal. MLN(PL) is only marginally worse than MLN(VP) on CLL but loses substantially on AUC. Purely logical and purely probabilistic approaches all give poor results.

The results on Cora are shown in Tables 6.2 and 6.3. Again, MLNs with discriminative training outperform the other approaches. The performance of MLN(ML) is very poor due to the non-convergence of Gibbs sampling. MLN(PL) performs much worse than MLN(VP) on both CLL and AUC. The purely logical KB performs very poorly. CL performs better than KB, but still much worse than MLN(VP). Among the probabilistic approaches, BN performs marginally better than MLN(VP) on CLL on predicting citations, but significantly worse on AUC. On authors and venues, MLN(VP) outperforms all other approaches on both CLL and AUC.

Table 6.2: CLL results on the Cora database.

System	Citation	Author	Venue
MLN(VP)	-0.069 ± 0.001	-0.069 ± 0.008	-0.232 ± 0.006
MLN(ML)	-13.26 ± 0.013	-12.97 ± 0.086	-13.38 ± 0.034
MLN(PL)	-0.699 ± 0.000	-3.062 ± 0.046	-0.708 ± 0.002
KB	-8.629 ± 0.009	-8.096 ± 0.062	-8.475 ± 0.022
CL	-0.461 ± 0.000	-2.375 ± 0.069	-1.261 ± 0.022
NB	-0.082 ± 0.000	-0.203 ± 0.008	-0.233 ± 0.003
BN	-0.067 ± 0.000	-0.203 ± 0.008	-0.233 ± 0.003

6.5 Conclusion

In this chapter, we presented an algorithm for discriminative learning of MLN parameters. The algorithm is based on the voted perceptron algorithm proposed by Collins for learning HMMs. We generalized it to Markov logic, replacing Viterbi in the Collins algorithm by a weighted satisfiability solver. Our experiments show that this approach outperforms generative learning.

Table 6.3: AUC results on the Cora database.

System	Citation	Author	Venue
MLN(VP)	0.973±0.000	0.969±0.001	0.771±0.003
MLN(ML)	0.111±0.000	0.162±0.000	0.061±0.000
MLN(PL)	0.722±0.001	0.323±0.001	0.342±0.005
KB	0.149±0.000	0.180±0.000	0.096±0.000
CL	0.187±0.000	0.090±0.000	0.047±0.000
NB	0.945±0.000	0.734±0.006	0.339±0.001
BN	0.951±0.000	0.734±0.006	0.339±0.001

Chapter 7

A UNIFIED APPROACH TO ENTITY RESOLUTION

7.1 Introduction

In this chapter and the next, we will describe applications of Markov logic to two important real world problems. The first one, described in this chapter, is the problem of entity resolution. The next chapter describes the application of Markov logic to the problem of identifying social relationships in image collections.

Entity resolution is the problem of identifying which of the references in a given dataset refer to the same underlying entity or object in the real world. These are records that, while not syntactically identical, represent the same real-world entity. For instance, given a citation database, we may be interested in identifying the references that refer to the same underlying paper. These references, though referring to the same paper, may differ from each other, because of variations in the way authors names are written, conference names being abbreviated, spelling mistakes and so on. This problem is known by the name of entity resolution, record linkage, object identification, de-duplication, merge/purge, data association, identity uncertainty, reference reconciliation, and others.

The problem of entity resolution often occurs in the process of data cleaning and preparation which is the first stage in the data mining process, and in most cases it is by far the most expensive. Data from relevant sources must be collected, integrated, scrubbed and pre-processed in a variety of ways before accurate models can be mined from it. When data from multiple databases is merged into a single database, many duplicate records often result. Correctly merging these records and the information they represent is an essential step in producing data of sufficient quality for mining. In recent years this problem has received growing attention in the data mining community, with a related workshop at KDD-2003 [62] and a related task as part of the 2003 KDD Cup [29].

The entity resolution problem was first identified by Newcombe et al. [72], and given a statistical formulation by Fellegi and Sunter [26]. Most current approaches are variants of the Fellegi-Sunter model, in which entity resolution is viewed as a classification problem: given a vector of similarity scores between the attributes of two entities, classify it as “Match” or “Non-match.” A separate match decision is made for each candidate pair, followed by transitive closure to eliminate inconsistencies. Typically, a logistic regression model is used [1]. One line of research has focused on scaling entity resolution to large databases by avoiding the quadratic number of comparisons between all pairs of entities (e.g., [38, 67, 61, 11]). Another has focused on the use of active learning techniques to minimize the need for labeled data (e.g., [100, 89, 5]). Several authors have devised, compared and learned similarity measures for use in entity resolution (e.g., [10, 101, 4]). A number of alternate formulations have also been proposed (e.g., [9]). Entity resolution has been applied in a wide variety of domains (e.g., [74, 17]) and to different types of data, including text (e.g., [55]) and images (e.g., [40]). Winkler [105] surveys research in traditional record linkage.

Most recently, several authors have pointed out that match decisions should not be made independently for each candidate pair. While the Fellegi-Sunter model treats all pairs of candidate matches as i.i.d. (independent and identically distributed), this is clearly not the case, since each entity appears in multiple candidate matches. While this interdependency complicates learning and inference, it also offers the opportunity to improve entity resolution, by taking into account information that was previously ignored. For example, Singla and Domingos [94], Dong *et al.* [25] and Culotta and McCallum [14] allow the resolution of entities of one type to be helped by resolution of entities of related types (e.g., if two papers are the same, their authors are the same, which in turn is evidence that other pairs of papers by the same authors should be matched, etc.). McCallum and Wellner [63] incorporate the transitive closure step into the statistical model. Pasula *et al.* [76] incorporate parsing of entities from citation lists into a citation matching model. Bhattacharya and Getoor [3] use coauthorship relations to help match authors in citation databases. Milch *et al.* [66] propose a language for reasoning about entity resolution. Shen *et al.* [92] exploit various types of constraints to improve matching accuracy. Davis *et al.* [17] use inductive logic programming techniques to discover relational rules for entity resolution, which they then combine using a naive Bayes classifier.

One of the key problems with the approaches described above is that they address isolated aspects of the problem, e.g., transitivity. Further, most of them have been developed as standalone systems, which makes it difficult to compare and combine them with other approaches. Incorporating any new approaches is even more difficult. What is desirable is a unified approach, which is easy to understand and allows us to combine the benefits of various approaches into a single model.

In this chapter we propose a simple and mathematically sound formulation of the entity resolution problem based on Markov logic that incorporates the non-i.i.d. approaches described above, and can be viewed as a generalization of the Fellegi-Sunter model. Our model can seamlessly combine many different approaches by writing a few weighted formulas in Markov logic for each. This allows us to readily use the existing machinery of Markov logic for performing efficient learning and inference. We illustrate this by combining a few salient approaches to entity resolution, and applying the resulting system to a large citation database. We will first describe our proposed approach to entity resolution, followed by our experiments.

7.2 MLNs for Entity Resolution

7.2.1 Equality in Markov Logic

Most systems for inference in first-order logic make the *unique names assumption*: different constants refer to different objects in the domain. This assumption can be removed by introducing the *equality predicate* ($\texttt{Equals}(x, y)$ or $x = y$ for short) and its axioms [30]:

Reflexivity: $\forall x \;\; x = x$.

Symmetry: $\forall x, y \;\; x = y \Rightarrow y = x$.

Transitivity: $\forall x, y, z \;\; x = y \wedge y = z \Rightarrow x = z$.

Predicate equivalence: For each binary predicate R:

$\forall x_1, x_2, y_1, y_2 \;\; x_1 = x_2 \wedge y_1 = y_2 \Rightarrow (R(x_1, y_1) \Leftrightarrow R(x_2, y_2))$. Similar axioms are required for predicates of other arities and for functions, but binary predicates suffice for this dissertation.

Adding the formulas above with infinite weight to an MLN allows it to handle non-unique names. We can also add the reverse of the last one with finite weight:

Reverse predicate equivalence: For each binary predicate R: $\forall x_1, x_2, y_1, y_2 \;\; R(x_1, y_1) \wedge R(x_2, y_2) \Rightarrow (x_1 = x_2 \Leftrightarrow y_1 = y_2)$, and similarly for other arities and functions.

The meaning of this formula is most easily understood by noting that it is equivalent to the two clauses:

$$\forall x_1, x_2, y_1, y_2 \; R(x_1, y_1) \wedge R(x_2, y_2) \wedge x_1 = x_2 \Rightarrow y_1 = y_2$$
$$\forall x_1, x_2, y_1, y_2 \; R(x_1, y_1) \wedge R(x_2, y_2) \wedge y_1 = y_2 \Rightarrow x_1 = x_2$$

As statements in first-order logic, these clauses are false, because different groundings of the same predicate do not generally represent the same tuples of objects. However, when added to an MLN with a finite weight, they capture an important statistical regularity: *if two objects are in the same relation to the same object, this is evidence that they may be the same object*. Some relations provide stronger evidence than others, and this is captured by assigning (or learning) different weights to the formula for different R. For example, when de-duplicating citations, two papers having the same title is stronger evidence that they are the same paper than them having the same author, which in turn is stronger evidence than them having the same venue. However, even the latter is quite useful: two papers appearing in the same venue are much more likely to be the same than two papers about which nothing is known.

Remarkably, *the equality axioms and reverse predicate equivalence are all that is needed to perform entity resolution in Markov logic*. As we will see, despite its simplicity, this formulation incorporates the essential features of some of the most sophisticated entity resolution approaches to date, including the "collective inference" approaches of McCallum and Wellner [63] and Singla and Domingos [94]. A number of other approaches can be incorporated by adding the corresponding formulas. (We emphasize that our goal is not to reproduce every detail of these approaches, but rather to capture their essential features in a simple, consistent form.) Further, entity resolution and data mining can be seamlessly combined, and aid each other, by performing structure learning on top of the entity resolution MLN.

7.2.2 Problem Formulation

We now describe our proposed approach in detail. For simplicity, we assume that the database to be deduplicated contains only binary relations. This entails no loss of generality, because an n-ary relation can always be re-expressed as n binary relations. For example, if a citation database contains ground atoms of the form $\texttt{Paper}(\texttt{title}, \texttt{author}, \texttt{venue})$, they can be replaced by atoms of the form $\texttt{HasTitle}(\texttt{paper}, \texttt{title})$, $\texttt{HasAuthor}(\texttt{paper}, \texttt{author})$ and $\texttt{HasVenue}(\texttt{paper}, \texttt{venue})$. Each real-world entity (e.g., each paper, author or venue) is represented by one or more strings appearing as arguments of ground atoms in the database. For example, different atoms could contain the strings ICDM-2006, Sixth ICDM and IEEE ICDM'06, all of which represent the same conference. We assume that the predicates in the database (representing relations in the real world) are *typed*; for example, the first argument of the predicate $\texttt{HasAuthor}(\texttt{paper}, \texttt{author})$ is of type Paper, and the second is of type Author. The goal of entity resolution is, for each pair of constants of the same type (x_1, x_2), to determine whether they represent the same entity: is $x_1 = x_2$? Thus the query predicate for inference is equality; the evidence predicates are the (binarized) relations in the database, and other relations that can be deterministically derived from the database (see below). The model we use for entity resolution is in the form of an MLN, with formulas and weights that may be hand-coded and/or learned. The most likely truth assignment to the query atoms given the evidence is computed using MaxWalkSAT. Conditional probabilities of query atoms given the evidence are calculated using Gibbs sampling.

The model includes a unit clause for each query predicate. (A unit clause is a clause containing only one literal.) The weight of a unit clause captures (roughly speaking) the marginal distribution of the corresponding predicate, leaving non-unit clauses to capture the dependencies between predicates. Since most groundings of most predicates are usually false (e.g., most pairs of author strings do not represent the same author), it is clearest to use unit clauses consisting of negative literals, with positive weights. Since predicate arguments are typed, there is a unit clause for equality between entities of each type (e.g., $\texttt{paper1} = \texttt{paper2}$, $\texttt{author1} = \texttt{author2}$, etc.). From a discriminative point of view, the weight of a unit clause represents the threshold above which evidence must accumulate for a candidate pair of the corresponding type to be declared a match.

7.2.3 Field Comparison

We assume that each field in a database to be deduplicated is a string composed of one or more words (or, more generally, tokens), and define the predicate $\texttt{HasWord}(\texttt{field}, \texttt{word})$ which is true iff `field` contains `word`. Applied to this predicate, reverse predicate equivalence states that

$$\forall x_1, x_2, y_1, y_2\ \texttt{HasWord}(x_1, y_1) \wedge \texttt{HasWord}(x_2, y_2) \wedge\ y_1 = y_2 \Rightarrow x_1 = x_2$$

or, in other words, fields that have a word in common are more likely to be the same. When inserted into Equation 2.4, and assuming for the moment no other clauses, this clause produces a logistic regression for the field match predicate $x_1 = x_2$ as a function of the number of words n the two fields have in common: $P(x_1 = x_2 \mid n) = 1/(1 + e^{-wn})$, where w is the weight of the formula. Effectively, then, reverse predicate equivalence applied to $\texttt{HasWord}()$ implements a simple similarity measure between fields. This measure can be made adaptive, in the style of Bilenko and Mooney [4], by learning a different weight for each grounding of reverse predicate equivalence with a different word. (Groundings where $y_1 \neq y_2$ are always satisfied, and therefore their weights cancel out in the numerator and denominator of Equation 2.4, and are irrelevant. Reflexivity ensures the proper treatment of groundings where $y_1 = y_2$.)

It can also be useful to add the "negative" version of reverse predicate equivalence:

$$\forall x_1, x_2, y_1, y_2\ \neg\texttt{HasWord}(x_1, y_1) \wedge \texttt{HasWord}(x_2, y_2) \wedge\ y_1 = y_2 \Rightarrow x_1 \neq x_2$$

$$\forall x_1, x_2, y_1, y_2\ \texttt{HasWord}(x_1, y_1) \wedge \neg\texttt{HasWord}(x_2, y_2) \wedge\ y_1 = y_2 \Rightarrow x_1 \neq x_2$$

$$\forall x_1, x_2, y_1, y_2\ \neg\texttt{HasWord}(x_1, y_1) \wedge \neg\texttt{HasWord}(x_2, y_2) \wedge\ y_1 = y_2 \Rightarrow x_1 = x_2$$

Like other word-based similarity measures, this approach has the disadvantage that it treats misspellings, variant spellings and abbreviations of a word as completely different words. Since these are often a significant issue in entity resolution, it would be desirable to account for them. One way to do this efficiently is to compare word strings by the engrams they contain [36]. This can be done in our framework by defining the predicate $\texttt{HasEngram}(\texttt{word}, \texttt{engram})$, which is true iff `engram` is a substring of `word`. (This predicate can be computed on the fly from its arguments, or pre-computed for all relevant word-engram pairs and given as evidence.) Applying reverse predicate equivalence to this predicate results in a logistic regression model for the equality of two words as a function of the number of engrams they have in common. Combined with the logistic regression for field equality, this produces a two-level similarity measure, comparing fields as sets of words, which are in turn compared as strings. Cohen *et al.* [10] found such hybrid measures to outperform pure word-based and pure string-based ones for entity resolution. The maximum length of engrams to consider is a parameter of the problem. Linear-interpolation smoothing is obtained by defining different predicates for engrams of different length, with the corresponding weights for the corresponding versions of reverse predicate equivalence. (These can also be learned, using weight priors to avoid overfitting.) It is also possible to incorporate string edit distances like Levenshtein and Needleman-Wunsch [4] into an MLN. This involves stating formulas analogous to the recurrence relations used to compute these distances, with (negative) weights corresponding to the costs of insertion, deletion, etc. Pursuing this approach is an item for future work.

7.2.4 *The Fellegi-Sunter Model*

The Fellegi-Sunter model uses naive Bayes to predict whether two records are the same, with field comparisons as the predictors [26]. If the predictors are the field match predicates, Fellegi-Sunter is a special case of reverse predicate equality, with R as the relation between a field and the record it appears in (e.g., $\mathtt{HasAuthor}(\mathtt{paper}, \mathtt{author})$). If the predictors are field similarities, measured by the number of words present in both, either and none of the fields, Fellegi-Sunter is implemented by clauses of the form

$$\forall x_1, x_2, y_1, y_2 \;\; \mathtt{HasWord}(x_1, y_1) \wedge \mathtt{HasWord}(\mathtt{x_2}, \mathtt{y_2}) \wedge \; y_1 = y_2 \wedge R(z_1, x_1) \wedge R(z_2, x_2) \\ \Rightarrow z_1 = z_2$$

$$\forall x_1, x_2, y_1, y_2 \;\; \neg\mathtt{HasWord}(x_1, y_1) \wedge \mathtt{HasWord}(\mathtt{x_2}, \mathtt{y_2}) \wedge \; y_1 = y_2 \wedge R(z_1, x_1) \wedge R(z_2, x_2) \\ \Rightarrow z_1 \neq z_2$$

$$\forall x_1, x_2, y_1, y_2 \;\; \mathtt{HasWord}(x_1, y_1) \wedge \neg\mathtt{HasWord}(\mathtt{x_2}, \mathtt{y_2}) \wedge \; y_1 = y_2 \wedge R(z_1, x_1) \wedge R(z_2, x_2) \\ \Rightarrow z_1 \neq z_2$$

$$\forall x_1, x_2, y_1, y_2 \;\; \neg\mathtt{HasWord}(x_1, y_1) \wedge \neg\mathtt{HasWord}(\mathtt{x_2}, \mathtt{y_2}) \wedge \; y_1 = y_2 \wedge R(z_1, x_1) \wedge R(z_2, x_2) \\ \Rightarrow z_1 = z_2$$

$$\forall z_1, z_2 \;\; z_1 \neq z_2$$

for each field-record relation R. The last rule corresponds to the class priors implemented as a unit clause.

7.2.5 Relational Models

The combination of Fellegi-Sunter with transitivity produces McCallum and Wellner's [63] conditional random field (CRF) model, with field matches or field similarities as the features. (A logistic regression model is a CRF where all the query variables are independent; transitive closure renders them dependent. Discriminatively-trained MLNs can be viewed as relational extensions of CRFs.)

Reverse predicate equivalence applied to the relations in the database yields the CRF model of Singla and Domingos [94], with the field similarity measure described above instead of TF-IDF. It is also very similar to the CRF model of Culotta and McCallum [14]. The model of Dong *et al.* [25] is also of this type, but more *ad hoc*. All of these models have the property that they allow entities of multiple types to be resolved simultaneously, with inference about one pair of entities triggering inferences about related pairs of entities (e.g., if two papers are the same, their authors are the same; and vice-versa, albeit with lower weight).

We can also use coauthorship relations for entity resolution, in the vein of Bhattacharya and Getoor [3], by defining the $\texttt{Coauthor}(x_1, x_2)$ predicate using the formula

$$\forall x, y_1, y_2 \;\; \texttt{HasAuthor}(x, y_1) \wedge \texttt{HasAuthor}(x, y_2) \Rightarrow \texttt{Coauthor}(y_1, y_2)$$

with infinite weight, and applying reverse predicate equivalence to it. (We can also explicitly state that coauthorship is reflexive and symmetric, but this is not necessary.) Notice that this approach increases the likelihood that two authors are the same even if they are coauthors of a third author on *different* papers. While this is still potentially useful, a presumably stronger regularity is captured by the clause

$$\begin{aligned}\forall x_1, x_2, y_1, y_2, y_3, y_4 \; &\texttt{HasAuthor}(x_1, y_1) \wedge \texttt{HasAuthor}(x_2, y_2) \wedge \texttt{HasAuthor}(x_1, y_3) \\ &\wedge \texttt{HasAuthor}(x_2, y_4) \wedge x_1 = x_2 \wedge y_1 = y_2 \Rightarrow y_3 = y_4.\end{aligned}$$

This formula is related to reverse predicate equivalence, but (with suitably high weight) represents the non-linear increase in evidence that can occur when both the papers and the coauthors are the same.

So far, we have seen that an MLN with a small number of hand-coded formulas representing properties of equality is sufficient to perform state-of-the-art entity resolution. However, one of the key features of the entity resolution problem is that a wide variety of knowledge, much of it domain-dependent, can (and needs to) be brought to bear on matching decisions. This knowledge can be incorporated into our approach by expressing it in first-order logic. For example, the constraints listed by Shen *et al.* [92] can all be incorporated into an MLN in this way. Weighted satisfiability then performs the role of relaxation labeling in Shen at al. It is also possible to incorporate formulas learned independently using ILP techniques, as in Davis *et al.* [17], or to refine the hand-coded formulas and construct additional ones using MLN structure learning [47].

7.2.6 Scalability

In practice, even for fairly small databases there will be a large number of equality atoms to infer (e.g., 1000 constants of one type yield a million equality atoms). However, the vast majority of these will usually be false (i.e., non-matches). Scalability is typically achieved by performing inference only over plausible candidate pairs, identified using a cheap similarity measure (e.g., TF-IDF computed using a reverse index from words to fields). This approach can easily be incorporated into our framework simply by adding all the non-plausible matches to the evidence as false atoms. Most clauses involving these atoms will always be satisfied, and thus there is no need to ground them. We select plausible candidates using McCallum *et al.*'s canopy approach [61], with TF-IDF cosine as the similarity measure, but any other approach could be used. While some of the apparent non-matches might be incorrect, this is a necessary and very reasonable approximation. Notice that reverse predicate equivalence might be able to correct some of these errors, by indirectly inferring that two very different strings in fact represent the same object. We have developed a version of MaxWalkSAT and MCMC that lazily grounds predicates and clauses, effectively allowing predicates that are initially assumed false to be revisited, without incurring the computational cost of completely grounding the network (see Chapter 4). Incorporating this into our entity resolution system is an item for future work.

7.3 Experiments

7.3.1 Datasets

We used two publicly available citation databases in our experiments: Cora and BibServ. These datasets have already been described in previous chapters, but for the sake of completeness of this chapter, we will mention some of the important details again.

Cora

Cora dataset is a collection of 1295 different citations to computer science research papers from the Cora Computer Science Research Paper Engine. We used the version processed by Bilenko and Mooney [4] where each citation was segmented into fields (author, venue, title, publisher, year, etc.) using an information extraction system. We used this processed version of Cora. We further cleaned it up by correcting some labels. This cleaned version contains references to 132 different research papers. We used only the three most informative fields: first author, title and venue (with venue including conferences, journals, workshops, etc.). We compared the performance of the algorithms for the task of de-duplicating citations, authors and venues. For training and testing purposes, we hand-labeled the field pairs. The labeled data contains references to 50 authors and 103 venues. After forming canopies, the total number of match decisions was 61,177.

BibServ

BibServ.org is a publicly available repository of about half a million pre-segmented citations. It is the result of merging citation databases donated by its users, CiteSeer, and DBLP. We experimented on a subset of 10,000 records extracted randomly from the user-donated subset of BibServ, which contains 21,805 citations. As in Cora, we used the first author, title and venue fields. In order to focus only on hard decisions, we discarded all the canopies of size less than 10. This left us with a total of 15,954 decisions. Since we lacked labeled data for BibServ, we used the parameters learned on Cora (with appropriate modifications) to perform inference on BibServ. Word stemming was used to identify the variations of the same underlying root word both in Cora and BibServ.

7.3.2 Models

We compared the following models in our experiments.

NB. This is the naive Bayes model as described in Section 7.2.4. We use a different feature for every word.

MLN(B). This is the basic MLN model closest to naive Bayes. It has the four reverse predicate equivalence rules connecting each word to the corresponding field/record match predicate. With per-word weights, this yields thousands of weights. For speed, these are derived from the naive Bayes parameters. The model also has a unit clause, $\neg\texttt{SameEntity}(e1, e2)$, for each entity type being matched. The weights of these rules are learned discriminatively using the algorithm of Singla and Domingos [93]. When the weights of single predicate rules are set using the class priors in naive Bayes, the two models are equivalent. All the following models are obtained by adding specific rules to the basic MLN model and learning these rules discriminatively.

MLN(B+C). This is obtained by adding reverse predicate equivalence rules for the various fields to MLN(B). This achieves the flow of information through shared attribute values as proposed by Singla and Domingos [94].

MLN(B+T). This is obtained by adding transitive closure rules to MLN(B). It incorporates transitivity into the model itself as proposed by McCallum and Wellner [63].

MLN(B+C+T). This model has both reverse predicate equivalence and transitive closure rules and i.e. it has the enhancements proposed by both Singla and Domingos [94] and McCallum and Wellner [63].

MLN(B+C+T+S). This model is obtained by adding rules learned using the structure learning algorithm of Kok and Domingos [47] to MLN(B+C+T). An example of a rule added by structure learning is: if two papers have the same title and the same venue, then they are the same paper.

MLN(B+N+C+T). This model has a two-level learning/inference step. The first step involves learning a model to predict if two word mentions are the same based on the n-grams they have in common (we used n=3). This step incorporates word-level transitivity and reverse predicate equivalence rules. The second step involves learning an MLN(B+C+T) model on the words inferred by the first stage.[1] This model implements a hybrid similarity measure as proposed by Cohen *et al.* [10].

MLN(G+C+T). This model is similar to MLN(B+C+T) except that it does not have per-word reverse predicate equivalence rules. Rather, it has four global rules, each with the same weight for all words, and these weights are learned discriminatively, like the rest.[2]

7.3.3 Methodology

In the Cora domain, we performed five-fold cross validation. In the BibServ domain, because of the absence of labeled data, the naive Bayes model could not be learned. The weights of the inverse predicate equivalence rules for each word were fixed in proportion to the IDF of the word. This was used as a baseline for all the enhanced models. The weights of other rules were determined from the weights learned on Cora for the corresponding model.

For each model, we measured the conditional log-likelihood (CLL) and area under the precision-recall curve (AUC) for the match predicates. The advantage of the CLL is that it directly measures the quality of the probability estimates produced. The advantage of the AUC is that it is insensitive to the large number of true negatives (i.e., ground atoms that are false and predicted to be false). The CLL of a set of predicates is the average over all their groundings of the ground atom's log-probability given the evidence. The precision-recall curve for match predicates is computed by varying the threshold CLL above which a ground atom is predicted to be true. We computed the standard deviations of the AUCs using the method of Richardson and Domingos [86].

[1]This model was learned on raw words without any stemming, to see if the n-gram step could potentially achieve the effects of stemming.

[2]The rule $\neg\texttt{HasWord}() \wedge \neg\texttt{HasWord}() \Rightarrow \texttt{SameField}()$ has essentially no predictive power; we set its weight to 0.

7.3.4 Results

Cora

Tables 7.1 and 7.2 show the CLL and AUC for the various models on the Cora dataset, respectively. For the case of AUC in venues, there is monotonic increase in the performance as we add various collective inference features to the model, with the best-performing model being MLN(B+C+T). This trend shows how adding each feature in turn enhances the performance, giving the largest improvement when all the features are added to the model. For the case of CLL in venues, the performance tends to fluctuate as we add various collective inference features, but the best-performing model is still MLN(B+C+T). For the case of citations, the results are similar, although the improvements as we add features are not as consistent as in case of AUC in venues. For AUC in authors, we have similar results, although the performance gain is much smaller compared to venues and citations. There is more fluctuation in the case of CLL but the collective models are still the best.

MLN(B+C+T+S) helps improve the performance of MLN(B+C+T) on citations and authors (both CLL and AUC) but does not help on venues.

MLN(B+N+C+T) improves performance on authors but not on citations and venues. This shows that while stemming can be a good way of identifying word duplicates in most cases, the engram model is quite helpful when dealing with fields such as authors, where initials are used for the complete word and can not be discovered by stemming alone.

MLN(G+C+T) (the model with global word rules) performs well for citations but less so for authors and venues. In general, per-word rule models seem to be particularly helpful when there are few words from which to infer the relationship between two entities.

BibServ

Since we did not have labeled data for BibServ, we hand-labeled 300 pairs each for citations and venues, randomly selected from the set where the MAP prediction for at least one of the algorithms was different from the others. For authors, we labeled all the potential match decisions, as there were only 240 of them. The results reported below are over these hand-labeled pairs.

Tables 7.3 and 7.4 show the CLL and AUC for the various algorithms on the BibServ dataset. As in the case of Cora, for citations and authors, the best-performing models are the ones involving

Table 7.1: CLL results on the Cora database.

System	Citation	Author	Venue
NB	-0.637 ± 0.010	-0.133 ± 0.021	-0.747 ± 0.017
MLN (B)	-0.643 ± 0.010	-0.131 ± 0.022	-0.760 ± 0.017
MLN (B+C)	-0.809 ± 0.012	-0.386 ± 0.064	-1.163 ± 0.034
MLN (B+T)	-0.369 ± 0.003	-0.213 ± 0.036	-1.036 ± 0.029
MLN (B+C+T)	-0.597 ± 0.007	-0.171 ± 0.043	-0.704 ± 0.023
MLN (B+C+T+S)	-0.503 ± 0.006	-0.100 ± 0.033	-0.874 ± 0.027
MLN (B+N+C+T)	-0.879 ± 0.008	-0.096 ± 0.032	-0.781 ± 0.023
MLN (G+C+T)	-0.394 ± 0.004	-0.263 ± 0.053	-1.196 ± 0.031

collective inference features. MLN(B+N+C+T) gives the best performance for both CLL and AUC in authors, for the reasons cited before. It is also the best-performing model for AUC in citations, closely followed by other collective models. MLN(B+C) gives the best performance for CLL in citations.

Whereas MLN(G+C+T) performs quite poorly on citations and authors, it in fact gives the best performance on CLL in venues. On AUC in venues, MLN(G+C+T) and MLN(B) are the two best performers. Overall, even though BibServ and Cora have quite different characteristics, applying the parameters learned on Cora to BibServ still gives good results. Collective inference is clearly useful, except for AUC on venues, where the results are inconclusive.

7.4 Conclusion

In this chapter, we proposed a unifying framework for entity resolution. We showed how a small number of axioms in Markov logic capture the essential features of many different approaches to this problem, in particular non-i.i.d. ones, as well as the original Fellegi-Sunter model. Experiments on two citation databases evaluate the contributions of these approaches, and illustrate how Markov logic enables us to easily build a sophisticated entity resolution system.

Table 7.2: AUC results on the Cora database.

System	Citation	Author	Venue
NB	0.913±0.000	0.986±0.000	0.738±0.002
MLN (B)	0.915±0.000	0.987±0.000	0.736±0.002
MLN (B+C)	0.891±0.000	0.968±0.000	0.741±0.001
MLN (B+T)	0.949±0.000	0.994±0.000	0.745±0.002
MLN (B+C+T)	0.964±0.000	0.984±0.000	0.828±0.002
MLN (B+C+T+S)	0.988±0.000	0.992±0.000	0.807±0.002
MLN (B+N+C+T)	0.952±0.000	0.992±0.000	0.817±0.002
MLN (G+C+T)	0.973±0.000	0.980±0.000	0.743±0.002

Table 7.3: CLL results on the Bibserv database.

System	Citation	Author	Venue
MLN(B)	−0.008±0.003	−0.586±0.114	−0.806±0.121
MLN(B+C)	−0.001±0.000	−0.544±0.113	−1.166±0.151
MLN(B+T)	−0.006±0.003	−0.600±0.116	−0.827±0.123
MLN(B+C+T)	−0.006±0.004	−0.473±0.105	−1.146±0.149
MLN(B+C+T+S)	−0.006±0.004	−0.486±0.107	−1.133±0.148
MLN(B+N+C+T)	−0.018±0.005	−0.363±0.091	−0.936±0.133
MLN(G+C+T)	−0.735±0.101	−4.679±0.256	−0.716±0.112

Table 7.4: AUC results on the Bibserv database.

System	Citation	Author	Venue
MLN(B)	0.997±0.001	0.910±0.013	0.908±0.011
MLN(B+C)	0.999±0.000	0.887±0.007	0.876±0.012
MLN(B+T)	0.993±0.003	0.909±0.013	0.898±0.010
MLN(B+C+T)	0.998±0.000	0.928±0.009	0.876±0.012
MLN(B+C+T+S)	0.970±0.020	0.926±0.010	0.876±0.012
MLN(B+N+C+T)	1.000±0.000	0.940±0.008	0.897±0.012
MLN(G+C+T)	0.491±0.000	0.432±0.001	0.906±0.012

Chapter 8

DISCOVERY OF SOCIAL RELATIONSHIPS IN IMAGE COLLECTIONS

8.1 Introduction

This chapter describes the application of Markov logic to the problem of identifying social relationships in image collections pertaining to everyday users. Image collections are pervasive. Mining semantically meaningful information from such collections has been an area of active research in the machine learning and vision communities. There is a large body of work focusing on problems of face detection and recognition, detecting objects of certain types such as grass, water, and sky. Most of this work relies on using low-level features available in the image (such as color or texture). In recent years, there has been an increased focus on extracting semantically more complex information such as scene detection and activity recognition [56, 54]. For example, one might want to cluster pictures based on whether they were taken outdoors or indoors or cluster work pictures vs. leisure pictures. This work relies primarily on using the derived features, such as people present in the image, the presence or absence of certain kinds of objects in the image, and so on. Typically, the power of collective inference is used in such scenarios [60]. For example, it may be hard to tell for a particular picture if it is work or leisure, but by looking at other pictures that are similar in a spatio-temporal sense it becomes easier to arrive at the correct conclusion. This line of research aims to change the way we perceive digital image collections - from sets of pixels to highly complex objects that can be organized and queried in meaningful ways.

Our goal is to automatically detect social relationships in image collections. For example, given two faces appearing in an image, we would like to infer if the two people are spouses or merely friends. Even when information about age, gender, and identity of various faces is known, this task seems extremely difficult. In related work [70, 28], the intention is to learn the likelihood that particular groups will appear together in images to facilitate recognition. In Weng *et al.* [104], movies are analyzed to find groups of associated characters. In all of these works, the relationships within the groups are left undefined.

Given a single image of two people, it is difficult to determine whether the two are friends or spouses. However, when a group of pictures are considered collectively, the task becomes more tractable. An observer unfamiliar with the images' subjects might guess based on heuristic rules such as (a) couples often tend to appear together in images just by themselves as opposed to friends who typically appear in groups, and (b) couples with young children often appear with their children in the images. The power of this approach is that one can even make meaningful inferences even about relationships between people who never (or very rarely) appear together in an image. For example, if A (male) appears with a child in a group of images and B (female) appears with the same child in other images, and A and B appear together in a few other images, then is it likely they are spouses and are the child's parents.

Markov logic allows us to capture these heuristic rules (possibly incorrect and conflicting in many scenarios) in a mathematically sound and meaningful way. Each rule is seen as a soft constraint (as opposed to a hard constraint in logic) whose importance is determined by the real-valued weight associated with it. These weights are learned from hand-labeled training data. We also propose to learn new rules using the data, in addition to the rules supplied by the domain experts, thereby enhancing the background knowledge. These rules (and their weights) are then used to perform a collective inference over the set of possible relationships. As we will show, we can also build a model for predicting relationships, age and gender, using noisy predictors (for age and gender) as inputs to the system. Inference is performed over all images, age, and gender simultaneously to allow each component to influence the others in the context of our model, thereby improving the accuracy of the prediction. We will first describe our model for predicting the social relationships in image collections, followed by our experimental evaluation.

8.2 Model

Our model is expressed in Markov logic. We will describe our objects of interest, predicates (properties of objects and relationships among them), and the rules that impose certain constraints on those predicates. We will then pose our learning and inference tasks.

8.2.1 Objects and Predicates

Objects

We have three kinds of objects in our domain:

- **Person:** A real person in the world.
- **Face:** A specific appearance of a face in an image.
- **Image:** An image in the collection.

We model two kinds of predicates defined over the objects of interest.

Evidence Predicates

The value of these predicates is known from the data at the time of the inference. An example evidence predicate is $\texttt{OccursIn}(\texttt{face}, \texttt{img})$, which represents the truth value of whether a particular face appears in a given image or not. We use evidence predicates for the following properties/relations:

- Number of people in an image: $\texttt{HasCount}(\texttt{img}, \texttt{cnt})$
- The age of a face appearing in an image: $\texttt{HasAge}(\texttt{face}, \texttt{age})$
- The gender of a face appearing in an image: $\texttt{HasGender}(\texttt{face}, \texttt{gender})$
- Whether a particular face appears in an image: $\texttt{OccursIn}(\texttt{face}, \texttt{img})$
- Correspondence between a person and his/her face: $\texttt{HasFace}(\texttt{person}, \texttt{face})$

The age (gender) of a face is the estimated age (gender) value estimated from the face from an image. Note that this is distinct from the actual age (gender) of a person, which is modeled as a query predicate. The age (gender) associated with a face is inferred from a classification model trained separately on a collection of faces using various facial features. We implemented age and gender classifiers following the examples of Li and Fei-Fei [51] and Yedidia *et al.* [107]. Note that different faces associated with the same person will likely have different estimated age and gender values. We model the age using five discrete bins: child, teen, youth, adult, and senior.

For this application, we assume the presence of face detection and recognition and therefore we know exactly which face corresponds to which person. Relaxing this assumption and folding face detection and recognition into the model is an important direction for future work.

Query Predicates

The value of these predicates is not known at the time of the inference and needs to be inferred. An example of this kind of predicate is $\texttt{HasRelation}(\texttt{person1}, \texttt{person2}, \texttt{relation})$, which represents the truth value of whether two persons share a given relationship. We use the following query predicates:

- The relationship between two persons: $\texttt{HasRelation}(\texttt{person1}, \texttt{person2}, \texttt{relation})$
- Age of a person: $\texttt{PersonHasAge}(\texttt{person}, \texttt{age})$
- Gender of a person: $\texttt{PersonHasGender}(\texttt{person}, \texttt{gender})$

We model two different kinds of settings.
Two-Class: In this basic setting, we model only two relationships in the domain: friend or relative. All the relations are mapped onto one of these two relationships. Relative follows the intuitive definition of being a relative. Anyone who is not a relative is considered as a friend.
Multi-Class: In the second setting, we model seven different kinds of social relationships: relative, friend, acquaintance, child, parent, spouse, and childfriend. Relative includes any relative (by blood or marriage) not including child, parent, or spouse. Friends are people who are not relatives and satisfy the intuitive definition of friendship. Childfriend models the friends of children. It is important to model the childfriend relationship, as children are pervasive in image collections and often appear with their friends. In such scenarios, it becomes important to distinguish between children and their friends. Any non-relatives, non-friends are acquaintances. For our purposes and in our data, spouses always have opposite gender.

8.2.2 Rules

We formulate two kinds of rules for our problem. All the rules are expressed as formulas in first-order logic.

Hard Rules

These describe the hard constraints in the domain, i.e., they should always hold true. An example of a hard rule is $\texttt{OccursIn}(\texttt{face}, \texttt{img1}) \wedge \texttt{OccursIn}(\texttt{face}, \texttt{img2}) \Rightarrow (\texttt{img1} = \texttt{img2})$, which simply states that each face occurs in at most one image in the collection. Here are some of the other hard rules that we use:

- Parents are older than their children.
- Spouses have opposite gender.
- Two people have a unique relationship between them.

Note that we assume there is a unique relationship between two people. Relaxing this assumption (e.g. two people can be both relatives and friends) is an item for future work.

Soft Rules

These rules describe the interesting set of constraints that we expect to usually, but not always, be true. An example of a soft rule is $\texttt{OccursIn}(\texttt{person1}, \texttt{img}) \wedge \texttt{OccursIn}(\texttt{person2}, \texttt{img}) \Rightarrow \neg\texttt{HasRelation}(\texttt{person1}, \texttt{person2}, \texttt{acquaintance})$. This rule states that two people who occur together in a picture are less likely to be mere acquaintances. Each additional instance of their occurring together (in different pictures) further decreases this likelihood. Here are some of the other soft rules that we use:

- Children and their friends are of similar age.
- A youth occurring solely with a child is one of the child’s parents.
- Two people of similar age and opposite gender appearing together are spouses.

- Friends and relatives are clustered across images: if two friends appear together in an image, then a third person occurring in the same image is more likely to be a friend. The same holds true for relatives.

Proper handling of the combination of hard and soft constraints together provides the power of our approach. We seek a solution that satisfies all the hard constraints (presumably such a solution always exists) and at the same time satisfies the (weighted) maximum number of soft constraints.

Singleton Rule

Finally, we have a rule consisting of a singleton predicate $\texttt{HasRelation}(\texttt{person1}, \texttt{person2}, +\texttt{rel}-\texttt{ation})$ ($+$ indicates a unique weight is learned for each relation), that essentially represents the prior probability of a particular relationship holding between any two random people in the collection. For example, the “friends” relationship is more common than the “parent-child” relationship. Similarly, we have the singleton rules $\texttt{HasAge}(\texttt{person}, +\texttt{age})$ and $\texttt{HasGender}(\texttt{person}, +\texttt{gender})$. These represent (intuitively) the prior probabilities of having a particular age and gender, respectively. For example, it is easy to capture the fact that children tend to appear in images more often by giving a high weight to the rule $\texttt{HasAge}(\texttt{person}, \texttt{child})$.

8.2.3 Learning and Inference

Given the model (the rules and their weights), inference consists of finding the marginal probabilities of all groundings of the query predicates `HasRelation`, `HasGender` and `HasAge` given all the evidence atoms. Since we have to handle a combination of hard (deterministic) and soft constraints, we use the MC-SAT algorithm of Poon and Domingos [82] as implemented in Alchemy [48].

Given the hard and soft constraints, learning corresponds to finding the optimal weights for each of the soft constraints. We find the MAP weights with a Gaussian prior centered at zero. We use a weight learner [58] implemented in Alchemy. We use the structure learning algorithm of Kok and Domingos [47] to refine (and learn new instances) of the rules that help us predict the target relationships. The original algorithm as described by them (and as implemented in Alchemy) does not allow the discovery of partially grounded clauses. This is important for us as we need to learn the different rules for different relationships. The rules may also differ for specific age groups and/or genders (for example, one might imagine that males and females differ in who they tend to appear with). The change needed in the algorithm to incorporate this feature is straightforward. We allow the addition of all possible partial groundings of a predicate as we search for the extensions of a clause. (Only certain variables (i.e. relationship, age, and gender) are allowed to be grounded in these predicates to avoid blowing up the search space.) After learning, the inference proceeds as previously described. The basic run of the structure learning algorithm did not produce any interesting rules (that were not already part of the hand-coded knowledge base). For our experiments, we simply report the results for the hand-coded KB. Experimenting further with learning new rules is a part of the future work.

8.3 Experiments

8.3.1 Dataset

We experimented on a dataset consisting of personal images collections of 13 different owners. The collectors came from diverse demographics in terms of age, gender, and ethnicity. There are about a couple hundred images for each collector and the total number of images is 1926 (we account only for images in which at least one person appears). The faces are detected and recognized, i.e. there is a one-to-one mapping between a face and a person in the real world. Each collection owner labeled their relationship to each person appearing in their image collection. The relationship label domain is a set of 30 different relationships such as mother, father, son, daughter, friend, son-in-law, and so on. Each of these relationship is associated with one of the broader relationship categories (two for the two-class case and seven for the multi-class case). Each collection owner also labeled the current age of each person appearing in the collection. The gender of each person was labeled by looking at their name and appearance.

8.3.2 Models

We compared five different models as explained below.

- **Random:** This is the simplest of all models. We randomly select the detected relationship one out of all the possible relationships using a uniform distribution.

- **Prior:** Using the prior distribution from the training data, one of the all possible relationships is selected as the detected relationship.

- **Hard:** This model picks uniformly at random one of the possible relationships while enforcing the common-sense hard constraints. For example, if two people are of same gender, then the spouse relationship is ruled out and we can pick only among the remaining relationships. The number of hard constraints used depends on the setting (multi-class/two-class) and will be detailed in the respective sections.

- **Hard-Prior**: This model is a combination of hard and prior models. The true relationships are selected using the prior probability of the relationships while ensuring the hard constraints are satisfied.

- **MLN:** This is the full-blown model, which uses a combination of soft and hard constraints, with weights learned for the soft rules using the training data. The prior information is incorporated into the model using singleton (soft) constraints which state that a particular kind of relationship holds. The number of rules used for multi-class/two-class cases will be detailed in the respective sections.

8.3.3 Methodology

We performed two sets of experiments: two-class and multi-class, as detailed in the model section. For the two-class setting, no age or gender information was used in the constraints. In the multi-class experiment, we assume the gender and age of each person is known. In this case, everything except the `HasRelation` predicate is treated as evidence (at learning as well as inference time).

For all our experiments, the age attribute was divided into five bands: child ($<$13), teen (13-20), youth (20-40), adult (40-60) and senior ($>$60). Since we had labeled data only for relationships between the collectors and the people appearing in their collections, we restricted ourselves to working with the relationships of various people with the corresponding image collectors (instead of predicting all possible pairs of relationships). We assumed that we know the identity of the image collector during learning as well as inference. The rules described in our model can easily (and in obvious manner) be adapted to this setting. Note that we fixed the above formulation to evaluate our model(s) in a fair manner.

We performed leave-one-out cross validation, learning on 12 image collectors' data and predicting on the remaining one. Each experiment predicts the relationship between the collection owner and each person in the image collection, for a total of 286 predictions across the 13 collections. For each model on each test set, we measure the accuracy (ACR), conditional log-likelihood (CLL), and area under the precision-recall curve (AUC) for the query predicates. ACR is a basic and intuitive measure of how well the model is doing. CLL directly measures the quality of the probability estimates produced. AUC gives a measure of how well the model works overall in precision-recall space. AUC is especially useful when the distribution of positives and negatives is skewed (as in our case out of n possible relationships, only one holds). The CLL of a query predicate is the average over all its groundings of the ground atom's log-probability given the evidence. The precision-recall curve for a predicate is computed by varying the threshold CLL above which a ground atom is predicted to be true. We computed the standard deviations of the AUCs using the method of Richardson and Domingos [86].

8.3.4 Results

Two-Class

In the two-class setting, four soft constraints were used. No hard constraints were used. The soft constraints simply state the following regularities: acquaintances appear in few images, friends occur in large groups, friends and relatives are clustered across images. Note that none of these soft constraints uses age or gender information. The goal of this experiment is to show that our approach leverages information from the soft constraints in a very simple setting. Table 8.1 details the results [1]. Clearly, the MLN model has the best performance (except for CLL where the prior model wins marginally), followed by the prior model. Figure 8.1 shows the precision-recall curves that compare all the models. These results establish the benefit of our approach in a very basic setting. Next, we move on to the more involved multi-class setting.

[1]The models "hard" and "hard-prior" are absent as no hard constraints are used in this setting

Table 8.1: Results comparing the different models for the two-class setting.

Model	ACR	CLL	AUC
Random	48.8±3.1	-0.693±0.000	49.6±0.0
Prior	50.4±3.1	-0.693±0.001	54.4±0.3
MLN	64.7±3.0	-0.709±0.031	66.7±0.4

Multi-Class

For the case of full observability, we used 5 hard constraints and 14 soft constraints (see the model section for examples).

Table 8.2 details the results. As expected, there is a gradual increase in performance as we move from the most basic model (random) to the most sophisticated model (MLN). Figure 8.2 shows the precision-recall curves for multi-class setting. The MLN model dominates over other models at all points of the precision-recall curve, clearly demonstrating the benefit of our soft rules.

It is interesting to examine the weights that are learned for the soft rules. More importance is placed on rules with higher weights. The following three rules received the highest weights (in decreasing order) in our MLN.

- If a non-child and a child appear together in an image, the former is a parent of the latter.
- Same rule as above, except the image has exactly two people.
- If a person is friends with a child, then the child and the person have the same age.

Figure 8.3 shows the predicted social relationships from the Markov Logic Network for five people from an image collection.

8.4 Conclusion

Automatically predicting social relationships in image collections is important for semantic understanding of everyday images and has a wide range of applications. Humans typically use heuristic

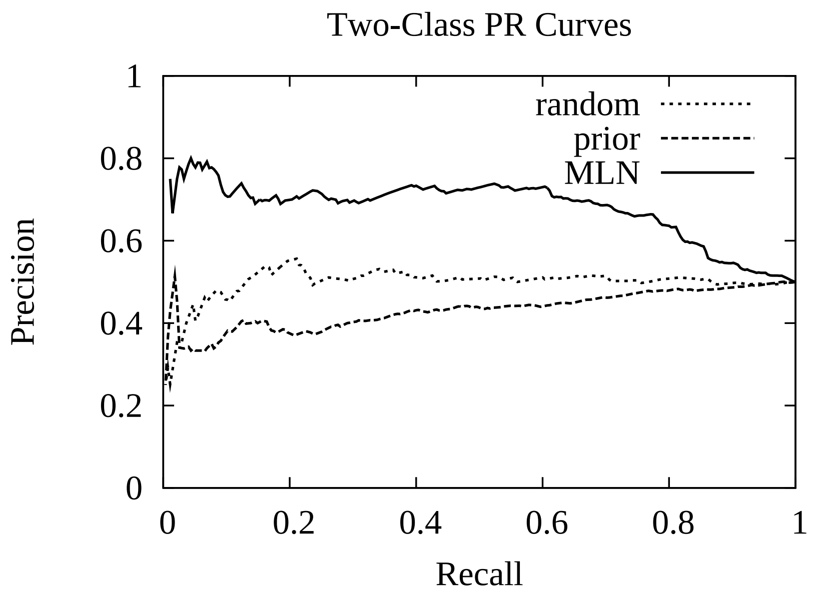


Figure 8.1: Precision-recall curves for the two-class setting.

rules to detect these social relationships. Our contribution in this dissertation is to use the power of Markov logic to formulate these heuristic rules as soft constraints in a mathematically sound and meaningful way. A combination of hard and soft constraints is used. To the best of our knowledge, out approach is unique in the literature. Our approach performs better than a combination of various basic approaches and suggests further investigation of the problem, leading to a better understanding of social relationships that can be extracted from images collections.

Table 8.2: Results comparing the different models for the multi-class setting.

Model	ACR	CLL	AUC
Random	12.4±2.1	-0.410±0.015	9.4±0.2
Prior	26.4±2.7	-0.404±0.015	21.0±0.2
Hard	14.3±2.2	-0.372±0.013	21.0±0.2
Hard-Prior	26.4±2.7	-0.370±0.013	23.3±0.2
MLN	29.9±2.9	-0.352±0.013	29.7±1.0

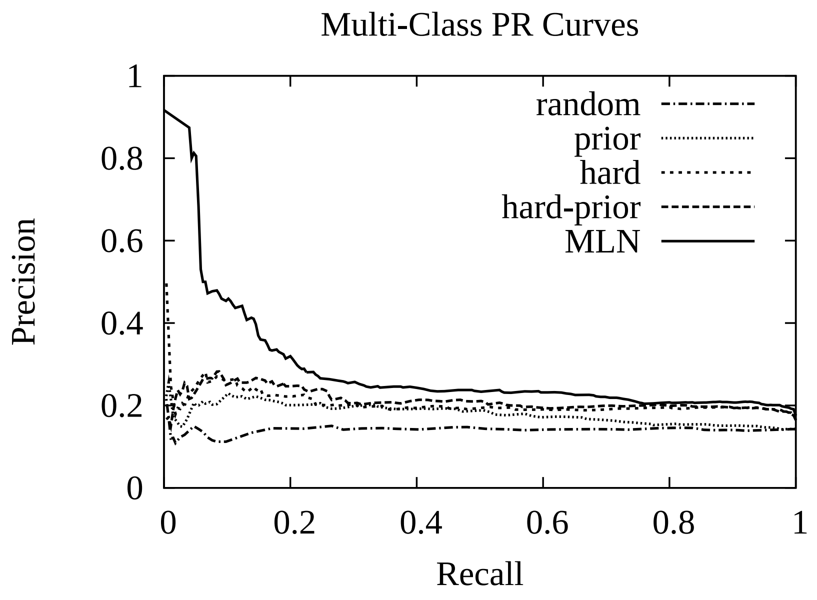


Figure 8.2: Precision-recall curves for the multi-class setting.

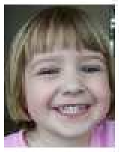
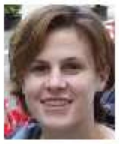
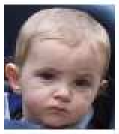
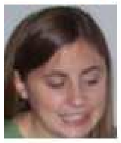
	Age	True Relationship	Predicted Relationship
	3	Child	Child
	27	Spouse	Relative
	1	Child	Child
	20	Relative	Relative
	34	Relative	Relative

Figure 8.3: For four of five people from this collection, the relationship predictions are correct using the Markov logic network.

Chapter 9
CONCLUSION

Markov logic is a simple yet powerful approach to combining logic and probability in a single representation. In this dissertation, we have extended its semantics to handle infinite domains, developed a series of efficient learning and inference algorithms, and successfully applied it to two domains. All the algorithms described in this dissertation are implemented in the Alchemy open source software package [48].

9.1 Contributions of this Dissertation

The contributions of this dissertation can be summarized as follows.

- We extended the semantics of Markov logic to infinite domains using the theory of Gibbs measures. We gave sufficient conditions for the existence and uniqueness of a measure consistent with the local potentials defined by an MLN. We also described the structure of the set of consistent measures when it is not a singleton, and showed how the problem of satisfiability can be cast in terms of MLN measures.

- Satisfiability testing is very effective for inference in relational domains, but is limited by the exponential memory cost of propositionalization. We proposed the LazySAT algorithm, which overcomes this problem by exploiting the sparseness of relational domains. Our algorithm greatly reduces memory requirements compared to WalkSAT, without sacrificing speed or solution quality.

- We presented a general framework for lifting probabilistic inference, and the first application of lifted inference to real-world domains. Our approach constructs a network of supernodes and superfeatures, corresponding to sets of nodes and features that are indistinguishable given the evidence, and applies the inference algorithm to this network. Our experiments using belief propagation show that lifted inference yields very large efficiency gains compared to the ground version, in both time and memory.

- We developed an algorithm for discriminative learning of MLN parameters by combining Collins's voted perceptron algorithm with a weighted satisfiability solver. We experimentally showed that this approach outperforms generative learning.

- We presented applications of Markov logic to two important real world problems. The first one is the problem of entity resolution. We showed how a small number of axioms in Markov logic capture the essential features of many different approaches to this problem, in particular non-i.i.d. ones, as well as the original Fellegi-Sunter model. This allows us to build a state-of-the-art entity resolution system. We then presented a model based on Markov logic for identifying social relationships in image collections. Various "heuristic rules" are combined together in a mathematically meaningful way by expressing them as soft constraints in Markov logic, giving much better solutions to the problem compared to the baseline.

9.2 Directions for Future Work

There are a number of directions for future work. On the theoretical front, these include deriving alternative conditions for existence and uniqueness of distribution(s) over infinite MLNs, analyzing the structure of consistent measure sets in more detail, extending the theory to non-Herbrand interpretations and recursive random fields [59], and studying interesting special cases of infinite MLNs.

We would like to analyze the effect of changing the balance between greedy and random moves (modifying p in Algorithm 2) on the LazySAT performance. One would expect that a bias towards greedy moves will help LazySAT performance (since fewer active clauses are created) but further experiments are needed to verify this thesis. Another direction to explore would be to compare the performance of LazySAT and lifted belief propagation (in the max-product case) for doing MAP inference. This question relates to the larger question of the relationship between lazy and lifted inference in general, and of whether the latter subsumes the former.

We described lifted inference in the context of a fixed given evidence. Analyzing what happens when additional evidence is provided online is another direction for future work. A simple way to handle additional evidence is to further refine the supernodes (superfeatures) but this may not always be optimal, as some of them may now actually be merged to form a larger supernode (superfeature).

Lifted inference gives a potential approach for performing inference in infinite domains. Developing this theory further and coming up with a set of real-world infinite domains where lifted inference can be applied is another interesting direction for future work.

In general, we would like to develop a unified theory of lifted inference which matches the way human perception works. It is now well known in the vision community that, while analyzing a scene, the human brain first builds a very crude model of the high-level objects and entities [39]. This model is refined further to fill in lower-level details as more processing time is given. Can we develop a similar model of lifted inference which first performs the high-level inference? This would result in a crude approximation of the underlying probabilities. In our terminology, an approximate lifted network is constructed and inference is done over this network. Lower-level details are then added as and when needed, given the availability of resources. This corresponds to further refining the inference results given by the approximate lifted network (while reusing most of the work done earlier).

On the application side, we would like to apply Markov logic to other domains, especially with missing information (or hidden variables), where EM could be potentially used. We would also like to experiment with large social networks (such as Facebook) and with biological domains.

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Research Interests

Machine Learning, Data Mining, Satisfiability Testing, Probabilistic Inference, Social Network Analysis

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Publications

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- Jiebo Luo, Parag Singla, Henry Kautz and Andrew Gallagher. Discovery of Social Relationships in Consumer Photo Collections using Markov Logic CVPR Workshop on Semantic Learning and Applications in Multimedia, 2008 (pp. 1 - 7).

- Parag Singla and Matthew Richardson. Yes, There is a Correlation - From Social Networks to Personal Behavior on the Web. Seventeenth International Conference on World Wide Web, 2008 (pp. 655 - 664).

- Pedro Domingos, Stanley Kok, Daniel Lowd, Hoifung Poon, Matthew Richardson and Parag Singla. Markov Logic. In Probabilistic Inference and Logic Programming (edited by L. De Raedt, P. Frasconi, K. Kersting and S. Muggleton.). To appear.

- Parag Singla and Pedro Domingos. Markov Logic in Infinite Domains. Twenty-Third Conference on Uncertainty in Artificial Intelligence, 2007 (pp. 368 - 375).

- Parag Singla and Pedro Domingos. Entity Resolution with Markov Logic. Sixth International Conference on Data Mining, 2006 (pp. 572 - 582).

- Parag Singla and Pedro Domingos. Memory-Efficient Inference in Relational Domains. Twenty-First National Conference on Artificial Intelligence, 2006 (pp. 488 - 493).

- Pedro Domingos, Stanley Kok, Hoifung Poon, Matthew Richardson and Parag Singla. Unifying Logical and Statistical AI. Twenty-First National Conference on Artificial Intelligence, 2006 (pp. 2 - 7).

- Parag Singla and Pedro Domingos. Discriminative Training of Markov Logic Networks. Twentieth National Conference on Artificial Intelligence, 2006 (pp. 868 - 873).

- Parag Singla and Pedro Domingos. Object Identification with Attribute-Mediated Dependences. Ninth European Conference on Principles and Practice of Knowledge Discovery in Databases, 2005 (pp. 297 - 308).

- Parag and Pedro Domingos. Multi-Relational Record Linkage. KDD-2004 Workshop on Multi-Relational Data Mining, 2004 (pp. 31-48).

- B. Aditya, Soumen Chakrabarti, Rushi Desai, Arvind Hulgeri, Hrishikesh Karambelkar, Rupesh Nasre, Parag and S. Sudarshan. User Interaction in the BANKS System. Nineteenth International Conference on Data Engineering, 2003 (pp. 786 - 788).

- B. Aditya, Gaurav Bhalotia, Soumen Chakrabarti, Arvind Hulgeri, Charuta Nakhe, Parag and S. Sudarshan. BANKS: Browsing and Keyword Searching in Relational Databases. Twenty-Eighth International Conference on Very Large Data Bases, 2002 (pp. 1083 - 1086).

RESEARCH AND PROFESSIONAL EXPERIENCE

- **University of Washington, Seattle** **Jan 04 - till date**

  Position: Research Assistant

  Projects:

  – Algorithms for efficient learning and inference in Markov logic
  – Extending the semantics of Markov logic to infinite domains
  – Application of Markov logic to entity resolution
  – Object-Identification using collective information

- **Kodak Research Labs, Rochester** **Jun 07 - Aug 07**

  Position: Summer Intern.

  Project: Discovering social relationships from personal photo collections using Markov logic.

- **Microsoft Research, Redmond** **Jul 06 - Sep 06**

  Position: Summer Intern.

  Project: Finding a correlation between the personal behavior of people on the web (i.e. keyword searches, demographics etc.) and their social behavior (i.e. talking characteristics on IM).

- **IIT Bombay, Mumbai** **Jul 01 - Aug 02**

  Position: Undergraduate Researcher.

  Project: Supporting web like keyword search in databases.

- **IBM India Research Lab, New Delhi** **May 01 - Jul 01**
  Position: Summer Intern.
  Project: Agglomerative clustering of a set of proper nouns using the features extracted from the web.

TEACHING EXPERIENCE

University of Washington, Seattle. *Teaching Assistant.*

- CSE 142/143: Computer Programming (Undergraduate) **Au 02, Wi 03**
- CSE P546: Data Mining (Professional Masters) **Sp 03, Au 04**
- CSE 531: Computability and Complexity (Graduate) **Au 03**

PATENTS AND SOFTWARE

Patents Filed:

- Matthew Richardson and Parag Singla. Using Joint Communication and Search Data. Microsoft Corporation, 2007.
- Jiebo Luo, Parag Singla, Henry Kautz and Andrew Gallagher. Discovering Social Relationships from Personal Photo Collections. Eastman Kodak Company, 2008 (*in process of filing*)

Software Developed:

- Alchemy: System for Statistical Relational AI.
  http://alchemy.cs.washington.edu.
  (Along with various other contributors.)

Professional Activities

- Reviewer for
  - ACM Transactions on Knowledge Discovery from Data
  - Annals of Mathematics and Artificial Intelligence
  - International Conference on Data Mining
- Volunteer for Engineering Open House, University of Washington, 2007.

Academic Achievements

- Winner of a Student Travel Award at ICDM-06. **2006**
- Winner of the Best Paper Award at PKDD-05. **2005**
- In the Joint Entrance Examination for securing admission to the IIT, was placed **Ninety Nine** in India among approximately 100,000 competitive students who took the examination. **1998**
- Recipient of Merit Certificate under National Scholarship Scheme for CBSE (Central Board for Secondary Education) Grade Twelve Examination, India. **1998**
- Ranked **1st** in the whole District for the High School (Grade Ten) Examination, India. **1996**

Extra-Curricular Activities

- Board Member, Hindu YUVA, University of Washington. **2004 - till date**
- Coordinator, Group for Rural Activities, IIT Bombay. **2001 - 2002**
- Recipient of the Organizational Color, IIT Bombay. **2002**

References

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