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AG5



# Learning Rules With Categorical Attributes from Linked Data Sources

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*To my father Cicero, my mother Marlene and my sister Carolina*

- Andre



# *Abstract*

Inductive Logic Programming (ILP) is a consolidated technique for mining Datalog rules in knowledge bases. Nevertheless, it's inherently expensive and the hypothesis search space grows combinatorially with the knowledge base size. This problem is even more dramatic when literals with constants are considered, therefore, it usually requires very aggressive pruning for making it feasible. With the objective of efficiently learning rules with ranges for numerical attributes, we propose a preprocessing step and an extension to ILP top-down algorithm, that suggests the most interesting categorical constants to be added in the refinement step. It consists of building a lattice that expresses the correlations between a root numerical attribute and multiple categorical relations and their constants. This lattice is then queried by the core ILP algorithm in the refinement step and provides a list of refinement suggestions ordered by a defined interestingness measure. This thesis discusses how to efficiently build the lattice, how it's incorporated in the core learning algorithm and evaluates different interestingness measures.



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# Contents

<b>Abstract</b>	<b>vi</b>
<b>Acknowledgements</b>	<b>viii</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Motivation . . . . .	3
1.2 Contributions . . . . .	5
1.3 Outline . . . . .	5
<b>2 Related Work</b>	<b>7</b>
2.1 Logic Programming . . . . .	7
2.2 Inductive Logic Programming . . . . .	8
2.2.1 Searching the Hypothesis Space . . . . .	10
2.2.2 Top-Down ILP . . . . .	11
2.2.3 ILP Complexity . . . . .	13
2.3 Association Rule Mining . . . . .	13
2.3.1 Measures . . . . .	13
2.3.2 Anti-monotonicity of Support . . . . .	14
2.3.3 Itemset Lattice . . . . .	15
2.3.4 Apriori Algorithm . . . . .	15
2.4 Discretization of Numerical Attributes . . . . .	16
2.4.1 Equal Width . . . . .	18
2.4.2 Equal Frequencies . . . . .	18
2.5 Mining Optimized Rules for Numeric Attributes . . . . .	18
2.6 Information Theoretic Measures . . . . .	19
2.6.1 Shannon's Entropy . . . . .	20
2.6.2 Kullback-Leibler Divergence . . . . .	20
2.6.3 Mutual Information . . . . .	21
2.7 Semantic Web Applications . . . . .	22
2.8 Linked Open Data Applications . . . . .	23
<b>3 Learning Rules With Numerical and Categorical Attributes</b>	<b>25</b>
3.1 Interesting Rule Definition . . . . .	25
3.2 Categorical Property Definition . . . . .	26
3.2.1 Numerical Properties as Categorical . . . . .	28

3.2.2	Combination Categorical Property with Linking Relation . . . . .	28
3.2.3	Absence or Presence of a Property as Categories . . . . .	28
3.2.4	Notation Used . . . . .	29
3.3	Preprocessing . . . . .	30
3.3.1	Relation Preprocessing . . . . .	30
3.3.2	. . . . .	33
3.4	Correlation Lattice . . . . .	33
3.4.1	Building the Lattice . . . . .	34
3.4.2	Pruning Opportunities . . . . .	36
3.4.3	Entropy Divergence Measures . . . . .	39
3.4.4	Heuristics . . . . .	40
3.5	Bucketing the Numerical Attributes . . . . .	41
3.6	Incorporating Correlation Lattice into the Core ILP Algorithm . . . . .	42
3.6.1	Querying the Correlation Lattice . . . . .	42
<b>4</b>	<b>Algorithmic Framework</b>	<b>47</b>
4.1	Knowledge Base Backend . . . . .	47
4.2	Preprocessing . . . . .	47
4.2.1	Correlation Lattice . . . . .	47
<b>5</b>	<b>Experiments</b>	<b>51</b>
	 <b>List of Figures</b>	 <b>51</b>
	 <b>List of Tables</b>	 <b>57</b>
	 <b>Bibliography</b>	 <b>59</b>

# Chapter 1

## Introduction

In the last years, the volume of semantic data available, in particular in RDF format, has dramatically increased. Initiatives like the W3C Semantic Web and the Linked Open Data have great contribution in such development. The first provides a common standard that allows data to be shared and reused across different applications and the latter provides linkages between different datasets that were not originally interconnected. Moreover, advances in information extraction have also made a strong contribution, by crawling multiple non-structured resources in the Web and extracting RDF facts.

Nevertheless, information extraction still has its limitations and many of its sources might contain contradictory or uncertain information. Therefore, many of the extracted datasets suffer from incompleteness, noise and uncertainty. The first one means that there are facts that are not existent in the dataset, the second one means that the dataset might contain facts that are not true and the latter one means that the truth of the facts is not certain. These problems make it much more challenging to automatically learn rules from the data.

In order to reduce such problems, one can apply a set of inference rules that describes its domain to the knowledge base. With that, it's possible to resolve contradictions as well as strengthen or weaken their confidence values. It's also possible to derive new facts that are originally not existent due to incompleteness. Such inference rules can be of two types:

1. *Hard Rules*: Consistency constraints which might represent functional dependencies, functional or inverse-functional properties of predicates or mutual exclusion. For example:

- $marriedTo(X, Y) :- marriedTo(Y, X), (X \neq Y)$

- $grandChildOf(X, Y) :- childOf(X, Z), childOf(Z, Y)$
- $parentOf(X, Y) :- childOf(Y, X)$
- $(Z = Y) :- wasBornIn(X, Z), wasBornIn(X, Y)$

2. *Soft Rules*: Weighted Datalog rules that frequently, but not always hold in the real world. As they might also produce incorrect information, derived facts can have a level of uncertainty which is represented by a confidence value. For example, it's known that married people usually live in the same place as their partner:

$$livesIn(X, Y) :- marriedTo(X, Z) livesIn(Z, Y)$$

So, if we have an incomplete knowledge base, which lacks information about where *Michelle Obama* lives, but we know that she's married to *Barack Obama* and he lives in *Washington, D.C.*, we could then apply this soft rule to derive the fact  $livesIn(michelleObama, washingtonDC)$ .

Such rules are rarely known beforehand, but the data itself can be used to mine these rules using Inductive Logic Programming (ILP). It is a well-established framework for inductively learning relational descriptions (in the form of logic programs) from examples and background knowledge. Given a logical database of facts, an ILP system will generate hypothesis in a pre-determined order and test them against the examples. However in a large knowledge base, ILP becomes too expensive as the search space grows combinatorially with the knowledge base size and the larger the number of examples, the more expensive it is to test each hypothesis.

Although it is very expensive to learn rules with constants, such kind of rules can be extremely interesting as they can express particular characteristics of specific groups. For example, the rule  $speaks(X, Y) :- livesIn(X, Z)$  is not very meaningful, it simply tells that people that live in anywhere will speak some language. Nevertheless, if we consider setting constant values for  $Y$  and  $Z$ , we can learn much more valuable rules such as  $speaks(X, english) :- livesIn(X, australia)$  or  $speaks(X, spanish) :- livesIn(X, mexico)$ .

The problem of that, is that for such example, it would be necessary to test rules with all combinations of country and languages, what surely can lead to a very expensive process when applied on large databases. Given the huge size of search space and the great interestingness of rules with constants, it is appropriate to reduce the search space by pruning constants or combinations of constants that do not add interesting information to the hypothesis.

[Talk more about ILP]

## 1.1 Motivation

For numerical properties it might be also relevant to search for interesting constants. Nevertheless, for very large or infinite numerical domains such as the real numbers for example, setting a numerical constant as an individual value will very likely have a single entity associated to it. In such case it would be equivalent to simply specifying a constant for this given entity without the necessity of adding the numerical property

For example, it is extremely unlikely that a country has the exact same GDP or population as any other country. If we have the following rule with the *hasPopulation*, whose domain is the positive integer numbers  $\mathbb{N}^+$ :

$$speaks(X, portuguese) :- livesIn(X, Z), hasPopulation(Z, 193946886)$$

As Brazil is the only country with a population of 193,946,886 inhabitants, this same rule would be equivalent to:

$$speaks(X, portuguese) :- livesIn(X, brazil)$$

Of course, if we have to choose between one of the two rules, the latter one would be preferred as it is shorter and specifies the country in a clearer manner. Moreover, by setting numerical constants punctually, we would end up having a huge number of different constants to test in the hypothesis and most of them would be most likely discarded because of low support.

Therefore, it is interesting to split the attribute's domain into categories by discretizing it. Subsequently check if any of the buckets present different confidence in comparison to its correspondent numerical constant-free rule (which we will call base-rule).

For example if we test the hypothesis and we find support=100 and confidence=0.4:

$$isMarriedTo(X, Y) :- hasAge(X, Z)$$

and then we split  $Z$  into three buckets:

- $b_1 : Z \in [0, 20]$
- $b_2 : Z \in (20, 40]$
- $b_3 : Z \in (40, \infty]$

we then generate three refined-rules by restricting the base-rule's domain from variable  $Z$ :

- $isMarriedTo(X, Y) :- hasAge(X, Z), z \in [0, 20]$   
support=40, confidence=0.1
- $isMarriedTo(X, Y) :- hasAge(X, Z), z \in (20, 40]$   
support=40, confidence=0.5
- $isMarriedTo(X, Y) :- hasAge(X, Z), z \in (40, \infty]$   
support=20, confidence=0.8

for  $b_2$  and  $b_3$ , the hypothesis has significant gain by specifying numerical constants. Adding a relation to the body might produce totally different support and confidence distributions along the buckets. For example, if we add the relation  $hasChild(X, A)$ , we could obtain other interesting rules:

Base-rule:

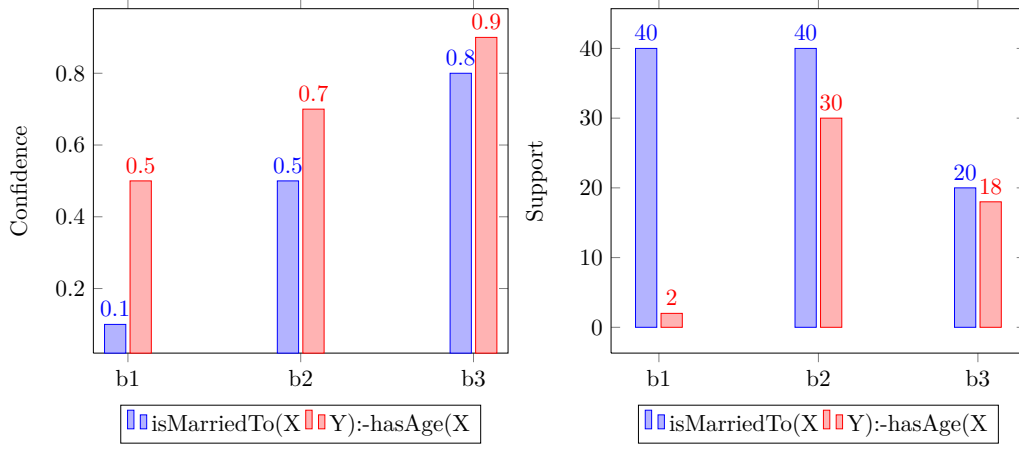
- $sMarriedTo(X, Y) :- hasAge(X, Z), hasChild(X, A)$   
support=50, confidence=0.625

Refined-rules:

- $isMarriedTo(X, Y) :- hasAge(X, Z), hasChild(x, a), Z \in [0, 20]$   
support=2, confidence=0.5
- $isMarriedTo(X, Y) :- hasAge(X, Z), hasChild(x, a), Z \in (20, 40]$   
support=30, confidence=0.7
- $isMarriedTo(X, Y) :- hasAge(X, Z), hasChild(x, a), Z \in (40, \infty]$   
support=18, confidence=0.9

Adding a given predicate to the rule might not bring any gain or even loss in confidence to the base-rule, but when bucketing per age, present a different confidence and support distribution and might even produce gain in confidence for some specific buckets.

Nevertheless, adding a predicate with no correlation to the rule might not generate any gain. Thus, it's necessary to carefully choose the relations and eventual constants and discard the ones with no correlation to the rule.



## 1.2 Contributions

In this thesis, we propose a pre-processing step to build a graph we call Correlation Lattice for each numerical property we want to for interesting intervals. In each graph, that has a numerical property as root, we first query the examples distribution on the numerical attribute, and build a histogram by splitting them into  $k$  buckets. Subsequently, we pick a set of  $c$  categorical properties that can be joined with the root, extract the frequencies histogram and analyze how the distribution of sub-population created by joining them with the root is affected. Afterwards, we try to combine the categories and check whether they still produce interesting sub-populations creating a lattice, like in frequent set mining apriori algorithm.

We discuss the pruning opportunities and also evaluate different heuristics and interest-iness measures and their efficiency in finding rules with numerical intervals.

With information about different examples distributions contained in the generated lattice, once we add one of the root properties during the core ILP algorithm, we can then search for the most interesting categorical properties that could result in different confidence distributions. For every categorical property we can also suggest the most interesting constants and other categorical properties to be combined in a subcategory of both.

## 1.3 Outline





## Chapter 2

# Related Work

In this chapter relevant work related to the thesis topic will be briefly presented. In section 2.1...

### 2.1 Logic Programming

[?] [?] In this section, basic logic programming and deductive database terminology such as *literal*, *clause*, *program clause*, *datalog clause* and *hypothesis* will be presented. Firstly, it is important to mention that variables are represented as uppercase letters followed by a string of lowercase letters and/or digits. Function and predicate symbols are lowercase letters also followed by a string of lowercase and/or digits.

An *atomic formula*  $L$  is a predicate symbol followed by a bracketed n-tuple of *terms*. A *term* can be a variable or a function symbol followed by a bracketed n-tuple of terms. A constant is a function symbol of arity 0. So for example, if  $f$ ,  $g$ , and  $h$  are function symbols and  $X$  a variable, then  $g(X)$  is term,  $f(g(X), h)$  is also a term and  $h$  is a *constant*.

A *literal* is an *atomic formula* which can be negated or not. So both  $L$  and its negation  $\bar{L}$  are literals for any *atomic formula*  $L$ . A clause  $c$  is a disjunction of literals, for example:

$$c = (L_1 \vee L_2 \vee \dots \bar{L}_i \vee \bar{L}_{i+1} \vee \dots) \equiv L_1 \vee L_2 \vee \dots \leftarrow L_i \wedge L_{i+1} \wedge \dots$$

Such disjunction of literals can also be written in following way:

$$\{L_1, L_2, \dots, \bar{L}_i, \bar{L}_{i+1}, \dots\}$$
$$L_1, L_2, \dots \leftarrow L_i, L_{i+1}, \dots$$

A *program clause* is a clause which contains exactly one positive literal. That is, it has the form:

$$\underbrace{T}_{\text{head}} \leftarrow \underbrace{L_1, L_2, \dots}_{\text{body}}$$

A *datalog clause* is a program clause with no function symbols with arity greater different from zero. That means that only variables and constants can be used as predicate arguments. A datalog clause is considered *safe* if all the variables present in the head literal  $T$  are also present in the body. Moreover, it may also allow negated literals in the body, as long as every variable existent in a negated body literal are also be present in a non-negated body literal.

## 2.2 Inductive Logic Programming

[? ] Inductive Logic Programming (ILP) is a machine learning technique that combines inductive machine learning with the logic programming representation. Given a known background knowledge and a set of training examples represented as a logical database of facts (literals without any variables), an ILP system will learn a hypothesis in the form of a logic program.

The clauses in the hypothesis aim at recognizing a concept  $\mathcal{C}$ , which is defined as a subset of objects  $\mathcal{C} \subseteq \mathcal{U}$ . For example,  $\mathcal{U}$  may be the set of all students in a University and  $\mathcal{C}$  all the students studying Informatics. Concepts and objects are described in a description language  $\mathcal{L}$ , typically a subset of first-order logic, but various languages have also been used in ILP, including propositional logic and first order predicate calculus.

The training data for learning a concept  $\mathcal{C}$  is a set of examples  $\mathcal{E}$ , where each examples is a grounded fact labeled as positive ( $\oplus$ ) if the object is an instance of  $\mathcal{C}$ , or negative ( $\ominus$ ) otherwise. We denote the set of positive examples as  $\mathcal{E}^+$  and the set of negative examples as  $\mathcal{E}^-$ .

The background knowledge  $\mathcal{B}$  is a prior knowledge which contributes in learning the hypothesis. It indirectly restricts the hypothesis search space, as the learned hypothesis  $\mathcal{H}$  should be consistent with the background knowledge as well as the training examples.

A hypothesis  $\mathcal{H}$  is said to cover an example  $e$  given a background knowledge  $\mathcal{B}$  ( $\text{covers}(\mathcal{B} \cup \mathcal{H}, e)$ ) if the example satisfies the hypothesis and background knowledge. In logic programming where the  $\mathcal{H}$  is a set of program clauses and an example is a ground fact, it means that  $e$  is entailed by  $\mathcal{B} \cup \mathcal{H}$ .

$$\text{covers}(\mathcal{B} \cup \mathcal{H}, e) = \text{true} \quad \text{if} \quad \mathcal{B} \cup \mathcal{H} \models e$$

We can also define a covering function for a set of examples which returns a subset with the examples entailed by  $\mathcal{B} \cup \mathcal{H}$ :

$$\text{covers}(\mathcal{B} \cup \mathcal{H}, \mathcal{E}) = \{e \in \mathcal{E} \mid \mathcal{B} \cup \mathcal{H} \models e\}$$

Therewith, we can define two important concepts in inductive learning:

- **Completeness:** A hypothesis  $\mathcal{H}$  is complete with respect to background knowledge  $\mathcal{B}$  and examples  $\mathcal{E}$  if all the positive examples are covered, or in other words:  $\text{covers}(\mathcal{B}, \mathcal{H}, \mathcal{E}^+) = \mathcal{E}^+$
- **Consistency:** A hypothesis  $\mathcal{H}$  is consistent with respect to background knowledge  $\mathcal{B}$  and examples  $\mathcal{E}$  if no negative examples are covered, or in other words:  $\text{covers}(\mathcal{B}, \mathcal{H}, \mathcal{E}^-) = \emptyset$

The objective of learning a concept requires a hypothesis that is complete and consistent with respect to the given concept training examples and background knowledge. The example shown in table ?? (presented in [? ]) illustrates a simple problem of learning a hypothesis for the target relation  $\text{daughter}(X, Y)$ .

**Table 2.1:** A simple ILP problem: learning the *daughter* relation.

Training Examples	Background Knowledge
$\text{daughter}(\text{mary}, \text{ann}) \oplus$	$\text{parent}(\text{ann}, \text{mary}).$
$\text{daughter}(\text{eve}, \text{tom}) \oplus$	$\text{parent}(\text{ann}, \text{tom}).$
$\text{daughter}(\text{tom}, \text{ann}) \ominus$	$\text{parent}(\text{tom}, \text{eve}).$
$\text{daughter}(\text{eve}, \text{ann}) \ominus$	$\text{parent}(\text{tom}, \text{ian}).$
	$\text{female}(\text{ann}).$
	$\text{female}(\text{mary}).$
	$\text{female}(\text{eve}).$

If we consider, for example, the language of safe datalog clauses, it is possible to formulate the following complete and consistent hypothesis:

$$\mathcal{H} = \text{daughter}(X, Y) \text{ :- } \text{female}(X), \text{parent}(Y, X)$$

### 2.2.1 Searching the Hypothesis Space

In ILP, the hypothesis space is determined by the language of the programs  $\mathcal{L}$  consisting of the possible program clauses allowed by the language. Also, the vocabulary of predicate symbols is determined by the predicates from the background knowledge  $\mathcal{B}$ .

It is useful to structure the search space with partial ordering into a set of clauses based on  $\theta$ -subsumption in order to systematically search the program clauses space. A clause  $c$   $\theta$ -subsumes  $c'$  if there's a substitution  $\theta$  such that clause  $c\theta \subseteq c'$ . This also introduces a notion of generality, where clause  $c$  is at least as generally as  $c'$ , or in other words,  $c'$  is a specialization of  $c$ .

For example, if we have the following  $c$  and  $c'$ :

$$\begin{aligned} c &= \text{daughter}(X, Y) \text{ :- } \text{parent}(Y, X) \\ c' &= \text{daughter}(X, Y) \text{ :- } \text{female}(X), \text{parent}(Y, X) \end{aligned}$$

we know that for that  $c'$  is a specialization of  $c$  because for  $\theta = \emptyset$ ,  $c \subseteq c'$  since:

$$\{\text{daughter}(X, Y), \neg \text{parent}(Y, X)\} \subset \{\text{daughter}(X, Y), \neg \text{female}(X), \neg \text{parent}(Y, X)\}$$

To better illustrate it, if we have:

$$\begin{aligned} c &= \text{livesIn}(X, Y) \text{ :- } \text{marriedTo}(X, Z), \text{livesIn}(Z, Y) \\ c' &= \text{livesIn}(X, \text{germany}) \text{ :- } \text{marriedTo}(X, Z), \text{livesIn}(Z, \text{germany}) \end{aligned}$$

we know that  $c'$  is a specialization of  $c$  because with the substitution  $\theta = \{Y/\text{germany}\}$ ,  $c\theta = c'$ .

This notion gives us an important property that can be used for pruning parts of the search space:

- When generalizing from  $c$  to  $c'$ , all the examples covered by  $c$  are also covered by  $c'$ . So if  $c$  is inconsistent, then all its generalizations are inconsistent as well.
- When specializing from  $c$  to  $c'$ , an example not covered by  $c$  will neither be covered by  $c'$ . So if  $c'$  does not cover any positive examples, neither do any its specializations.

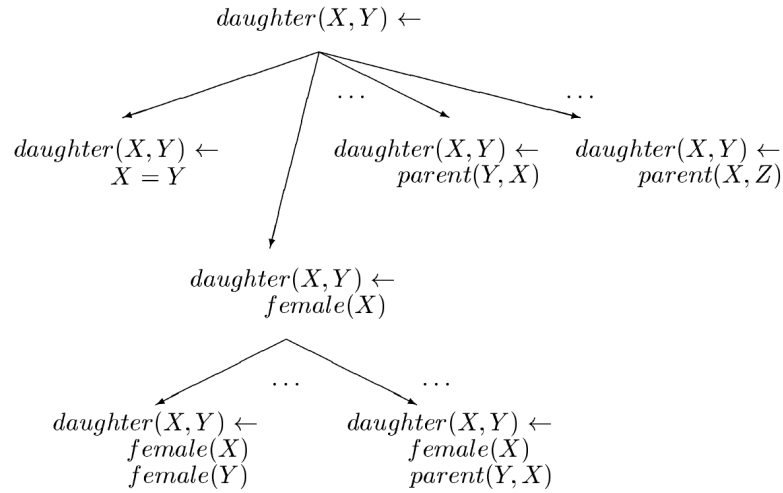
These properties are the basis for two main search approaches:

- Bottom-up: starts with less general clauses and searches least general generalizations
- Top-down: starts with more general clauses and searches for most general consistent specializations

As in this thesis we work only with the top-down approach, we will discuss it in more details in the next subsection. Further information about bottom-up approach can be found in [? ].

### 2.2.2 Top-Down ILP

The search space of program clauses can be viewed as a lattice, structured by  $\theta$ -subsumption generality ordering. Such lattice is called a *refinement graph*, which can be used to direct the search from most general to specific hypothesis. The figure ?? illustrates a part of the refinement graph for the family relation example shown in table ??.



**Figure 2.1:** Part of the refinement graph for the family relations problem

In such graph, nodes are program clauses and arcs are refinement operations, which can be of two kinds:

- Apply a substitution on the clause
- Add a literal to the body of the clause

The top-down algorithm consists basically of a specialization loop that refines a clause ensuring consistency embedded inside a covering loop that adds clauses to the hypothesis

ensuring completeness. Each loop has a stopping criterion, the covering loop iterates until it satisfies a sufficiency criterion and the specialization loop iterates until it satisfies a necessity criterion. The algorithm 1 shows in more details how the generic top-down ILP works.

---

**Algorithm 1:** Generic top-down specialization ILP algorithm

---

**Input:**  $\mathcal{E}$ : Training examples,  $\mathcal{B}$ : Background knowledge

**Result:**  $\mathcal{H}$ : Learned hypothesis

// Initialize the current training set and hypothesis

$\mathcal{E}_{cur} \leftarrow \mathcal{E}$  ;

$\mathcal{H} \leftarrow \emptyset$  ;

**repeat**Covering Loop

    // Initialize clause with empty body

$c \leftarrow T := \emptyset$  ;

**repeat**Specialization Loop

$c_{best} \leftarrow$  Best refinement of  $c$ ;  $c \leftarrow c_{best}$  ;

**until** *Necessity Stopping Criterion is satisfied*;

    // Add clause to the hypothesis

$\mathcal{H} \leftarrow \mathcal{H} \cup \{c\}$  ;

    // Remove positive examples covered by the new hypothesis

$\mathcal{E}_{cur} \leftarrow \mathcal{E}_{cur} - \text{covers}(\mathcal{B} \cup \mathcal{H}, \mathcal{E}_{cur}^+)$  ;

**until** *Sufficiency Stopping Criterion is satisfied*;

---

In domains with perfect data, the stopping criteria require that all positive examples are covered (completeness) and no negative examples are covered (consistency). However, in practice many datasets have imperfect data. Such imperfection is usually of the following kinds, as described in [? ]:

- Noise: random errors in the training examples and background knowledge
- Insufficiently covered example space: too sparse training examples from which it is difficult to reliably detect correlations
- Inexactness: inappropriate or insufficient description language which does not contain an exact description of the target concept
- Missing values in the training example

In order to avoid the effects of imperfect data, ILP can use heuristics as stopping criteria which tolerate some level of incompleteness and inconsistency. The simplest heuristic is the expected accuracy of a clause, which is defined as the probability that an example covered by the clause is labeled as positive:

$$A(c) = P(e \in \mathcal{E}^+ | c) = \frac{n^+(c)}{n^+(c) + n^-(c)} \quad (2.1)$$

where  $n^+(c)$  is the number of positive and  $n^-(c)$  the number of negative examples covered by  $c$ .

### 2.2.3 ILP Complexity

As discussed in [? ], the complexity of ILP resides at the second level of polynomial hierarchy and it is  $\Sigma_2^P$ -complete. Thus, there are two sources of complexity:

- Choice problem:
- Checking problem: checking if a choice was good or not

As ILP complexity grows exponentially with the number of literals, it is common to restrict the number of literals allowed in a clause in order to reduce execution time. [Sampling,MaxLiterals]

## 2.3 Association Rule Mining

[? ] [? ]

Association Rule Mining is method for discovering interesting relations between variables in large databases. It is intended to work on a database composed by a set of transactions  $\mathcal{D} = \{t_1, t_2, \dots, t_m\}$  and a set of items  $\mathcal{I} = \{i_1, i_2, \dots, i_n\}$ . Each transaction  $\mathcal{T}$  consists of a set of items which is subset of  $\mathcal{I}$ , which is usually represented by a binary vector of size  $n$  indicating the presence of absence of items in the transaction.

The objective of association rule mining is to learn inference rules of the form  $X \Rightarrow Y$ , where  $X, Y \subseteq \mathcal{I}$  and  $X \cap Y = \emptyset$ . Rules are selected according to various interestingness measures that will be subsequently discussed.

### 2.3.1 Measures

In this subsection we will discuss measures used for selecting interesting rules in the mining process.

We say a transaction  $\mathcal{T}$  supports an itemset  $\mathcal{X} \subseteq \mathcal{I}$  if  $\mathcal{X} \subseteq \mathcal{T}$ . The support measure  $supp(\mathcal{X})$  is defined as the ratio between the number of transactions supporting  $\mathcal{X}$  and the total size of the database  $\mathcal{D}$ :

$$supp(X) = \frac{|\{\mathcal{T} \in \mathcal{D} | X \subseteq \mathcal{T}\}|}{|\mathcal{D}|} \quad (2.2)$$

The support of a rule  $X \Rightarrow Y$  is defined as:

$$supp(X \Rightarrow Y) = supp(X \cup Y) \quad (2.3)$$

The confidence of a rule  $X \Rightarrow Y$ , which can may be interpreted as the probability of the the head given the body  $P(Y|X)$ , is defined as:

$$conf(X \Rightarrow Y) = \frac{supp(X \cup Y)}{supp(X)} \quad (2.4)$$

Confidence and support are the two measures used in classical association rule mining. Albeit, there are other relevant measures such as *lift*. It measures how different the observed rule support is in comparison to that expected if  $X$  and  $Y$  were independent:

$$lift(X \Rightarrow Y) = \frac{supp(X \Rightarrow Y)}{supp(X)supp(Y)} \quad (2.5)$$

A lift value 1 would imply that  $X$  and  $Y$  are independent, therefore any rule involving both itemsets does not make sense. A lift value greater than 1, provides information about the level of dependence between both variables. Higher lift values makes a rule potentially more interesting.

### 2.3.2 Anti-monotonicity of Support

An important characteristic of the support measure is the anti-monotonicity. It means that for any itemset  $X \subseteq \mathcal{I}$  if we have another itemset  $Y \subseteq \mathcal{I}$  such that  $X \subseteq Y$ , then the support of  $Y$  cannot be greater than the support of  $X$ . In other words, all subsets from a frequent itemset are also frequent, and all supersets from an infrequent item are also infrequent.

When searching for frequent itemsets, this characteristic plays a key role in pruning the search space, which grows exponentially with the number of items  $n$ . The set of possible itemsets is the power set over  $\mathcal{I}$ , which has size  $2^n - 1$ . As association rules are usually required to satisfy a specified minimum support, if we know that a given itemset does not satisfy it, we can automatically prune all its supersets.



### 2.3.3 Itemset Lattice

The problem of searching frequent itemsets (FI), i.e., itemsets that satisfy the specified minimum support, can be structured in a lattice. Firstly, an itemset is frequent if it has support greater or equal than an arbitrarily specified minimum support.

There are two special kinds of itemsets:

- Maximal frequent itemset (MFI): a frequent itemset is maximal if none of its immediate supersets are frequent.
- Closed frequent itemset (CFI): a frequent itemset is closed if all of its immediate supersets have lower support.

Each of these kinds of itemsets has an special property. By knowing all the maximal itemsets of a database, we also know all the frequent itemsets. Nevertheless, it is not possible to know the support of each of the frequent itemsets. By knowing all the closed of a database, it is possible to know the all the frequent itemsets as well as their supports.

In the example of database  $\mathcal{D}$  shown in table ?? with resulting itemset lattice shown in figure 2.2, frequent itemsets are shown with thicker border. The minimum support threshold was set to  $\frac{2}{5}$ , so the frequent itemsets are the ones with frequency greater than or equal to 2. For this example, we would have as maximal itemset  $\{ABCE\}$  and as closed itemsets  $\{ABCE, BCE, BE\}$

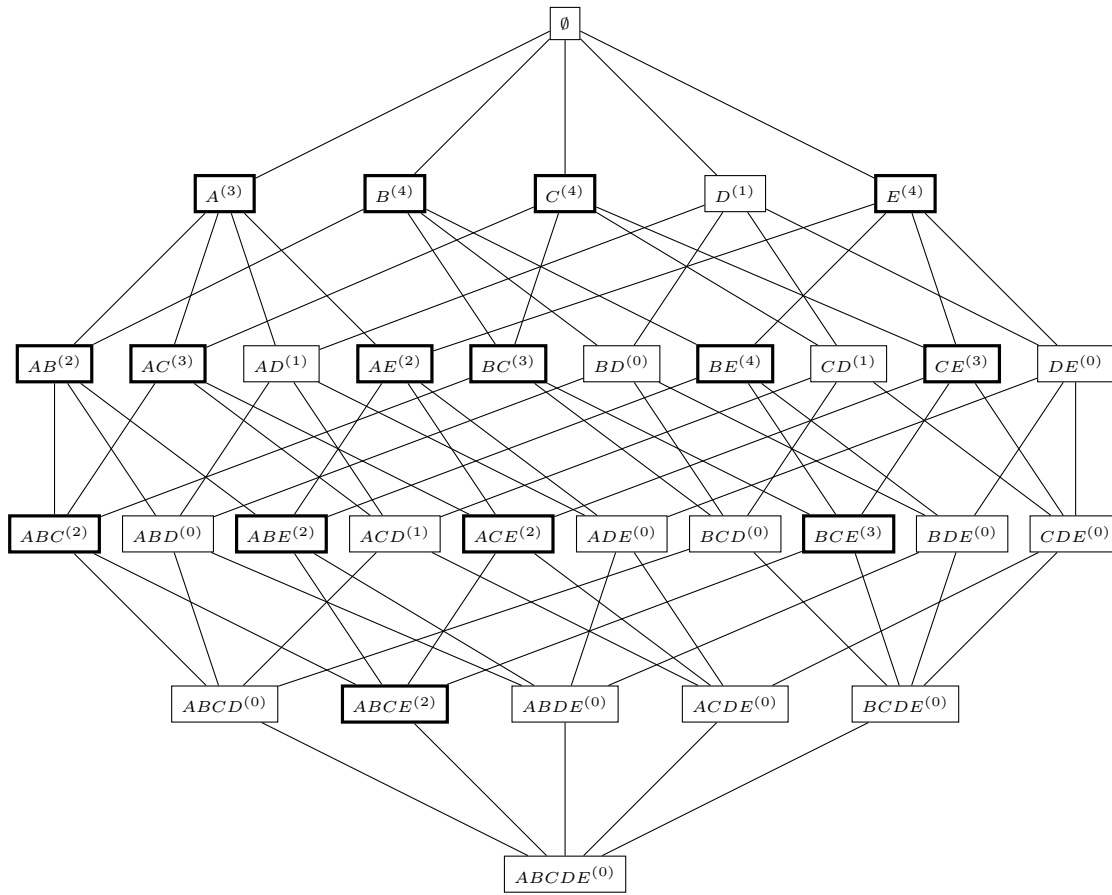
TID	Items			
1	A	C	D	
2	B	C	E	
3	A	B	C	E
4	B	E		
5	A	B	C	E

**Table 2.2:** Example of transaction database  $\mathcal{D}$  [?] ]

[...]

### 2.3.4 Apriori Algorithm

The apriori algorithm is a method for searching frequent itemsets which explores the anti-monotonic property of the support measure. It computes the itemsets support iteratively, by ascending order of size. The process takes  $k$  iterations where  $k$  is the size

**Figure 2.2:** Itemset Lattice example

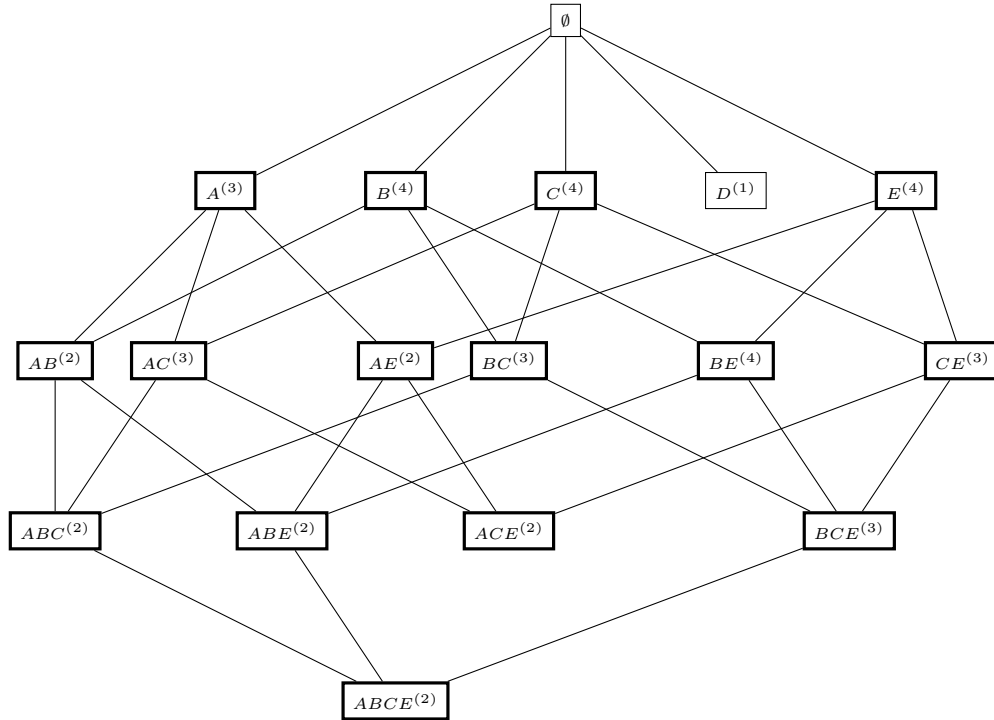
of the largest frequent itemset. In each iteration  $i \leq k$ , the database is scanned once and all the support of all itemsets of size  $i$  are computed.

In the first iteration, all itemsets of size 1 have their supports computed. On the  $1 < i \leq k$  subsequent iterations, a set of candidates  $C_i$  is created by joining the frequent itemsets of size  $i - 1$  found in the previous iteration. Two itemsets of size  $i$  can only join if they share  $i - 1$  items, so their union can form an itemset of size  $i + 1$ . Only after finding the set of candidate itemsets  $C_1$ , the database is scanned in order to determine the support of each of them. The algorithm 2 shows in more details how the apriori algorithm works.

For the previous example of database ??, the itemset lattice generated by the apriori algorithm is shown in figure 2.2.

## 2.4 Discretization of Numerical Attributes

Discretization of continuous features is a very important tool frequently used in statistics, data mining and machine learning. It is a pre-processing technique which is used for

**Algorithm 2:** Apriori frequent itemset discovery**Input:**  $\mathcal{D}$ : Database of transactions**Result:**  $\mathcal{H}$ : Learned hypothesis $L_1 \leftarrow$  Frequent itemsets of size 1 ; $L \leftarrow L_1$  ; $k \leftarrow 1$  ;**while**  $L_{k-1} \neq \emptyset$  **do**     $C_k \leftarrow \text{aprioriGen}(L_{k-1})$  ;    **forall** the  $t \in \mathcal{D}$  **do**         $C_t \leftarrow \{c | c \in C_k \wedge c \subseteq t\}$  ;        **forall** the  $c \in C_t$  **do**             $c.\text{frequency} \leftarrow c.\text{frequency} + 1$  ;     $L_k \leftarrow \{c | c \in C_k \wedge c.\text{frequency} \geq \text{minSupport}\}$  ;     $L \leftarrow L \cup L_k$  ;     $k \leftarrow k + 1$  ;**return**  $L$  ;**Figure 2.3:** Itemset Lattice example

reducing the effects of observation errors. It is basically a form of quantization where the original data values in a given interval are replaced by a representative value of that interval.

Discretization techniques can be divided in supervised and unsupervised methods. The first requires the objects to be labeled with classes, and the domain is discretized with the objective of reducing the class entropies. The second one doesn't consider object

classes, only object frequencies. Unsupervised methods normally require the number of buckets to be arbitrarily defined.

Various different supervised and unsupervised methods for discretization of continuous features are discussed in [? ]. To build the lattice we don't use labels for the examples so we just use unsupervised methods.

Supervised methods can be used for finding interesting intervals in the rules, by considering positive and negative examples as labels. However, it is out of the scope of this thesis, thus we will not discuss them in details.

### 2.4.1 Equal Width

This unsupervised discretization method consists of simply querying both the maximum and minimum values of the root's numerical attribute, then for splitting this interval into  $k$  buckets of same width  $w$ :

$$w = \frac{max - min}{k} \quad (2.6)$$

It's the simplest and most straightforward discretization method, but its main problem is that it is highly sensitive to outliers that may drastically skew the resulting distribution.

### 2.4.2 Equal Frequencies

In this also unsupervised discretization method, the domain is divided in buckets with equal frequency. That is, given a total frequency  $m$ , the domain is discretized in  $k$  buckets such that each has frequency  $\frac{m}{k}$ . Multiple objects with same numerical attribute value might make it impossible to find bucket boundaries that equally distribute the frequencies.

The greatest advantage of this method is that it always results in a distribution with lowest possible entropy, i.e. distribution is always uniform or as close to uniformity as possible.

## 2.5 Mining Optimized Rules for Numeric Attributes

In [1], a technique for efficient learning association rules with interesting ranges for numerical attributes is presented. It focuses on finding numerical intervals which optimize

a specific interestingness measure, given the confidence and support distribution of a rule along a numerical attribute.

Such rules have the form  $(A_1 \in [l_1, u_1]) \wedge C_1 \rightarrow C_2$ , where  $A_1$  is a numerical attribute,  $l_1$  and  $u_1$  are the lower and upper boundaries of  $A_1$ , and  $C_1$  and  $C_2$  contain only instantiated conditions.

The authors propose algorithms for determining values for the boundaries  $l_1$  and  $u_1$  for the following cases:

- Optimized confidence: the rule confidence is maximized and support of the condition  $(A_1 \in [l_1, u_1]) \wedge C_1$  is at least the specified minimum support.
- Optimized support: the support of the condition  $(A_1 \in [l_1, u_1]) \wedge C_1$  is maximized and the rule confidence is at least the specified minimum confidence.
- Optimized gain: the rule gain is maximized and the confidence is at least the specified minimum confidence.

[Add pseudo-algorithm and some more discussion]

## 2.6 Information Theoretic Measures

Information-theoretic measures are widely used in various different learning processes. Its importance lies on its power to measure importance of attributes and relationships between attributes. An attribute is considered important in data mining if regularities are encountered in smaller populations obtained based on the values of such attribute, but not in the larger population. Such regularities are identifiable by lower entropy values, indicating that interesting attributes lead to entropy reduction. More specifically, the entropy reduction is the difference between the entropy of the decision attribute and the conditional entropy of the decision attribute given a particular attribute, whose importance we want to investigate.

Let's say we have  $X$  as decision attribute and it divides the set of objects  $\mathcal{U}$  into a group of disjoint subsets defined by the value  $x \in \mathcal{X}$  of  $X$ , where  $\mathcal{X}$  is the non-empty set of values for  $X$ . Also, let's define  $I_X : \mathcal{U} \rightarrow \mathcal{X}$  is an information function that gives the value of attribute  $X$  for an object  $t \in \mathcal{U}$ . The set of objects  $m(X = x) \subseteq \mathcal{U}$ , whose value for  $X$  is  $x$  is defined as follows:

$$m(X = x) = m(x) = \{t \in \mathcal{U} | I_X(t) = x\} \quad (2.7)$$

With that, the probability distribution of  $X$  is defined by:

$$P(X = x) = P(x) = \frac{|m(x)|}{|\mathcal{U}|}, \quad x \in \mathcal{X} \quad (2.8)$$

Information theoretic measures are defined over probability distributions. They can measure the importance of an attribute, attribute association, or dissimilarity or similarity of populations. In the next subsections, we will discuss some of the most important measures.

### 2.6.1 Shannon's Entropy

The Shannon's entropy measure  $H$  is a non-negative function which may be interpreted as a measure of the information content or uncertainty about an attribute  $X$ . It is defined over a probability distribution of  $X$ :

$$\begin{aligned} H(P(X)) = H(X) &= E_{P(X)}[-\log P(X)] \\ &= - \sum_{x \in \mathcal{X}} P(x) \log P(x) \end{aligned} \quad (2.9)$$

The entropy of  $X$  is maximum if its probability distribution is uniform and minimum if the whole population is concentrated on a specific value  $x_c \in \mathcal{X}$ , i.e.  $P(x_c) = 1$  and  $P(x) = 0, x \neq x_c$ . The higher the entropy, the higher the uncertainty about  $X$  attribute value, and an entropy zero means complete certainty about the value of  $X$  since  $P(x_c) = 1$ .

### 2.6.2 Kullback-Leibler Divergence

The Kullback-Leibler divergence  $D(P||Q)$  between the population distributions  $P(X)$  and  $Q(X)$ , also known as  $I$ -divergence, measures the degree of deviation of  $P$  from another distribution  $Q$ :

$$\begin{aligned} D_{KL}(P||Q) &= E_{P(X)} \left[ \frac{P(X)}{Q(X)} \right] \\ &= \sum_{x \in \mathcal{X}} P(x) \log \left( \frac{P(x)}{Q(x)} \right) \end{aligned} \quad (2.10)$$

This divergence measure is a premetric but not a metric distance. It is non-negative and it becomes zero if  $P(x) = Q(x)$ ,  $\forall x \in \mathcal{X}$ , but it doesn't satisfy the symmetry and the triangle inequality properties.

There are symmetrized divergence measures based on the Kullback-Leibler, e.g. the  $J$ -divergence<sup>2.11</sup> and the Jensen-Shannon divergence<sup>2.12</sup>:

$$D_J(P||Q) = D_{KL}(P||Q) + D_{KL}(Q||P) \quad (2.11)$$

$$D_{JS}(P||Q) = \frac{1}{2}D_{KL}(P||M) + \frac{1}{2}D_{KL}(Q||M) \quad (2.12)$$

where  $M$  is the average of the two distributions,  $M = \frac{1}{2}(P + Q)$ .

The Jensen-Shannon divergence also has the advantage that the difference is always a finite value ( $0 \leq D_{JS}(P||Q) \leq 1$ , for the base 2 logarithm). Although, it still does not satisfy the triangle inequality property, its square root does and, therefore, is a metric.

### 2.6.3 Mutual Information

The divergence measure can be used for computing the degree of independence between two attributes  $X$  and  $Y$ . This is done by simply measuring the divergence between the observed joint distribution  $P(X, Y)$  and the independent distribution formed by the marginals  $P(X)P(Y)$ . We call such measure mutual information:

$$\begin{aligned} I(X; Y) &= D(P(X, Y)||P(X)P(Y)) \\ &= E_{P(X, Y)} \left[ \log \frac{P(x, y)}{P(x)P(y)} \right] \\ &= \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} P(x, y) \log \frac{P(x, y)}{P(x)P(y)} \end{aligned} \quad (2.13)$$

Completely independent attributes have mutual information zero, and the greater the level of dependence, the greater the mutual information.

[2] [ ? ]

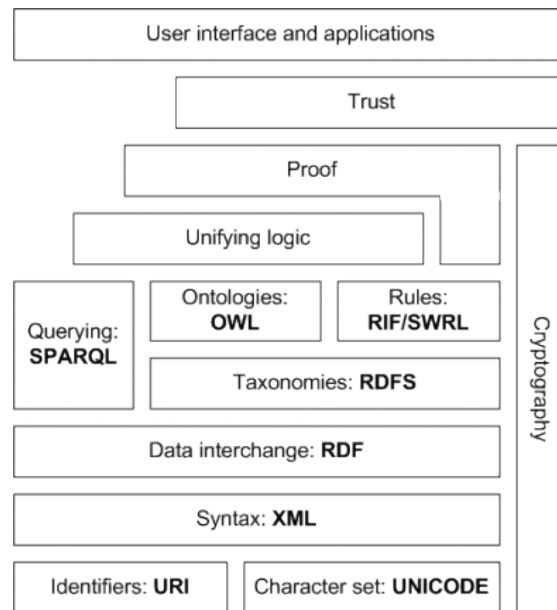


Figure 2.4: Semantic Web stack

## 2.7 Semantic Web Applications

The Semantic Web is, according to its official website, a technology created by the World Wide Web Consortium (W3C) to enable the so-called “Web of data”, enabling computers to do more useful work and develop systems that can support trusted interactions over the network.

It consists of a set of technologies and formats which aim to make web resources more readily accessible to automated processes. The semantic web stack, in figure ?? <sup>1</sup>, illustrates the semantic web architecture showing how its standards are organized and how it extends the classical hypertext web.

- Resource Description Framework (RDF): a framework for creating statements in the form of triples composed by subject, predicate and object. It uses URIs to name the predicates as well as the entities, which may be the subject or object in a triple. RDF can be encoded in a variety of formats, such as RDF/XML, N3, Turtle and N-Triples.
- RDF Schema (RDFS): a RDF vocabulary description language which provides basic elements for the description of ontologies (or RDF vocabularies) intended to structure RDF resources known as constructs (RDFS classes, associated properties, and utility properties).

<sup>1</sup>Semantic Web - XML2000, slide 10". W3C: <http://www.w3.org/2000/Talks/1206-xml2k-tbl/slide10-0.html>



- Web Ontology Language (OWL): a semantic markup language for publishing and sharing ontologies on the web. It is a vocabulary extension of RDF that allows an ontology to be described with a set of axioms which places constraints on classes and the types of relationships permitted between them.
- SPARQL: an RDF query language for databases which can be used to express queries across diverse data sources. It consists of triple patterns, conjunctions, disjunctions and optional patterns.
- Rule Interchange Format (RIF): defines a standard for exchanging rules among rule systems. It focuses on exchange rather than defining a single one-fits-all rule language, different databases might have different characteristics with different necessities.
- Semantic Web Rule Language (SWRL): a proposal for rule language combining sublanguages of OWL with the Unary/Binary Datalog Rule Markup Language (RuleML).

## 2.8 Linked Open Data Applications

The Semantic Web does not need only access to reachable and manageable data in a standard format, but also relationships among data from different sources. Therewith, it is possible to create a huge collection of interrelated datasets in the Web, also referred as Linked Data.

Linked Data is a fundamental part of the Semantic Web essence, facilitating a large scale integration and reasoning on data on the Web. A typical example of Linked dataset is DBpedia<sup>2</sup>. It basically extracts information from Wikipedia and make it available in RDF incorporating links to other datasets on the web, such as Geonames<sup>3</sup>, YAGO<sup>4</sup>, LinkedMDB<sup>5</sup> and USCensus<sup>6</sup>. With such linkage, it allows applications to exploit the extra information these datasets can provide, integrating facts from various different sources. Figure ?? shows the Linked Open Data cloud diagram,

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<sup>2</sup><http://www.dbpedia.org/>

<sup>3</sup><http://www.geonames.org/>

<sup>4</sup><http://www.mpi-inf.mpg.de/yago-naga/yago/>

<sup>5</sup><http://www.linkedmdb.org/>

<sup>6</sup><http://www.linkedmdb.org/>



<http://lod-cloud.net>

## Chapter 3

# Learning Rules With Numerical and Categorical Attributes

In this chapter we will discuss what kind of rules we are interested in, define what categorical properties are, describe in more details a Correlation Lattice, how to build it and integrate it in the core ILP learning algorithm.

### 3.1 Interesting Rule Definition

In this section we formally define what kind of rules we are interested in obtaining with the algorithm proposed in this thesis. As briefly explained in the introduction, the objective is to learn rules with numerical properties, focusing on searching ranges in the numerical attribute's domain that satisfy support and confidence thresholds.

Searching numerical intervals for a base-rule that already satisfies confidence threshold is not so interesting. The base-rule itself implicitly specifies an interval which covers the whole numerical attribute domain from any possible refined-rules. Moreover, even if for some specific range we have a higher confidence value, the gain in comparison to the base-rule would not be so great as the base-rule already present a high confidence value (at least higher than the specified threshold).

More precisely, if we have a confidence threshold  $TS_{conf}$  and defining confidence gain from a refined-rule  $r_2$  in comparison to a base-rule  $r_1$  as  $g_{r_2, r_1}$  as:

$$g_{r_2, r_1} = \frac{conf_{r_2}}{conf_{r_1}} \quad (3.1)$$

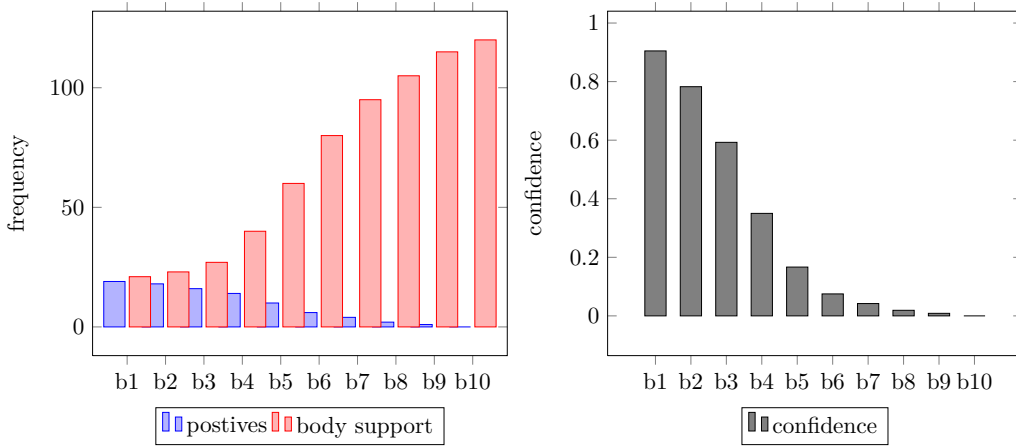
As we know that  $r_1 \geq TS_{conf}$ , then  $g_{r_2, r_1}$  is upper-bounded by:

$$g_{r_2, r_1} \leq \frac{1}{TS_{conf}} \quad (3.2)$$

More interesting for us would be base rules which satisfy the support threshold but does not satisfy the confidence threshold, or which satisfies a quite low confidence threshold. In such case, if we have a non-uniform confidence distribution along the buckets, it is possible that, for some specific intervals, its correspondent refined-rule satisfies both thresholds, therefore potentially having a significant confidence gain.

In figure ??, we illustrate that with an ideal example where positive examples and body support have completely different distributions and thus produce a very interesting confidence distribution. Such distribution is obtained thanks to the divergent rule's positives and body support distributions. This is shown in figure ??, where we obtained these distributions by normalizing the frequency histograms from the rule's positive examples and body support.

**Figure 3.1:** Example of frequency histograms from body support and positives support (left), and resulting confidence distribution (right)

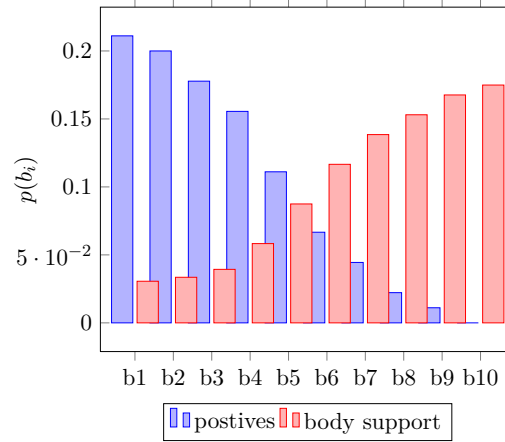


## 3.2 Categorical Property Definition

In this section, we formally define a categorical property as used in the Correlation Lattice.

First of all, a candidate relation must be joined with root join variable variable  $X$

A candidate categorical relation  $r(X, Z)$ , where  $X \in \mathcal{X}$  is the join variable and  $Z$  is within a categorical domain  $\mathcal{Z}$  with a finite number of categories  $\{z_1, z_2, \dots, z_n\}$ , such that:

**Figure 3.2:** Support distribution of body and positives from figure ??

$$\mathcal{X}_{z_i} = \{x | x \in \mathcal{X} \wedge \exists r(x, z_i)\}$$

Typically,  $\sum_{i=1}^k |\mathcal{X}_{z_i}| \ll k$  and  $\mathcal{X}_{z_i} \subseteq \mathcal{X}$  with  $|\mathcal{X}_{z_i}| < |\mathcal{X}|$

hasIncome(john,20000)	hasSex(john,male)
hasIncome(mike,30000)	hasSex(mike,male)
hasIncome(anne,25000)	hasSex(anne,female)
hasIncome(mary,5000)	hasSex(mary,female)
hasIncome(lisa,10000)	hasSex(lisa,female)
hasIncome(paul,0)	hasSex(paul,male)

For the table 3.2.2, if we define  $\mathcal{X} = \{x | \exists hasIncome(x, Y), Y \in \mathcal{Y}\}$ , then we would have the following sub-populations of  $\mathcal{X}$ :

$$\begin{aligned}
 \mathcal{X}_{male} &= \{x | x \in \mathcal{X} \wedge \exists hasSex(x, male)\} \\
 &= \{john, mike, paul\} \\
 \mathcal{X}_{female} &= \{x | x \in \mathcal{X} \wedge \exists hasSex(x, female)\} \\
 &= \{anne, mary, lisa\}
 \end{aligned}$$

The *rdf:type* property, for example, is also covered by this definition with the entity types being the categories.

A categorical property can be overlapping, i.e. with intersecting categories, or not. A non-overlapping categorical property  $r(X, Z)$ , such as *hasSex*, is defined as:

$$\mathcal{X}_{z_i} \cap \mathcal{X}_{z_j} = \emptyset, \quad \forall z_i, z_j \in \mathcal{Z}, i \neq j$$

This definition of categorical property might be too restrictive, therefore, in the next sections, we broaden this definition by applying different techniques.

### 3.2.1 Numerical Properties as Categorical

Numerical properties with very large or infinite domain can also be dealt as categorical, by simply applying a bucketing function that maps its numerical domain into a finite set of  $k$  buckets. For example, we can use a discretization function  $b$  to turn a numerical property  $r(X, Z)$ , with  $Z \in \mathbb{R}$ , into a non-overlapping categorical property:

$$b : \mathbb{R} \rightarrow \mathcal{B}, \text{ where } \mathcal{B} = \{1, 2, \dots, k\}$$

$$r(X, b(Z)) \equiv r'(X, B), \quad B \in \mathcal{B}$$

### 3.2.2 Combination Categorical Property with Linking Relation

We can also broaden this definition by composing a categorical property with linking relations. Therewith, it is possible to use categorical relations that do not directly join with root's join variable  $X$

If a functional relation  $r_1$  and a categorical  $r_2$ :

$$r_1(X, W) \equiv f_1 : \mathcal{X} \rightarrow \mathcal{W}$$

$$r_2(W, Z), \quad Z \in \mathcal{Z} = \{z_1, z_2, \dots, z_k\} \text{ is a categorical domain and}$$

Then  $r'(X, Z) \equiv r_1(X, W), r_2(W, Z) \equiv r_2(f_1(X), Z)$  is a composed categorical relation.

With that, different knowledge bases can be interconnected by simply applying this definition with *owl:sameAs* as linking relation. This allows to broaden the set of categorical properties to be analyzed in the Correlation Lattice to those contained in interlinked datasets.

<code>owl:sameAs(john,johnSmith)</code>	<code>hasProfession(johnSmith,teacher)</code>
<code>owl:sameAs(mike,mikeBell)</code>	<code>hasProfession(mikeBell,actor)</code>
<code>owl:sameAs(anne,anneSmith)</code>	<code>hasProfession(anneSmith,doctor)</code>
<code>owl:sameAs(lisa,lisaBell)</code>	<code>hasProfession(lisaBell,teacher)</code>

### 3.2.3 Absence or Presence of a Property as Categories

Another possibility is to define categories for presence or absence of supporting examples for properties. With this approach, one can also include non-categorical properties

into the Correlation Lattice and have insight about how the presence or absence of such property affects the distribution of root's numerical attribute.

In this case we must consider a property which does not have examples for all its domain. For example, the property  $isParentOf(x,y)$  has as both domain and range type Person. If not all the Person instances of the knowledge base have supporting facts for the relation  $isParentOf$ , then we can split the instances in two categories: the ones that are covered by the property and the ones that are not. For example, let  $hasIncome$  be the root property and let's assume we have a knowledge base with the following facts:

```
hasIncome(john,20000)  isParentOf(john,mary)
hasIncome(mike,30000)  isParentOf(mike,paul)
hasIncome(anne,25000)  isParentOf(anne,paul)
hasIncome(mary,5000)   isParentOf(lisa,mary)
hasIncome(lisa,10000)
hasIncome(paul,0)
```

Then we could split the root node set  $\mathcal{X}$  in two categories  $\mathcal{X}_{parent} \in \mathcal{X}$  and its complement  $\mathcal{X}_{parent}^c \in \mathcal{X}$ :

$$\begin{aligned}\mathcal{X}_{parent} &= \{x | x \in \mathcal{X} \wedge \exists isParentOf(x, Z)\} \\ &= \{john, mike, anne, lisa\} \\ \mathcal{X}_{parent}^c &= \{x | x \in \mathcal{X} \wedge x \notin \mathcal{X}_{parent}\} \\ &= \{mary, paul\}\end{aligned}$$

As in this thesis we are under open world assumption and we don not consider negated literals in the hypothesis, we ignore the absence and just include the presence of relations in the lattice.

### 3.2.4 Notation Used

As we will see in the next sections, in the Correlation Lattice all the relations are joined by the variable of root's join argument  $X$ . So we will denote the presence of a property  $a(X, Z)$  category as simply  $a$ , where the variable  $Z$  is free and not set to any constant. If we have a categorical property  $a(X, z_i)$  with  $k$  different categories  $z_i \in \mathcal{Z} = \{z_1, z_2, \dots, z_k\}$ , we denote each of the  $a(X, z_i)$  as  $a_i$ .

So for example if we set the root relation  $r = hasIncome(X, Y)$  and categorical relations:

$$\begin{aligned} a(X, Z) &= isMarriedTo(X, Z) \\ b(X, W) &= hasSex(X, W), \quad W \in \mathcal{W} = \{male, female\} \\ c(X, V) &= bornInMonth(X, V), \quad V \in \mathcal{V} = \{january, february, \dots, december\} \end{aligned}$$

With such notation, we can write large clauses in a much more concise way, such as in the examples below:

$$\begin{aligned} rab_1c_3 &= hasIncome(X, Y), isMarriedTo(X, Z), hasSex(X, male), bornInMonth(march) \\ rab_2c_{11} &= hasIncome(X, Y), isMarriedTo(X, Z), hasSex(X, female), bornInMonth(november) \end{aligned}$$

### 3.3 Preprocessing

In this section, we will present the preprocessing steps required by our proposed algorithm. It basically consists of first building a joinable relations map for each join pattern, according to relations domain and range types as well as support threshold. Afterwards, we search the available categorical properties for each numerical relation that will be used in the Correlation Lattice. At last we build the so called Correlation Lattice, which belongs to the preprocessing step but will be discussed in the next section.

#### 3.3.1 Relation Preprocessing

In this step, we focus on creating a map of joinable for each join pattern between two relations. As in this thesis we are working with RDF triples, we have four possible join patterns:

- Argument 1 on Argument 1: e.g.  $hasIncome(\mathbf{X}, Y)hasAge(\mathbf{x}, zZ)$
- Argument 1 on Argument 2: e.g.  $hasIncome(\mathbf{X}, Y)isMarriedTo(Z, \mathbf{x})$
- Argument 2 on Argument 1: e.g.  $livesIn(Y, \mathbf{X})isLocatedIn(\mathbf{X}, Z)$
- Argument 2 on Argument 2: e.g.  $livesIn(Y, \mathbf{X})wasBornIn(Z, \mathbf{X})$

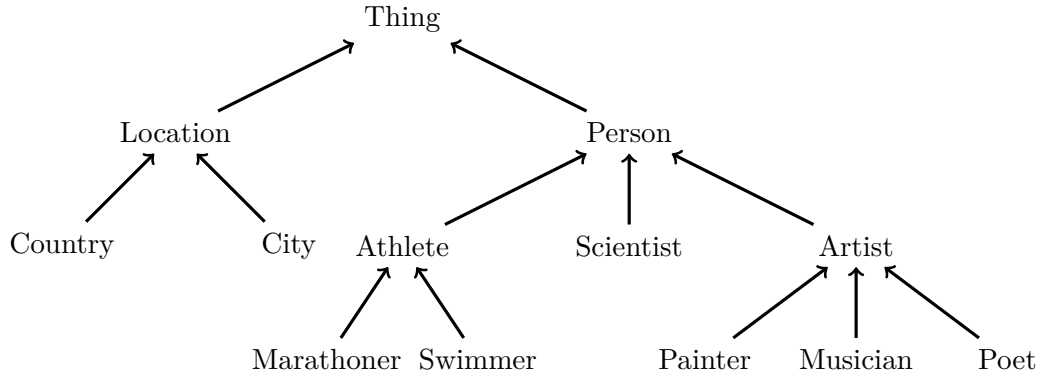
With that we could easily obtain all the possible pair of joinable relations for each join pattern, avoiding testing hypothesis containing invalid join pairs.



### 3.3.1.1 Exploiting Relation Range and Domain Types

A knowledge base is expected to have an ontology defining the structure of the stored data (the types of entities and their relationships). Additionally, every relation's range (type of 1<sup>st</sup> argument) and domain (type of 2<sup>nd</sup> argument) should be defined. These information can help us identify the allowed joining relations for each join pattern.

**Figure 3.3:** Type hierarchy example



Assuming that the knowledge base has its type hierarchy described with the relation *rdfs:subClassOf*, such as the example shown in figure ??, where in each arrow means that the tail is a subclass of the head. Also, we assume that every property has both argument types declared with *rdfs:domain* and *rdfs:range*. With such information, it is a straightforward task to prune out the pairs of joining relations not allowed by the type hierarchy.

For every possible pair of relations, we simply try to match the joining argument types from the 2 joining relations. We check whether they are equal or if one can be subsumed by the other. If so, then it is allowed to join the pair of relations on the given joining arguments, or in other words, the type hierarchy does not prevent them from joining. The pseudo-code for performing such task is shown in the Algorithm 3:

Nevertheless, it might be that in the knowledge base, the cardinality of such join might be zero or simply not exceed the support threshold. Thus, it is worth to that beforehand, and that is what will be explained in the next section.

### 3.3.1.2 Exploiting Support Monotonicity

Support is a monotonically decreasing measure in top-down ILP. So we know that by adding any literals to the hypothesis, we can only get a smaller or equal support. Therefore, for each pair of joinable relations in each of the join patterns, we can query the knowledge base and check whether they have enough supporting facts.

**Algorithm 3:** Function *checkTypes*

Checks whether two relations are joinable for a given join pattern

**Input:**  $r_i, r_j$ : Joining relations,  $arg_i, arg_j$ : Joining arguments**Output:** True if  $arg_i$  from  $r_i$  joins with  $arg_j$  from  $r_j$ , False otherwise

---

```

switch  $arg_i$  do
  case 1
     $type_i \leftarrow r_i.domain$  ;
  case 2
     $type_i \leftarrow r_i.range$  ;
switch  $arg_j$  do
  case 1
     $type_j \leftarrow r_j.domain$  ;
  case 2
     $type_j \leftarrow r_j.range$  ;
if  $type_i = type_j$  or  $subsumes(type_i, type_j)$  or  $subsumes(type_j, type_i)$  then
  | return true;
else
  | return false;

```

---

Thus, if any pair of relations does not reach the minimum support for a given join pattern, we know that any clause containing such join will therefore fail the support test as well, so we do not need to test such hypothesis in the core ILP algorithm.

**Algorithm 4:** Function *checkSupport*

Checks whether join support exceeds threshold

**Input:**  $r_i, r_j$ : Joining relations,  $arg_i, arg_j$ : Joining arguments, *supportThreshold*:

Support threshold

**Output:** True if join support exceeds threshold, False otherwise

---

```

switch ( $arg_i, arg_j$ ) do
  case (1, 1)
     $query \leftarrow \text{"select count distinct ?x where \{ ?x <r_i> ?y . ?x <r_j> ?z \}"} ;$ 
  case (1, 2)
     $query \leftarrow \text{"select count distinct ?x where \{ ?x <r_i> ?y . ?z <r_j> ?x \}"} ;$ 
  case (2, 1)
     $query \leftarrow \text{"select count distinct ?x where \{ ?y <r_i> ?x . ?x <r_j> ?z \}"} ;$ 
  case (2, 2)
     $query \leftarrow \text{"select count distinct ?x where \{ ?y <r_i> ?x . ?z <r_j> ?x \}"} ;$ 
 $joinSupport \leftarrow executeQuery(query);$ 
if  $joinSupport \geq supportThreshold$  then
  | return true;
else
  | return false;

```

---

The preprocessing is done by algorithm 5, which applies 3 and 4 on all the possible join pair combinations and extracting the valid ones, we can build 4 joining maps, one for each join pattern. Each map has relations as keys and a set of joinable relations as value. In the refinement step at the ILP algorithm, these maps will be queried in order to obtain suggestions of literals to be added.

---

**Algorithm 5:** Preprocessing algorithm

---

**Input:**  $r$ : Set of Relations, *supportThreshold*: The support threshold

**Result:**  $L_{m,n}(r_i)$ : List of joinable relations, where  $m, n \in \{1, 2\}, r_i \in r$

// Lists initialization

**foreach**  $r_i \in r$  **do**

$L_{1,1}(r_i) \leftarrow r_i$  ;

$L_{2,2}(r_i) \leftarrow r_i$  ;

$L_{1,2}(r_i) \leftarrow \emptyset$  ;

$L_{2,1}(r_i) \leftarrow \emptyset$  ;

// For every possible pair of relations

**foreach**  $r_i \in r$  **do**

**foreach**  $r_j \in r$  **and**  $j \geq i$  **do**

**if**  $r_i \neq r_j$  **then**

**if** *checkTypes*( $r_i, r_j, 1, 1$ ) **and** *checkSupport*( $r_i, r_j, 1, 1$ ) **then**

$L_{1,1}(r_i) \leftarrow L_{1,1}(r_i) \cup r_j$  ;

$L_{1,1}(r_j) \leftarrow L_{1,1}(r_j) \cup r_i$  ;

**if** *checkTypes*( $r_i, r_j, 2, 2$ ) **and** *checkSupport*( $r_i, r_j, 2, 2$ ) **then**

$L_{2,2}(r_i) \leftarrow L_{2,2}(r_i) \cup r_j$  ;

$L_{2,2}(r_j) \leftarrow L_{2,2}(r_j) \cup r_i$  ;

**if** *checkTypes*( $r_i, r_j, 1, 2$ ) **and** *checkSupport*( $r_i, r_j, 1, 2$ ) **then**

$L_{1,2}(r_i) \leftarrow L_{1,2}(r_i) \cup r_j$  ;

$L_{2,1}(r_j) \leftarrow L_{2,1}(r_j) \cup r_i$  ;

**if** *checkTypes*( $r_i, r_j, 2, 1$ ) **and** *checkSupport*( $r_i, r_j, 2, 1$ ) **then**

$L_{2,1}(r_i) \leftarrow L_{2,1}(r_i) \cup r_j$  ;

$L_{1,2}(r_j) \leftarrow L_{1,2}(r_j) \cup r_i$  ;

---

### 3.3.2

## 3.4 Correlation Lattice

The idea is to build during preprocessing a graph inspired in the itemset lattice that describes the influence of different categorical relations on a given numerical attribute's distribution. We call such graph a Correlation Lattice. Comparing to a Itemset Lattice, in a Correlation Lattice we have a set of categorical relations (that are joined with root property) instead of items. In addition, Each node in the graph has an associated histogram with the support distribution over the root's numerical attribute.

To illustrate the idea, let's analyze a simple real-world example with the  $hasIncome(X, Y)$  relation. If we have two categorical relations, one strongly correlated to income, e.g.  $hasEducation$ , and one uncorrelated (or very weakly correlated), e.g.  $wasBornInMonth$ .

Let's assume that for the relation  $wasBornInMonth(X, Z)$  we have the 12 months from the Gregorian Calendar as constants and for  $hasEducation(X, Z)$  we can have 10 different categorical constants for  $Z$ : "Preschool", "Kindergarten", "ElementarySchool", "MiddleSchool", "Highschool", "Professional School", "Associate's degree", "Bachelor's degree", "Master's degree" and "Doctorate degree".

It's expected that the income distribution will be roughly the same for people born in any of the months, whereas for different education levels, e.g. Elementary School and Doctoral Degree, their income distribution are expected to be different from each other them and different from the overall income distribution.

Based on this idea, we basically check how different categorical relations affect a numerical distribution. Such information, together with other measures such as support, provides valuable cues on what categorical attributes and what categorical constants might be the most interesting to be added to the hypothesis in the core ILP algorithm.

### 3.4.1 Building the Lattice

We first start with the chosen numerical property, for example  $hasIncome(X, Y)$ , which should have at least two arguments, one being a joining variable  $X$  and the other the numerical attribute variable  $Y$ . Firstly, we query the examples distribution along the numerical attribute  $Y$ , arbitrarily choose a number of buckets  $k$  and discretize its  $Y$ 's domain into buckets  $b_1, b_2, \dots, b_k$  using any unsupervised discretization method.

We then build a frequency histogram of the root node with the its overall population. We define the histogram of a node  $n$  with numerical attribute variable  $Y$  as a  $k$ -dimensional vector  $h(n)$  where:

$$h(n) = \langle h_1(n), h_2(n), \dots, h_k(n) \rangle \quad (3.3)$$

where  $h_i(n) = \text{supp}(n|Y \in b_i)$ , and therefore:

$$|h(n)|_1 = \sum_{i=1}^k h_i(n) = \text{supp}(n) \quad (3.4)$$

Every node in the lattice is composed by conjunctive clause of non-negated literals and contains a frequency histogram of its population. For the sake of comparison between, all histograms are built on the same buckets defined in the root node.

Subsequently, for the chosen set of categorical relations, we do the same with each subpopulation of examples from each category obtained by joining the root with its corresponding categorical literal. For every category a node in the lattice is created with associated frequency histogram. In addition, the edges of the lattice are created by setting the root as parent node, and adding the new nodes as children from the root.

In a further step, we try to join every possible pair of categorical relations and including the constants. For the given, example with the relations *hasEducation* and *wasBornInMonth* we would then create the nodes:

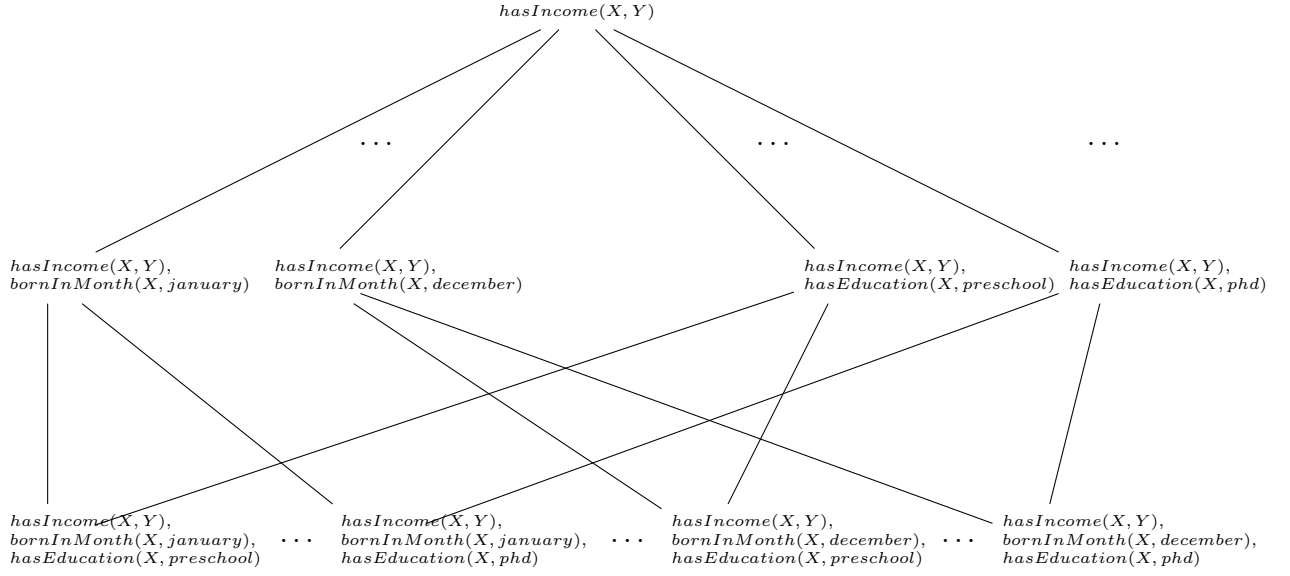
*hasIncome(X, Y)wasBornInMonth(x, "January"),hasEducation(x, "Preschool")*  
*hasIncome(X, Y)wasBornInMonth(x, "January"),hasEducation(x, "Kindergarten")*  
 ...  
*hasIncome(X, Y)wasBornInMonth(x, "January"),hasEducation(x, "Doctorate Degree")*

*hasIncome(X, Y)wasBornInMonth(x, "February"),hasEducation(x, "Preschool")*  
*hasIncome(X, Y)wasBornInMonth(x, "February"),hasEducation(x, "Kindergarten")*  
 ...  
*hasIncome(X, Y)wasBornInMonth(x, "February"),hasEducation(x, "Doctorate Degree")*

...

*hasIncome(X, Y)wasBornInMonth(x, "December"),hasEducation(x, "Preschool")*  
*hasIncome(X, Y)wasBornInMonth(x, "December"),hasEducation(x, "Kindergarten")*  
 ...  
*hasIncome(X, Y)wasBornInMonth(x, "December"),hasEducation(x, "Doctorate Degree")*

This process works just like in an itemset lattice until a predetermined maximum level or until all the possible combinations are exhausted. Figure 3.5 shows how a Correlation Lattice looks like.

**Figure 3.4:** Combination of relations *hasEducation* and *bornInMonth*

### 3.4.2 Pruning Opportunities

In this section we discuss about safe pruning opportunities that can be explored whilst building the Correlation Lattice: support and conditional independence. As these might not be sufficient to reduce lattice size to a feasible level, later, in section(??), we will also discuss possible pruning techniques.

#### 3.4.2.1 Support

As described in ([3]), in top-down ILP every refinement causes the support to decrease, therefore we know that for every node in the Correlation Lattice, its support will be greater or equal than any of its children, so support is a monotonically decreasing measure so we can safely prune a node that does not reach the minimum support threshold.

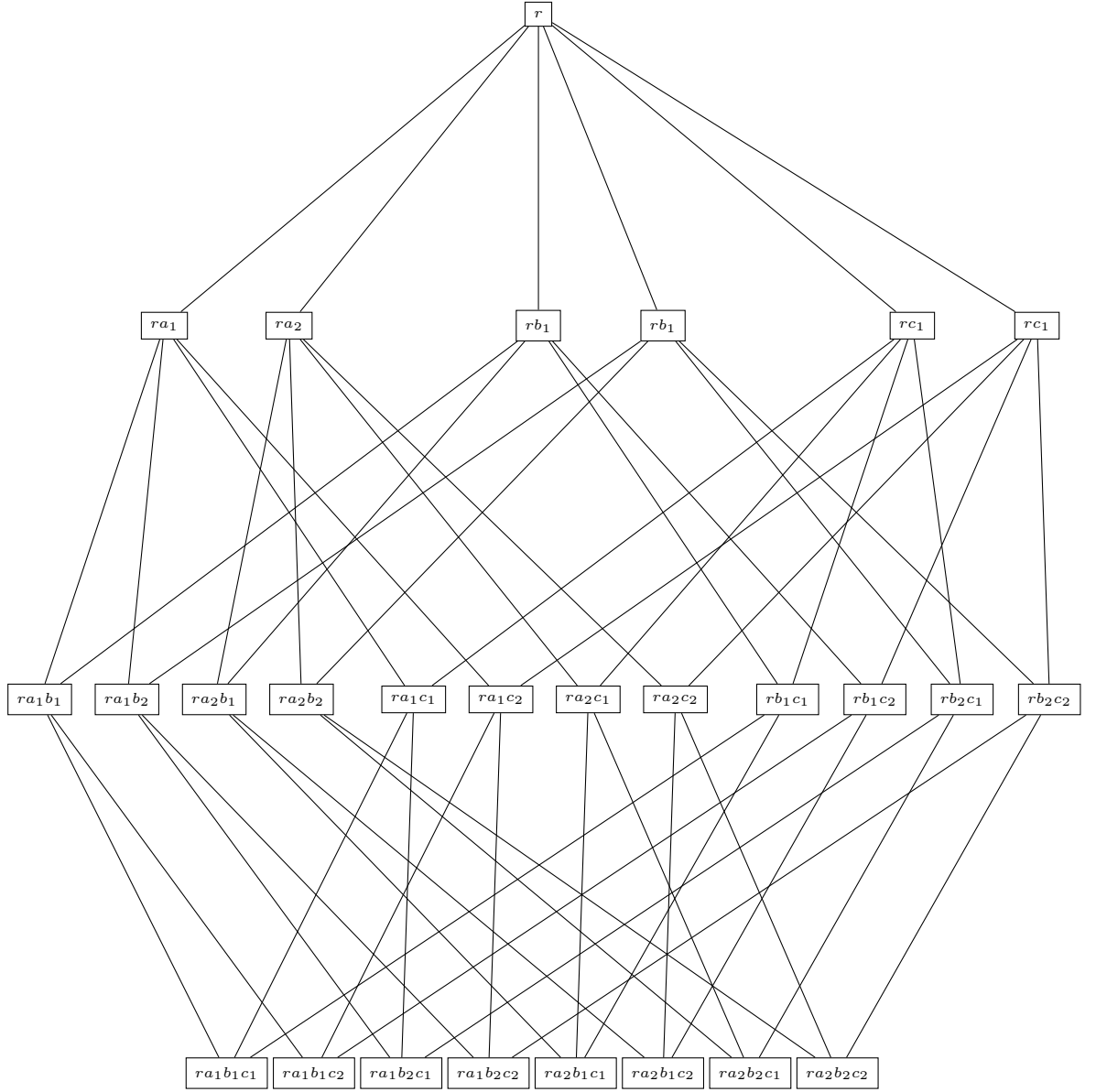
In this thesis, we define support as the absolute frequency of supporting facts. So the support of a node *n* is defined as:

$$supp(n) = |x| x \in n|$$

#### 3.4.2.2 Independence Checks

By simplicity, we assume that every possible pair of categorical relations are independent given their common parent and we search for evidence to prove the contrary.

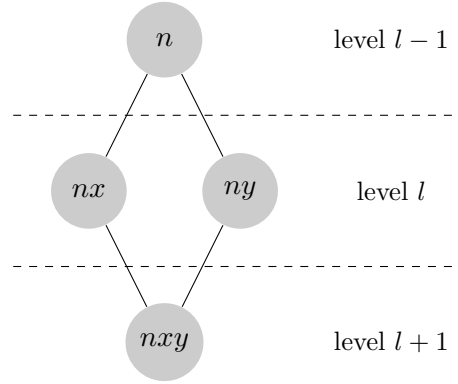
Figure 3.5: Correlation Lattice example



For 2 nodes to be joined, they must have a common parent, i.e. two nodes at level  $l$  (with  $l + 1$  literals) are joinable if they share  $l$  literals. Therefore, it is straightforward to calculate the conditional probabilities of each of the joining nodes given the common parent, and estimate the frequency distribution for the conditional independence case.

Let's say we have the following join case:

In the example shown in figure 3.6,  $x$  and  $y$  are literals and  $n$  is a node with clause  $c_n$ , such that  $x \neq y$  and  $x, y \notin c_n$ . The nodes  $nx$  and  $ny$  are formed by adding  $x$  and  $y$  to  $n$ , so  $c_{nx} = \{c_n, x\}$  and  $c_{ny} = \{c_n, y\}$ . With the histogram from these three nodes, we can calculate the conditional probability  $p_i(x|n)$  and  $p_i(y|n)$ , then calculate  $\hat{h}_i(nxy)$ , which is

**Figure 3.6:** Node join example for independence test

the estimation of  $h_i(nxy)$  assuming that  $x$  and  $y$  are independent given common parent  $n$ .

$$p_i(x|ny) = p_i(x|n)$$

$$= \frac{h_i(nx)}{h_i(n)}$$

$$p_i(y|nx) = p_i(y|n)$$

$$= \frac{h_i(ny)}{h_i(n)}$$

$$\hat{h}_i(nxy) = p_i(x|ny)p_i(y|n) * h_i(n)$$

$$= p_i(x|p)h_i(y|p)$$

$$\hat{h}_i(nxy) = p_i(y|nx)p_i(x|n) * h_i(n)$$

$$= p_i(y|p)h_i(x|p)$$

After that, we query the actual frequency distribution on the knowledge base and do a Pearson's chi-squared independence test. As null hypothesis and alternative hypothesis we have:

- $H_0 = x$  and  $y$  are conditionally independent given their common parent  $p$
- $H_1 = x$  and  $y$  are conditionally dependent given their common parent  $p$

Number of degrees of freedom is the number of buckets minus one:

$$df = k - 1$$



We calculate the critical value  $\chi^2$ :

$$\chi^2 = \sum_{i=1}^k \frac{(h_i - \hat{h}_i)^2}{\hat{h}_i} \quad (3.5)$$

[4]

Then it is possible to obtain the p-value and check whether there is enough confidence to reject the null hypothesis  $H_0$ .

In other words if we find out that  $x$  and  $y$  are conditionally independent given  $p$ , we could rewrite the equation ?? as the following rules being equivalents, with similar accuracy distributions:

$$x \leftarrow py \equiv x \leftarrow p \quad \text{and} \quad y \leftarrow px \equiv y \leftarrow p$$

Therefore, we know that if we have  $x$  fixed as head of clauses in the core ILP, and we currently have  $x \leftarrow p$  joining the node  $px$  with  $py$  to obtain the rule  $x \leftarrow py$  does not add any valuable information. The same applies for having  $y$ , and obtaining  $y \leftarrow px$  from  $y \leftarrow p$  by joining the same pair of nodes. This property plays an important role in the integration of the correlation lattice into the core ILP as we will explain in more details later in Section (??).

Nevertheless it cannot be safely pruned from the lattice.

This applies to nodes at any level  $l$ , with  $p \leq l$  parents and  $C_2^p$  possible join pairs. If any of the join pairs has enough evidence of being dependent, then 2 edges are created connecting each of the joined nodes to the result of their join

### 3.4.3 Entropy Divergence Measures

As seen in the previous sections, we are interested in rules whose base-rule has accuracy below threshold, but contains one or multiple specific intervals with accuracy above threshold. For this to happen, we need a rule with non-uniform accuracy distribution, or in other words, divergent body support and rule positive examples distributions.

Therefore, we are interested in adding categories that produces distributions different from their parent nodes'. In order to measure such divergence between distributions, some of the state-of-the-art such as the following ones can be used.

- Kullback-Leibler [5]:

$$D_{KL}(P||Q) = \sum_i \ln \left( \frac{P(i)}{Q(i)} \right) * P(i) \quad (3.6)$$

- Chi-squared ( $\chi^2$ ):

$$D_{\chi^2}(P||Q) = \sum_i \frac{(P(i) - Q(i))^2}{P(i)} \quad (3.7)$$

- Jensen-Shannon [6]:

$$D_{JS}(P||Q) = \frac{1}{2}D_{KL}(P||M) + \frac{1}{2}D_{KL}(Q||M), \quad (3.8)$$

Where  $P$  and  $Q$  are discrete distributions to be compared and  $M = \frac{1}{2}(P + Q)$ . In the lattice context, these distributions would be the frequency histogram normalized to 1, and nodes directly connected by edges would have their distributions compared.

As discussed in [6], although Jensen-Shannon is computationally more expensive, it has the advantage of being a symmetric and smoothed version of the Kullback-Leibler measure.

These divergence measures are important for identifying potential accuracy distributions. If the divergence between the frequency distributions of a parent and child node is big, that means that if we have a rule with the parent node as body and the additional literal from the child as head, its accuracy distribution will be not uniform and therefore potentially interesting for searching for refined-rules with numerical intervals.

### 3.4.4 Heuristics

As seen before, the number of nodes in Correlation Lattice grows exponentially with the number of categorical relations and its constants. For  $n$  categorical relations, each with  $m$  constants, the total number of nodes is  $2^{nm}$ . As we limit the number of levels in the lattice to  $l$ , the total number of nodes reduces to:

$$\sum_{i=1}^l \binom{nm}{i} \quad (3.9)$$

if  $l = nm$ :

$$\sum_{i=1}^{mn} \binom{nm}{i} = 2^{nm} \quad (3.10)$$

Pruning by support is usually not sufficient to make it feasible and it is necessary to apply heuristics to prune it more aggressively.

Pruning by divergence is clearly not safe. Let's suppose we have a root numerical property  $r(x, y)$ , and two categorical relations  $a(x, z)$  with constants  $A_1$  and  $A_2$  and  $b(x, w)$  with constants  $B_1$  and  $B_2$ . For simplicity, let's assume  $y$  is divided in two buckets and root  $r$  has an uniform distribution  $[0.5 \ 0.5]$  from frequencies  $[2 \ 2]$ . It is possible to have  $ra_1$  and  $ra_2$  as well as  $rb_1$  and  $rb_2$  with the same uniform distribution with frequencies  $[1 \ 1]$ . Nevertheless when combined we can have the following:

$ra_1b_1 : [1.0 \ 0.0]$   
 $ra_1b_2 : [0.0 \ 1.0]$   
 $ra_2b_1 : [0.0 \ 1.0]$   
 $ra_2b_2 : [1.0 \ 0.0]$

As shown above, divergence is not a monotonically decreasing measure, thus it can only be used as heuristics.

Moreover, using a divergence measure alone might also be problematic. Histograms with low support are more likely to present a higher divergence than histograms with higher support, supposing that they were drawn from the same original distribution. Consequently, an algorithm using only the divergence as heuristics would end up giving preference to nodes with lower support. Therefore, it is important to use divergence combined with support as pruning heuristics. [Restructure, it's confusing]

As seen in Section (??), checking for conditional independence of categories is very insightful and can detect equivalent rules like in Figure 3.6 where we know that  $x \leftarrow py \equiv x \leftarrow p$  and  $y \leftarrow px \equiv y \leftarrow p$ . Nevertheless, we cannot prune the node  $pxy$  from the lattice as  $x$  and  $y$  might not be independent given  $pz$ , and for instance, a rule  $x \leftarrow pyz$  might not be equivalent to  $x \leftarrow py$ .

### 3.5 Bucketing the Numerical Attributes

So far we have mentioned that the root's numerical attribute domain should be discretized by dividing it in buckets in order to build frequency histograms and compare distributions. In this section, we will discuss about how to perform such discretization.

The buckets used throughout the Correlation Lattice should be consistent, and the bucketing method as well as the boundaries are specified in the very beginning with the root node. It should have as input an arbitrarily defined number of buckets  $k$ .

Since we don't consider any labels for the examples, we use one of the unsupervised discretization methods presented in section 2.4: equal frequencies or equal width. We choose the method according to the domain characteristics and define the bucket boundaries based on the overall population distribution.

### 3.6 Incorporating Correlation Lattice into the Core ILP Algorithm

The ILP core learning algorithm requires some modifications in order to support the Correlation Lattice. As stated before, we use the top-down search, starting from the most general clauses then further refining them by introducing new substitutions or literals until stopping criteria is reached.

[...]

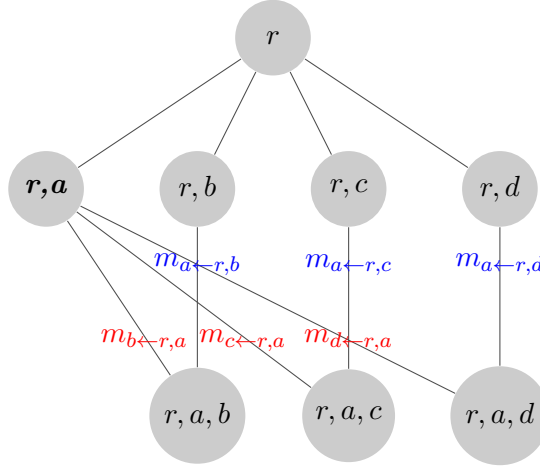
#### 3.6.1 Querying the Correlation Lattice

In the ILP there is a fixed head literal and such literal can and should be included in the Correlation Lattice. In case it is present in the lattice, it plays a key role in the search. Once the root property is added in a clause that does not exceed the accuracy threshold.

In such case we are interested in searching the most interesting literals to add. First step would be to search in the lattice the literals already present in both head and body of the clause that are joined with the root. Nevertheless, what we are not really interested in the benefit of adding a literal to the conjunction of rule's head and body, but in the benefit of adding the head to a body with a new literal.

For example, if we have the clause  $a \leftarrow r$ ,  $r$  is the root of a Correlation Lattice and the head  $a$  is included in it. After searching in the graph for the literals joined with root present in the clause we would come to node  $ra$ . We are not searching for the most interesting child from  $ra$ , but for the children, which has a parent without the head literal that has the highest interestingness measure when adding the head.

As shown in Figure 3.7, if we can add  $b$ ,  $c$  or  $d$  to  $ra$ , we are interested about the measures in blue instead of the ones in red. Nevertheless, searching for values for  $m_{a,rb}$ ,  $m_{a,rc}$

**Figure 3.7:** Interestingness of adding a literal to the body of a clause

and  $m_{a,rd}$  is a bit tricky. It is necessary to check for all children of  $ra$ , which ones have parents without head literal  $a$ , then gather all the measures and rank them.

In order to make it simpler, we can create a suggestions map during lattice build. This map would contain an entry for all node it is joined to, with head as key and literals to add sorted by measure as value. So for example when we are obtaining the node  $rab$  by joining  $ra$  and  $rb$ , we add to  $ra$  an entry with  $a$  as key,  $b$  as new literal and associated measure  $m_{a,rb}$  and we also add to  $rb$  an entry with  $b$  as key,  $a$  as new literal and associated measure  $m_{b,ra}$ . This is shown more clearly in algorithm 6.

---

**Algorithm 6:** Suggestion map build when joining nodes during lattice build

---

**Input:**  $nx, ny$ : Joining nodes,  $n$ : Common parent node

```

 $\hat{h}(nxy) \leftarrow h(nx)h(ny)/h(n)$  ;
 $h(nxy) \leftarrow \text{queryFrequencyHistogram}(nxy)$  ;
 $\chi^2 \leftarrow \sum_{i=1}^k (h_i(nxy) - \hat{h}_i(nxy))^2 / (\hat{h}_i(nxy))$  ;
 $dof \leftarrow k - 1$  ;
 $pValue = \text{criticalValue}(\chi^2, dof)$  ;
if  $pValue \geq minPValue$  then
     $m_{x,ny} \leftarrow \text{interestingness}(h(nxy), h(ny))$  ;
     $m_{y,nx} \leftarrow \text{interestingness}(h(nxy), h(nx))$  ;
     $nx.suggestionsMap(x) \leftarrow (y, m_{x,ny})$  ;
     $ny.suggestionsMap(y) \leftarrow (x, m_{y,nx})$  ;

```

---

In the example of Figure 3.7,  $ra$  would contain the following map:

a	b [ $m_{a,rb}$ ]
	c [ $m_{a,rc}$ ]
	d [ $m_{a,rd}$ ]

As in this example the node  $ra$  has only two literals, and the root  $r$  cannot be the head, we use the node  $ra_1b_1$  in Figure 3.5 to better illustrate it:

a1	c1 $[m_{a_1,rb_1c_1}]$
	c2 $[m_{a_1,rb_1c_2}]$
b1	c1 $[m_{b_1,ra_1c_1}]$
	c2 $[m_{b_1,ra_1c_2}]$

In a node at level  $l$  with  $l + 1$  literals (one being the root), we can have up to  $l$  keys in the map. Therewith, we can much more easily find the best suggestions for any possible head literal without having to visit other nodes.

First we need to introduce a new refinement operator that extracts the support and accuracy distributions along a chosen numerical property and searches for interesting ranges. With that there are

---

**Algorithm 7:** Refinement step

---

**Input:** *clause*: Set of literals from the clause, *lattice*( $r_{root}$ ): Set of existent Correlation Lattices, *lit<sub>body</sub>*: Literal in clause that will be joined with new Literal, *lit<sub>new</sub>*: Literal to be added to the clause, *arg<sub>body</sub>*: Join argument from body literal, *arg<sub>new</sub>*: Join argument from new literal

**Output:** True if *arg<sub>i</sub>* from  $r_i$  joins with *arg<sub>j</sub>* from  $r_j$ , False otherwise

$r_{new} \leftarrow lit_{new}.relation$  ;

**if** *arg<sub>new</sub>* = 1 **and**  $r_{new}$  is numerical **and**  $\exists lattice(r_{new})$  **then**

$node \leftarrow lattice(r_{new}).root.search(head)$  ;

**foreach** *lit<sub>i</sub>*  $\in clause.body$  **do**

$node \leftarrow node.search(lit_i)$  ;

$checkNumericalRanges(clause, lit_{new}, node)$  ;

---



---

**Algorithm 8:** checkNumericalRanges

---

**Input:**

**Output:**

$v \leftarrow$  Numerical variable from *lit<sub>new</sub>* ;

$acc \leftarrow queryAccuracyDistribution(clause, v)$  ;

$sup \leftarrow querySupportDistribution(clause, v)$  ;

$intervals \leftarrow searchInterestingIntervals(acc, sup, accTS, supTS)$  ;

**foreach** *interval<sub>i</sub>*  $\in intervals$  **do**

$newClause \leftarrow \{clause \cup lit_{new} \cup \{v \in interval_i\}\}$  ;

    Add *newClause* to rule tree ;

$suggestions \leftarrow node.getSuggestions(clause.head)$  ;

**foreach** *lit<sub>i</sub>*  $\in suggestions$  **and**  $i \leq k$  **do**

$node_i \leftarrow node.search(lit_i)$  ;

$checkNumericalRanges(clause \cup lit_i, lit_{new}, node_i)$  ;

---

---

**Algorithm 9:** Check whether a clause has potential interesting numerical intervals

---

**Input:** *clause*: Clause with numerical literal, *lattice*: Lattice from **foreach**

*lit<sub>i</sub>* ∈ *suggestions* **and**  $i \leq k$  **do**

*node<sub>i</sub>* ← *node*.search(*lit<sub>i</sub>*) ;  
     checkNumericalRanges(*clause* ∪ *lit<sub>i</sub>*, *lit<sub>new</sub>*, *node<sub>i</sub>*) ;

---

In the specialization step, we can detect whether the clause contains any numerical property, which is root of a Correlation Lattice. If so, it can search for interesting ranges numerical ranges,





## Chapter 4

# Algorithmic Framework

### 4.1 Knowledge Base Backend

For storing and retrieving RDF data we use RDF3X [7]. It has the advantage of being specialized and optimized for RDF data, using a strong indexing approach with compressed B<sup>+</sup>-Tree indices for each of six permutations of *subject (S)*, *predicate (P)* and *object (O)*: *SPO*, *SOP*, *OSP*, *OPS*, *PSO* and *POS*.

RDF3X particularities...

### 4.2 Preprocessing

#### 4.2.1 Correlation Lattice

##### 4.2.1.1 Graph Node

Every node essentially contains the following attributes:

- Set of pointers to parent nodes
- Set of pointers to child nodes
- Set of pointers to constant nodes
- Histogram with facts distribution over root numerical property

#### 4.2.1.2 Building the Correlation Lattice

For building the Correlation Lattice, we start with the root node, which has a numerical property as literal and no constants assigned, e.g. *hasIncome(x,y)*. We then query the distribution of positive examples over the property in the whole Knowledge Base.

*SELECT COUNT ?y WHERE { ?x <hasIncome> ?y } GROUP BY (?y)*

It's also necessary to specify the bucketing technique and the number of buckets in order to extract the histogram from the obtained query results. These buckets are used to build the histograms of all nodes in the graph.

Afterwards, we select the the categorical properties that will be used in the lattice. For each of the selected properties, we join them with the root numerical property (for simplicity we'll assume all the categorical properties are joined with both 1<sup>st</sup> arguments) and we query the distribution again. In the first level, it's necessary to extract a histogram for each of the categorical constants in the selected properties. Therefore, it's a good strategy to group the results also by these categorical constants so If we select *hasEducation* for example, we would then fire the following SPARQL query:

*SELECT COUNT ?z ?y WHERE { ?x <hasIncome> ?y . ?x <hasEducation> ?z }  
GROUP BY (?z,?y)*

With such query, it's possible to extract a histogram for the node *hasIncome(x,y)hasEducation(x,z)* and its correspondent constants.

#### 4.2.1.3 Searching Rules in Correlation Lattice

In the Correlation Lattice itself, it's possible to extract valuable rules. Given its characteristic of all the relations being joined on the same root argument, those rules represent how different categories are related along root's numerical constants.

For every non-root node in the Correlation Lattice, any of its parents can be seen as rule's body and the remaining literal as head, e.g.:

Let's denote  $a_i$  as a relation  $a(x, y)$  with constants  $A_i$  for  $y$ , so for example  $a_1 \equiv a(x, A_1)$ :

For the node  $ra_1b_1c_1$  with parents  $ra_1b_1$ ,  $ra_1c_1$  and  $rb_1c_1$ , we can extract and easily evaluate three rules:

$$Rule_1 : \quad a_1 \leftarrow b_1 c_1 r$$

$$supp_i(Rule_1) = h_i(ra_1 b_1 c_1)$$

$$acc_i(Rule_1) = \frac{h_i(ra_1 b_1 c_1)}{h_i(rb_1 c_1)}$$

$$Rule_2 : \quad b_1 \leftarrow a_1 c_1 r$$

$$supp_i(Rule_2) = h_i(ra_1 b_1 c_1)$$

$$acc_i(Rule_2) = \frac{h_i(ra_1 b_1 c_1)}{h_i(ra_1 c_1)}$$

$$Rule_3 : \quad c_1 \leftarrow a_1 b_1 r$$

$$supp_i(Rule_3) = h_i(ra_1 b_1 c_1)$$

$$acc_i(Rule_3) = \frac{h_i(ra_1 b_1 c_1)}{h_i(ra_1 b_1)}$$

Subsequently we can analyze the frequency and confidence distributions and determine whether any of the rules are interesting, using any of the techniques discussed in [??] and find possible interesting intervals.

#### 4.2.1.4



## Chapter 5

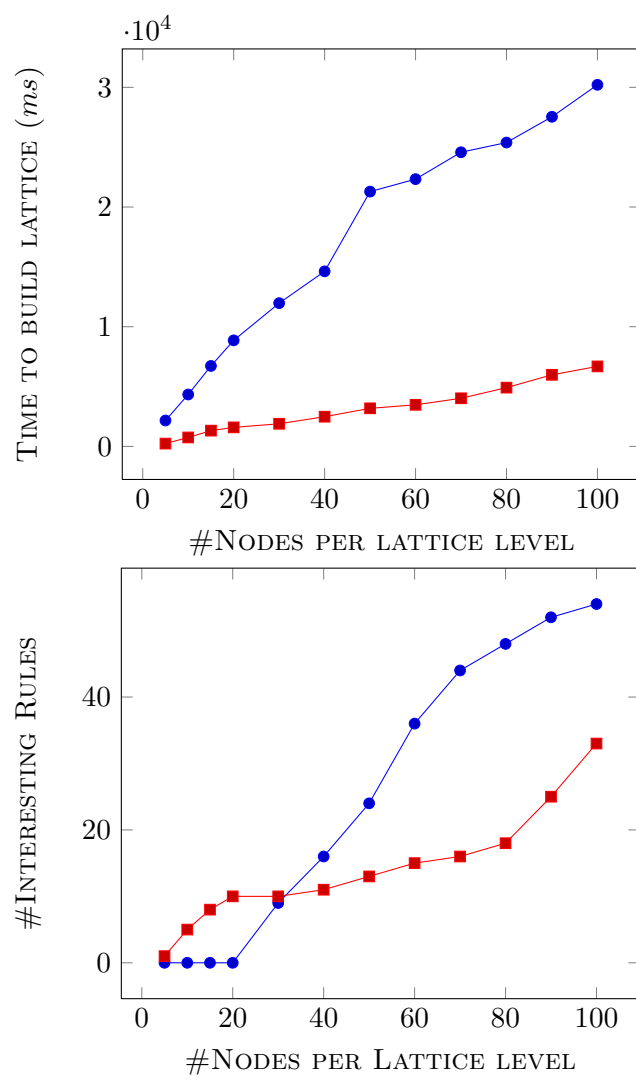
# Experiments

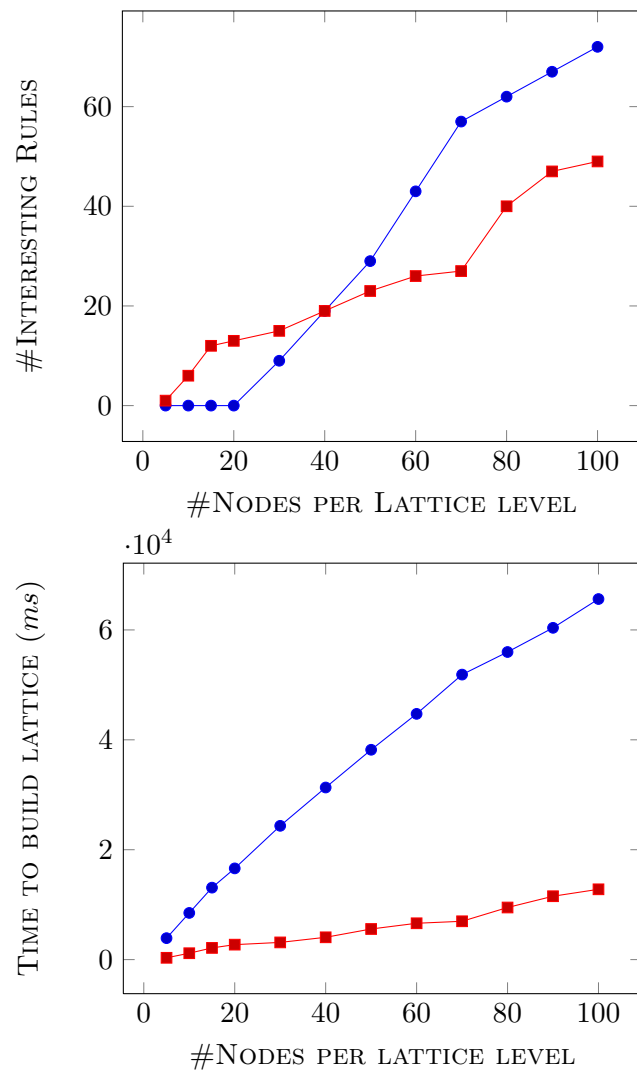
\*\*\*Roughly explaining the experiments I did so far, we want to evaluate whether the heuristics are good. So we use US Census data to build a lattice (for income property) with the limitation of having up to  $n$  nodes at each level. So far I compared the KL-divergence\*Support with support only as measures. For every level I sort the nodes by the measure (nodes with multiple parents will have multiple KL-divergence, in this case I take the maximum one) and try to join the nodes with highest measures first until  $n$  nodes for the next level is reached. In other words, I greedily build the a lattice with limited number of nodes per level.

After that, I try to extract rules with interesting ranges directly from the lattice and test them against a test partition. Interesting rules are defined as in ReferencesInteresting Rules with support threshold of 25 examples and accuracy threshold of 0.75. After that, I compare the number of interesting rules learned, the time taken to build the lattice and the accuracy and accuracy gain compared to the base rule.

Accuracy and accuracy gain seem to depend exclusively on the accuracy threshold, so they are roughly the same for both measures. Processing time is much smaller for the KL-divergence as it doesn't simply focus on huge relations and as expected, it also presents a greater number of rules with interesting ranges (at least for smaller number of nodes per level).

Hopefully I'll soon have results from applying the lattice in the core ILP. I managed to overcome some implementation problems I had when creating the lattice in YAGO.

**Figure 5.1:** Lattices with 3 levels

**Figure 5.2:** Lattice with 4 levels





# List of Figures

2.1	Part of the refinement graph for the family relations problem . . . . .	11
2.2	Itemset Lattice example . . . . .	16
2.3	Itemset Lattice example . . . . .	17
2.4	Semantic Web stack . . . . .	22
2.5	Linking Open Data cloud diagram, by Richard Cyganiak and Anja Jentzsch. <a href="http://lod-cloud.net">http://lod-cloud.net</a> . . . . .	24
3.1	Example of frequency histograms from body support and positives support (left), and resulting confidence distribution (right) . . . . .	26
3.2	Support distribution of body and positives from figure ?? . . . . .	27
3.3	Type hierarchy example . . . . .	31
3.4	Combination of relations <i>hasEducation</i> and <i>bornInMonth</i> . . . . .	36
3.5	Correlation Lattice example . . . . .	37
3.6	Node join example for independence test . . . . .	38
3.7	Interestingness of adding a literal to the body of a clause . . . . .	43
5.1	Lattices with 3 levels . . . . .	52
5.2	Lattice with 4 levels . . . . .	53



# List of Tables

2.1	A simple ILP problem: learning the <i>daughter</i> relation. . . . .	9
2.2	Example of transaction database $\mathcal{D}$ [?] . . . . .	15



# Bibliography

- [1] Sergey Brin, Rajeev Rastogi, and Kyuseok Shim. Mining optimized gain rules for numeric attributes. In *Proceedings of the Fifth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pages 135–144. ACM Press, 1999.
- [2] Toon Calders, Christian W. Günther, Mykola Pechenizkiy, and Anne Rozinat. Using minimum description length for process mining. In *SAC*, pages 1451–1455, 2009.
- [3] Nada Lavrac and Saso Dzeroski. *Inductive Logic Programming: Techniques and Applications*. Ellis Horwood, New York, 1994. URL <http://www-ai.ijs.si/SasoDzeroski/ILPBook/>.
- [4] Szymon Jaroszewicz and Dan A. Simovici. Pruning redundant association rules using maximum entropy principle. In *In Advances in Knowledge Discovery and Data Mining, 6th Pacific-Asia Conference, PAKDD'02*, pages 135–147, 2002.
- [5] S. Kullback and R. A. Leibler. On information and sufficiency. *Ann. Math. Statist.*, 22(1):79–86, 1951.
- [6] J. Briet and P. Harremos. Properties of classical and quantum jensen-shannon divergence. *Physical Review A: Atomic, Molecular and Optical Physics*, 79(5), May 2009. ISSN 1050-2947.
- [7] Thomas Neumann and Gerhard Weikum. The rdf-3x engine for scalable management of rdf data. *The VLDB Journal*, 19(1):91–113, February 2010. ISSN 1066-8888. doi: 10.1007/s00778-009-0165-y. URL <http://dx.doi.org/10.1007/s00778-009-0165-y>.