Generalizing Refinement Operators to Learn Prenex Conjunctive Normal Forms

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Abstract. Inductive Logic Programming considers almost exclusively universally quantified theories. To add expressiveness we should consider general prenex conjunctive normal forms which use existential variables. Learning with refinement operators is the most used learning method in ILP. To extend refinement operators to PCNF, we should first extend substitutions to PCNF. The usual substitutions often generalize a formula instead of specializing it because of the existential variables. In this article we define substitutions to specialize a given PCNF and a *weakly complete* downward refinement operator. Based on this operator, we have implemented a simple learning system PCL on some type of PCNF.

1 Introduction

Inductive Logic Programming learns a *correct* logic formula with respect to examples. The definition of correctness has to do with the way examples are presented. Suppose some interpretations are given as examples, formulas with these examples as models should be found. A *downward* refinement operator ρ can be used to search such a formula. If a searching process begins with $\top = \{\square\}$, it should be replaced by the set of its refinements in $\rho(\top)$ because $\square$ has no models. A refinement $\phi \in \rho(\top)$ may have to be replaced by its refinements again because some given interpretations are not its models. This process can go on until correct formulas are found.

Refinement operators have often been used ([S81, RD97]) to learn a correct universally quantified theory incrementally. If clause C subsumes clause D , then a *refinement chain* exists from C to D using *elementary substitutions* and adding literals. Let $C = p(x, y)$ and $D = p(x, x) \vee \neg q(f(x))$. Then a chain may be $p(x, y), p(x, y) \vee \neg q(z), p(x, y) \vee \neg q(f(u)), p(x, x) \vee \neg q(f(u)), p(x, x) \vee \neg q(f(x))$. If a correct universally quantified theory does exist, then a refinement chain from $\square$ to every clause in this theory exists because $\square$ subsumes every clause.

Until now almost all ILP researchers are only interested in universally quantified clauses, especially definite program clauses. However, we may want to learn a concept expressed by a formula ϕ with existential variables such as a prenex conjunctive normal form (PCNF). To solve such problems, one considers the universally quantified Skolem standard form ψ of ϕ . It is well known

that $\psi \models \phi$ but not $\phi \models \psi$. For instance, let the 3-ary predicate p be interpreted in the set of real numbers $\mathbf{R}$ as $p(x, y, z)$ is true iff $xy = z$. The concept that for an arbitrary $z \in \mathbf{R}$, there are x, y such that $xy = z$ can be expressed by $\phi = \forall z^2 \exists x \exists y p(x, y, z)$. A standard form of the formula ϕ is $\psi = \forall z p(f(z), g(z), z)$ for new function symbols f, g . A model of ϕ is also a model of ψ only when f and g are interpreted in certain ways, e.g. $f(z) = 2z$ and $g(z) = z/2$, but we would like to check the truth value of ϕ directly. In a database we may have an integrity constraint $\forall x \forall y \exists z \neg \text{sell}(x, y) \vee \text{supply}(x, y, z)$: if a shop x sells an item y , there must be a company z which supplies x with y . Of course we can define one particular supplier as $f(x, y)$ but we have to change f when we consider another supplier. To add expressiveness we should consider learning PCNF in general.

We would also like to use (elementary) substitutions to refine a PCNF. The usual substitutions often generalize a formula instead of specializing it because of the existential variables. Let $\phi = \forall x \exists y p(x, y)$ and $\psi = \forall x p(x, x)$. Then $\psi \models \phi$ but $\phi \not\models \psi$. Therefore we will define a new type of substitutions to specialize a PCNF. Based on our substitutions and adding literals, we can define a *downward* refinement operator ρ which is *weakly complete*: For every ϕ there is a refinement chain from $\top$ to ϕ , i.e., there is an n such that $\phi \in \rho^n(\top)$.

Generalizing and specializing a formula with existential quantifiers have also been considered in [GF96]. A formula there involves only one clause (actually a clause presented in a special form). The variables in the head of a clause are universally quantified. The variables not in the head are quantified separately in the body by existential and universal quantifiers. Some rules are given to manipulate the variables only in the body. It seems that the rules are motivated by the following principle: if the body is generalized, then the formula is specialized and vice versa. [GF96] adopts neither PCNF in general nor a uniform approach with substitutions.

In this article we begin with establishing some properties of PCNF. We then define (elementary) substitutions and a downward refinement operator. We use a refinement operator to search in the set of theories expressed in PCNF. This differs from a classic refinement operator which is defined in a search space of universally quantified clauses. Most proofs will be omitted (see [NLR99]). We explain then briefly our first step in implementation. If $I_1, I_2, \dots, I_n$ is a set of interpretations, the system PCL finds a PCNF ϕ such that every I_j is a model of ϕ . Hence we have generalized the Claudien system [RD97] which only deals with the standard forms.

2 Prenex Conjunctive Normal Forms

In the first subsection we give some well known basic definitions and results in logic (see [NW97]). In the second subsection we state two important lemmas of ours. In the last subsection we consider the effects of adding literals to a clause in a PCNF.

2.1 Preliminaries

Definition 1. An interpretation I with domain D of a first-order language L consists of the following: (a) Each n -ary function symbol f in L is assigned a mapping from D^n to D . (b) Each n -ary predicate symbol p in L is assigned a mapping from D^n to $\{\text{true}, \text{false}\}$.

Definition 2. Let I be an interpretation of the first-order language L with domain D . Let V be a set of variables, then a mapping $\theta : V \rightarrow D$ is called a variable assignment from V . Given a variable assignment θ from the set of variables in a formula ϕ , we can check if ϕ is true or false under I and θ . If ϕ is a closed formula, then the truth value of ϕ is independent of the variable assignment we choose. I is a model of the closed formula ϕ if ϕ is true in I . Formula ψ logically implies formula ϕ , denoted by $\psi \models \phi$, if every model of ψ is also a model of ϕ . ψ and ϕ are called logically equivalent, denoted by $\psi \Leftrightarrow \phi$, if they have the same models.

Definition 3. A clause is a disjunction of a finite number of literals. A prenex conjunctive normal form (PCNF) ψ is a closed formula $q_1x_1q_2x_2\ldots q_nx_n(C_1 \wedge C_2 \wedge \ldots \wedge C_m)$ where q_i is a quantifier ($\exists$ or $\forall$), $x_i \neq x_j$ if $i \neq j$ and C_j is a clause. $q_1x_1q_2x_2\ldots q_nx_n$ is the prenex of ψ and $C_1 \wedge C_2 \wedge \ldots \wedge C_m$ is the matrix of ψ . We denote ψ often by $q_1x_1q_2x_2\ldots q_nx_nM(x_1, \ldots, x_n)$ or $Q(x_1, \ldots, x_n)M(x_1, \ldots, x_n)$ or $Q(\bar{x})M(\bar{x})$ or $Q(\psi)M(\psi)$ or QM . We call variables in $Q(\psi)$ universal or existential; depending on how they are bound; the set of existential and universal variables are denoted by $eVar(\psi)$ and $uVar(\psi)$, respectively. We have $Var(\psi) = uVar(\psi) \cup eVar(\psi)$.

Note that if $\{y_1, \ldots, y_m\} \supseteq \{x_1, \ldots, x_n\}$, then $Q(\bar{y})M(\bar{x}) \Leftrightarrow Q(\bar{x})M(\bar{x})$.

Theorem 1. Let ϕ be a closed formula. Then there exists a PCNF ψ such that ϕ and ψ are logically equivalent.

2.2 Some properties of PCNF

We often need to check if some interpretation I is a model of a formula ψ . Lemma 1 in this subsection gives a necessary and sufficient condition for I to be a model of ψ . Lemma 2 tells that the truth value of a formula has often to do with the positions of variables in the prenex. Both lemmas will often be used for proving other results.

Example 1. Let $\psi = \exists x \forall y p(x, f(y))$ and $\phi = \forall y \exists x p(x, f(y))$. Then $\psi \models \phi$: Let I be an interpretation with domain D . Then ψ is true in I iff there is a $d \in D$ such that the formula $\forall y p(d, f(y))$ is true in I iff there is $d \in D$ such that for every $e \in D$, $p(d, f(e))$ is true. On the other hand, ϕ is true in I iff for every $e \in D$, $\exists x p(x, f(e))$ is true iff for every $e \in D$, there is $d \in D$ such that $p(d, f(e))$ is true. Notice that the choice of d here may depend on e . Since I is a model of ψ , for every $e \in D$, we can choose the same $d \in D$ such that $p(d, f(e))$ is true in I . Consider the Herbrand interpretation $I = \{p(t, f(t)) \mid t \text{ ground}\}$. Then I is

a model of ϕ . For an assignment $\sigma = \{x/t\}$, let $\gamma = \{y/t\}$ then $\phi(\sigma \cup \gamma)$ is true. We can not say I is a model of ψ because γ depends on σ . We can generalize this example to the following lemmas

Lemma 1. *Let $\phi = q_1x_1 \dots q_nx_nM(x_1, \dots, x_n)$. An interpretation I with domain D is a model of ϕ iff for every $\sigma : \text{uVar}(\phi) \rightarrow D$ there is a $\gamma : \text{eVar}(\phi) \rightarrow D$ such that the following two conditions are satisfied: (a) $M(\sigma \cup \gamma)$ is true in I . (b) the definition of γ on x_i depends only on how σ and γ are defined on $\{x_1, x_2, \dots, x_{i-1}\}$, i.e., an element in D can be assigned to x_i after the assignment of all $x_j, j < i$ has been done.*

Lemma 2. *Let*

$\psi = q_1x_1 \dots \exists x_i \dots \forall x_j \dots q_nx_nM, \phi = q_1x_1 \dots \forall x_j \dots \exists x_i \dots q_nx_nM$
and suppose there is no other existential variable between x_i and x_j in the prenexes of these two formulas. Then $\psi \models \phi$.

Proof . Suppose I is a model of ψ . We want to prove that I is also a model of ϕ by applying Lemma 1. Let $\sigma : \text{uVar}(\phi) \rightarrow D$. By Lemma 1, there is a variable assignment γ of $\text{eVar}(\psi)$ such that $M(\psi)(\sigma \cup \gamma)$ is true under I . The assignment of $x_k \in \text{eVar}(\psi)$ may depend on the definition of σ and γ on variables before x_k in $Q(\psi)$. Since $\text{uVar}(\psi) = \text{uVar}(\phi)$ and $M(\psi) = M(\phi)$, we have $M(\phi)(\sigma \cup \gamma)$ true under I . By Lemma 1, we can say I is a model of ϕ if γ in $x_k \in \text{eVar}(\phi)$ depends on the assignment of variables before x_k in $Q(\phi)$. Note that $Q(\phi)$ interchanges only the order of $\exists x_i$ and $\forall x_j$ in $Q(\psi)$. The assignment of x_i in γ depends only on the assignment of σ, γ on $x_1, \dots, x_{i-1}$ which appear before $\exists x_i$ in $Q(\phi)$. If $x_k \in \text{eVar}(\phi)$ is another existential variable, then it is not between x_i and x_j so $x_1, \dots, x_{k-1}$ are still before x_k in $Q(\phi)$. That means I is a model of ϕ .

2.3 Adding literals

A classic refinement step for a universal quantified PCNF extends a clause in the matrix with an extra literal containing new variables. This will also be done for our refinement operator for PCNF. For this we need the the following results which are based on the fact that the disjunctions of formulas is true if at least one of them is true.

Lemma 3. *Let $\psi = q_1x_1 \dots q_nx_nC_1 \wedge C_2 \dots \wedge C_m$ where every C_i is a clause. Let L be a literal which contains only variables $y_1, \dots, y_k$ that are new w.r.t. ψ . If $\phi = q_1x_1 \dots q_nx_n\forall y_1 \dots \forall y_k C_1 \wedge \dots \wedge (C_j \vee L) \dots \wedge C_m$, then $\psi \models \phi$.*

We call the action in Lemma 3 *adding a u-literal*. Similarly we can prove the following lemma which *adds an e-literal* to a formula.

Lemma 4. *Let $\psi = q_1x_1 \dots q_nx_nC_1 \wedge C_2 \dots \wedge C_m$ where every C_i is a clause. Let L be a literal which contains only new variables $y_1, \dots, y_k$ that are new w.r.t. ψ . If $\phi = \exists y_1 \dots \exists y_k q_1x_1 \dots q_nx_n C_1 \wedge \dots \wedge (C_j \vee L) \dots \wedge C_m$, then $\psi \models \phi$.*

3 Substitutions and Specializations

We are used to it that a substitution θ is defined by replacing some variables with terms. For a universally quantified clause C we have always $C \models C\theta$. This is not valid for PCNF as the following examples show. Thus we are motivated to define a new type of substitutions which specialize PCNF.

Example 2. Consider the following implications:

$$\begin{aligned} \forall x p(x) &\models p(a) \text{ and } p(a) \not\models \forall x p(x) \\ p(a) &\models \exists x p(x) \text{ and } \exists x p(x) \not\models p(a) \\ \exists x p(x, x) &\models \exists x \exists y p(x, y) \text{ and } \exists x \exists y p(x, y) \not\models \exists x p(x, x) \end{aligned}$$

A unification of two universally quantified variables does not always specialize a PCNF. Let $\psi = \forall x \exists y \forall z p(x, y, z)$, $\phi = \forall x \exists y p(x, y, x)$, $\phi' = \exists y \forall z p(z, y, z)$, and $I = \{p(t, f(t), t') \mid t, t' \text{ ground}\}$. Then I is a model of ψ and ϕ but not a model of ϕ' . For ϕ' true in I , we need an s such that $p(t, s, t)$ true for every t .

3.1 Elementary substitutions for PCNF

A matrix can be pictured as a tree, with the root on top. At each node, number downgoing branches 1, 2, 3, etc. from left to right. Each node and the tree hanging from it is given by the path that leads to it from the top. For example, let $M = p(x, y) \wedge (p(x, x) \vee \neg q(f(x)))$. The second clause has position $\langle 2 \rangle$. $\neg q(f(x))$ has position $\langle 2, 2 \rangle$, $f(x)$ has position $\langle 2, 2, 1 \rangle$, etc.

Definition 4. *An substitution for a matrix M has the form $\theta = \{(t_1/s_1, p_1), \dots, (t_n/s_n, p_n)\}$. $M\theta$ is a matrix formed by using M and θ : for every i , the term at position p_i in M is t_i and t_i should be replaced by s_i . For example, if $M = p(x, y) \wedge (p(x, x) \vee \neg q(f(x)))$ and $\theta = \{(x/f(z), \langle 1, 1 \rangle), (f(x)/g(z), \langle 2, 2, 1 \rangle)\}$, then $M\theta = p(f(z), y) \wedge (p(x, x) \vee \neg q(g(z)))$. It is easy to see that the old definition of a substitution is a special case of the new kind of substitutions. In such a case we use the old notation where the positions are not needed.*

Definition 5. *Let $\psi = q_1 x_1 \dots q_n x_n C_1 \wedge \dots \wedge C_m = Q(\psi)M(\psi)$ be a PCNF. There are the following 5 types of elementary substitutions for ψ :*

The first two types have to do with universal variables:

- *Let $x_i, x_j \in \text{uVar}(\psi)$ and $i < j$. An elementary u-unification $\theta = \{x_j/x_i\}$ for ψ can be applied to ψ such that $\psi\theta = q_1 x_1 \dots q_n x_n (M(\psi)\theta)$. For example let $\psi = \forall x \forall y p(f(x), y)$ and $\theta = \{y/x\}$. Then $\psi\theta = \forall x \forall y p(f(x), x)$ which is equivalent to $\forall x p(f(x), x)$.*
- *Let $x_i \in \text{uVar}(\psi)$. If $t = f(y_1, \dots, y_k)$, where $y_1, \dots, y_k$ are new distinct variables w.r.t. ψ , then $\theta = \{x_i/t\}$ is called an elementary u-substitution. Let $\psi\theta$ be the new formula constructed as follows. All x_i -occurrences in the matrix of ψ are replaced by t simultaneously, i.e. $M(\psi\theta) = M(\psi)\theta$. Moreover, the $\forall x_i$ in the prenex of ψ is replaced by $\forall y_1 \forall y_2 \dots \forall y_k$. For example, let $\psi = \forall x \exists y p(x, y)$ and $\theta = \{x/f(u, v)\}$. Then $\psi\theta = \forall u \forall v \exists y p(f(u, v), y)$.*

The next two types have to do with existential variables:

- Let $x_i \in \text{eVar}(\psi)$ and let $\{(x_i, p_1), \dots, (x_i, p_k)\}$ be a proper subset of the x_i -occurrences in $M(\psi)$. If z is a new variable, then $\theta = \{(x_i/z, p_1), \dots, (x_i/z, p_k)\}$ is called an elementary e-antiunification and $\psi\theta$ is the PCNF $q_1x_1 \dots \exists x_i \exists z q_{i+1}x_{i+1} \dots q_nx_n(M\theta)$. For example, let $\psi = \exists xp(x, x)$ and $\theta = \{x/z, \langle 2 \rangle\}$. Then $\psi\theta = \exists x \exists zp(x, z)$.
- Let $t = f(x_{i_1}, \dots, x_{i_m})$ which contains only distinct existential variables. Let $i_j = \max\{i_1, \dots, i_m\}$. Let $\{(t, p_1), \dots, (t, p_k)\}$ be occurrences in $M(\psi)$. If z is a new variable, then $\theta = \{(t/z, p_1), \dots, (t/z, p_k)\}$ is called an elementary e-substitution for ψ . We define $\psi\theta = q_1x_1 \dots q_{i_j}x_{i_j} \exists z q_{i_j+1}x_{i_j+1} \dots q_nx_n(M\theta)$. For example, let $\psi = \forall x \exists y \exists u \exists v p(x, u) \wedge (p(x, y) \vee \neg q(f(u, v)))$. If $\theta = \{(f(u, v)/z, \langle 2, 2, 1 \rangle)\}$, then $\psi\theta = \forall x \exists y \exists u \exists v \exists z p(x, u) \wedge (p(x, x) \vee \neg q(z))$.

The last type has to do with interchanging an existential with a universal variable:

- Suppose $x_i \in \text{eVar}(\psi)$, $x_j \in \text{uVar}(\psi)$ and $i < j$. If there is no other existential variable between x_i and x_j in $Q(\psi)$, then $\{(x_i, x_j)\}$ denotes an elementary eu-substitution. It interchanges the positions of x_i and x_j in $Q(\psi)$. For example, let $\theta = \{(x, y)\}$. Then $(\exists x \forall y p(x, y))\theta = \forall y \exists x p(x, y)$.

3.2 Substitutions and specializations

For every elementary substitutions θ w.r.t. ψ we can prove that $\psi \models \psi\theta$. For instance,

Lemma 5. Let $\psi = Q(\psi)M(\psi)$ be a PCNF. Let $\theta = \{(t/z, p_1), \dots, (t/z, p_m)\}$ be an elementary e-substitution. Then $\psi \models \psi\theta$.

Proof . Let I be a model of ψ . Let t contain only the existential variables $x_{i_1}, \dots, x_{i_k}$ where $i_1 < i_2 < \dots < i_k$. Then $\psi\theta = q_1x_1 \dots q_{i_k}x_{i_k} \exists z q_{i_k+1}x_{i_k+1} \dots q_nx_nM\theta$. $M(\psi)$ differs from $M(\psi\theta)$ only at position $p_1, p_2, \dots, p_k$. Clearly, $\text{uVar}(\psi\theta) = \text{uVar}(\psi)$ and $\text{eVar}(\psi\theta) = \text{eVar}(\psi) \cup \{z\}$. We want to prove for every variable assignment σ of $\text{uVar}(\psi\theta)$ to D , there is a variable assignment γ of $\text{eVar}(\psi\theta)$ to D such that $M(\psi)\theta(\sigma \cup \gamma)$ is true under I . Since I is a model of ψ , and the assignment σ is also an assignment of $\text{uVar}(\psi)$, by Lemma 1 there is a variable assignment γ of $\text{eVar}(\psi)$ to D such that $M(\psi)(\sigma \cup \gamma)$ is true under I . Moreover, if $x_i \in \text{eVar}(\psi)$, then $\gamma(x_i)$ depends only on how σ and γ behave on variables before x_i in $P(\psi)$. Notice that at every position p_j in $M(\psi)(\sigma \cup \gamma)$ we have in fact $t\gamma$. We consider the substitution $\gamma' = \gamma \cup \{z/t\gamma\}$. Then $M(\psi)(\sigma \cup \gamma) = M(\psi)\theta(\sigma \cup \gamma')$. Notice z is behind all variables $x_1, \dots, x_{i_k}$ in $P(\psi\theta)$. Thus z depends also only on how σ and γ' defined on the variables before it. By applying Lemma 1, we have I is a model of $\psi\theta$.

We can combine the elementary substitutions to get the following definition and theorem.

Definition 6. Let ψ be a PCNF. Suppose θ_1 is an elementary substitution w.r.t. ψ and θ_i is elementary w.r.t. $(\dots(\psi\theta_1)\theta_2\dots)\theta_{i-1}$ for every $i = 2, \dots, n$. Let $\theta = \theta_1 \dots \theta_n$ be the composition of these θ_i , i.e. $\psi\theta = (\dots(\psi\theta_1)\theta_2\dots)\theta_n$. Then θ is called a substitution w.r.t. ψ .

Theorem 2. For a PCNF ψ and a substitution θ defined as above, $\psi \models \psi\theta$.

4 Downward Refinement Operator

Let the search space S be the set of all PCNF of a first order logical language which has a finite number of function and predicate symbols. Let the top $\top \in S$ be the conjunction of a positive number of empty clauses, i.e. $\top = \square \wedge \square \dots \wedge \square$. The number of $\square$ is irrelevant because they are all equivalent to *false*. A refinement operator on S is a function $\rho : S \rightarrow 2^S$ (the set of all subsets of S). A refinement operator ρ is *downward* if for every ψ and $\phi \in \rho(\psi)$, we have $\psi \models \phi$. A *refinement chain* from ψ to ϕ is a sequence $\psi_0, \psi_1, \dots, \psi_k$ in S such that $\psi_0 \Leftrightarrow \psi$, $\psi_k \Leftrightarrow \phi$ and $\psi_i \in \rho(\psi_{i-1})$.

Definition 7. Let $\psi = q_1x_1 \dots q_nx_n C_1 \wedge C_2 \dots \wedge C_m$. Let ρ be a refinement operator on S defined by the following items.

Note that there are only a finite number of non-alphabetical variants in $\rho(\psi)$.

The first three items have to do with universal variables:

- 1. For an elementary u-unification $\theta = \{y/x\}$, where $x, y \in \text{uVar}(\psi)$ and x comes before y in $Q(\psi)$, let $\psi\theta \in \rho(\psi)$.
- 2. Let $x \in \text{uVar}(\psi)$ and an elementary u-substitution $\theta = \{x/f(y_1, \dots, y_k)\}$, let $\psi\theta \in \rho(\psi)$.
- 3. Let $L = p(y_1, \dots, y_k)$ or $\neg p(y_1, \dots, y_k)$ where $y_1, \dots, y_k$ are distinct variables new w.r.t. ψ . For an arbitrary $j = 1, \dots, m$, let ϕ_j be defined by adding a u-literal to ψ : $\phi_j = q_1x_1 \dots q_nx_n \forall y_1 \dots \forall y_k C_1 \wedge \dots \wedge (C_j \vee L) \wedge \dots \wedge C_m$. Then $\phi_j \in \rho(\psi)$.

The next 3 items have to do with existential variables:

- 4. Let $x \in \text{eVar}(\psi)$ and $\{(x, p_1), \dots, (x, p_k)\}$ be some (not all) x -occurrences in $M(\psi)$. For a new variable y and an elementary e-antiunification $\theta = \{(x/y, p_1), \dots, (x/y, p_k)\}$, let $\psi\theta \in \rho(\psi)$.
- 5. Let $(t, p_i) = (f(y_1, \dots, y_s), p_i)$, $i = 1, \dots, k$ be term occurrences in $M(\psi)$ such that all y_j are distinct and in $\text{eVar}(\psi)$. Then for the elementary e-substitution $\theta = \{(t/y, p_1), \dots, (t/y, p_k)\}$, let $\psi\theta \in \rho(\psi)$.
- 6. Let $L = p(y, \dots, y)$ or $L = \neg p(y, \dots, y)$ be a literal with new variable y . Then for $j = 1, \dots, m$, let $\phi_j \in \rho(\psi)$ be defined by adding an e-literal: $\phi_j = \exists y q_1x_1 \dots q_nx_n C_1 \wedge \dots \wedge (C_j \vee L) \wedge \dots \wedge C_m$.

The last item has to do with eu-substitutions:

- 7. Let $x \in \text{eVar}(\psi)$ and $y \in \text{uVar}(\psi)$ and suppose x comes before y in $Q(\psi)$. For the elementary eu-substitution $\theta = \{(x, y)\}$, let $\psi\theta \in \rho(\psi)$.

Theorem 3. If $\phi \in \rho(\psi)$, then $\psi \models \phi$, i.e. ρ is a downward refinement operator.

5 The Completeness of the Refinement Operator ρ

In this section we will show that the refinement operator ρ is *weakly complete* in S . That is to say, for every ϕ in S , there is a finite refinement chain from $\top$ to ϕ . We show this by the following steps. Example 3 will illustrate these steps more concretely.

1. Replace every existential variable in $M(\phi)$ by a new constant not in ϕ and remove all the existential variables from $Q(\phi)$. Let the new PCNF be ψ . Then the variables in ψ are universally quantified. Let $M(\psi) = C_1 \wedge C_2 \dots \wedge C_m$. We have then $\Box$ subsumes C_i ($\Box \succeq C_i$) for all i .
2. Similar to a result about the classic refinement refinement operator [S81,NW97], we can prove that there is a chain from $\Box$ to every C_i . The combination of these chains will give a chain from $\top$ to ψ .
3. By using the elementary e-substitutions (item 4 of ρ) we can change the constant occurrences in ψ back to existential variables. This establishes a refinement chain from ψ to ϕ' which looks almost like ϕ but all existential variables appear before the universal variables.
4. Using eu-substitutions (item 7 of ρ) we can move the existential variables to the right places in the prenex. This means there is a chain from ϕ' to ϕ . Thus we have the weak completeness of ρ .

Example 3. We will give an example to show what a concrete finite chain from $\top$ to a given $\phi = \forall x \exists y ((\neg p(x) \vee q(f(x)) \vee q(y)) \wedge r(y, a))$ looks like. Note that the chain is not unique. Such a chain exists for a general ϕ (Theorem 4) because of the following lemmas. We use an arrow $\xrightarrow{n}$ to denote a refinement step which uses the n -th item of ρ .

$$\begin{aligned}
& \Box \xrightarrow{3} \forall x \neg p(x) \xrightarrow{3,3,3} \\
& \forall x \forall u \forall v \forall w \forall w' ((\neg p(x) \vee p(u) \vee q(v)) \wedge r(w, w')) \xrightarrow{2} \\
& \forall x \forall u_1 \forall v \forall w \forall w' ((\neg p(x) \vee p(f(u_1)) \vee q(v)) \wedge r(w, w')) \xrightarrow{1,1} \\
& \forall x \forall v \forall w' (\neg p(x) \vee p(f(x)) \vee q(v)) \wedge r(v, w') \xrightarrow{2,2} \\
& \psi = \forall x (\neg p(x) \vee p(f(x)) \vee q(b)) \wedge r(b, a) \xrightarrow{5} \\
& \phi' = \exists y \forall x (\neg p(x) \vee p(f(x)) \vee q(y)) \wedge r(y, a) \xrightarrow{7} \\
& \phi = \forall x \exists y (\neg p(x) \vee p(f(x)) \vee q(y)) \wedge r(y, a)
\end{aligned}$$

Lemma 6. *Let C be a universally quantified clause. Then there is a finite chain of refinements from $\Box$ to C .*

Lemma 7. *Let $\psi = Q(\psi)M(\psi)$ be a universally quantified PCNF. Then there is a finite ρ -chain from $\top$ to ψ .*

Lemma 8. *Let $\phi = \exists y_1 \dots \exists y_n \forall x_1 \dots \forall x_m M(\phi)$ whose existential variables in the prenex appear before the universal variables. Let $b_1, \dots, b_n$ be different constants which do not appear in ϕ . Let the universally quantified ψ be ϕ after replacing variable y_i by b_i . Then there is a finite ρ -chain from ψ to ϕ .*

Theorem 4. *Given $\phi = Q(\phi)M(\phi)$, there is a finite ρ -chain from $\top$ to ϕ .*

6 Learning PCNF in Practice

Based on the refinement operator given in the previous sections, we have extended a simple version of the Claudien system (see [RD97]) to a learning system PCL (abbreviation of *PCNF Claudien*), and implemented it in Prolog. Learning by interpretations [R97] is used. Claudien learns a universal clausal theory w.r.t. a set of positive examples (interpretations), such that each example is a model of the theory. This clausal theory can be considered as a set of regularities (or integrity constraints) satisfied by these examples. PCL is able to learn a PCNF which is more expressive.

Consider a finite set of scenes (*bongard interpretations*) as positive examples. A scene contains several figures: each figure has properties like *shape*, *size*, ... and these figures are related to each other indicated by *in*, *above*, *left_of*, ... Claudien is able to find things like: $\forall x \forall y (shape(y, circle) \leftarrow figure(x), figure(y), in(x, y))$, i.e., for every figure x and y in a scene, when x is inside y , then y must be a circle. The following rule cannot be found by Claudien, but PCL can: $\forall x \exists y ((in(x, y) \leftarrow shape(x, triangle)) \wedge shape(y, circle))$, each triangle is in at least one circle.

To extend Claudien towards PCL, several issues have to be addressed. In the following subsections we discuss the most important ones.

6.1 Testing interpretation in a search space

In Claudien, a clause $head \leftarrow body$ is true for an example if the Prolog query $? - body, not(head)$ fails for that example. This works only if the clauses are *range restricted*, meaning that all variables in the head should also occur in the body. Indeed, consider a Herbrand interpretation $I = \{p(a, b), q(a)\}$ and $\phi = \forall x \forall y (p(x, y) \leftarrow q(x))$. ϕ is false because $p(a, a) \leftarrow q(a)$ is false. We get *No* as the answer of the query because there is a refutation of $false \leftarrow p(x, y)$ and $p(x, y) \leftarrow q(x)$.

For PCL, we also consider range restricted PCNFs. The following definition can be found in [N82]: a PCNF ϕ in S is *range restricted* iff

- If $x \in \text{uVar}(\phi)$ and x is in a positive literal of a clause C (in $head(C)$) in $M(\phi)$, then x must also appear in a negative literal of C (in $body(C)$).
- If $x \in \text{eVar}(\phi)$ and x is in a negative literal of a clause C (in $body(C)$) in $M(\phi)$, then there is a clause D in $M(\phi)$ with only positive literals (no body) such that x appears in every literal in D (in every atom of $head(D)$).

Intuitively, a range restricted formula is structured in such a way that for an interpretation, the range of a variable is restricted to the elements defined by some other relations in the same formula. For example, $\exists x (false \leftarrow p(x))$ is not range restricted. To test this kind of rule, we need an explicit domain for the variable x . Let $\phi = \forall x \exists y (r(y) \wedge (q(x) \leftarrow p(x, y)))$ and $I = \{q(a), r(a), p(b, a)\}$. Then ϕ is range restricted. To check if I is a model of ϕ , we need only to consider y where $r(y)$ is true, i.e. $\{y/a\}$.

A **search space** S for PCL consists of range restricted, function free PCNFs (the only functions are constants). Moreover, in a PCNF there are upper bounds for clauses in a matrix, literals in each clause, constants and variables, hence S is a finite set. The search space is further restricted by some language bias. For instance, the types of the arguments of each predicate must be declared. Also, a declaration is necessary for each type for which constants must be generated. This allows for example to specify some types where no constants should be generated,

6.2 The downward refinement operator

For the implementation of the refinement operator ρ , several issues must be addressed.

First, for efficiency it is necessary to optimize the refinement operator. We should try to avoid deriving equivalent PCNF. One way to do this is to define an order in which literals occur in each clause and an order of the clauses. This removes equivalencies obtained by applying associativity and commutativity rules. e.g. we can obtain $false \leftarrow p \wedge q$ in two ways: We can start from the empty clause $false$, first add p to obtain $false \leftarrow p$ and then add q to obtain $false \leftarrow p \wedge q$. We could also first add q to obtain $false \leftarrow q$ and then add p to obtain $false \leftarrow q \wedge p$ but the latter is not allowed because p comes alphabetically before q . Such orders are also considered in Claudien using the DLAB language bias.

Second, we need to address the following problem: For every i -th clause in a matrix with $n(\geq i)$ clauses, we can start from the conjunction of i empty clauses. Thus we have to search n trees. The computational cost of searching in the i -th tree grows very fast as i increases. We can solve this problem partially by reusing the formulas we have found. If $q_1x_1\dots q_kx_kC_1 \wedge \dots \wedge C_{i-1} \wedge C_i$ is a PCNF with i clauses which is correct w.r.t. the examples, then $q_1x_1\dots q_kx_kC_1 \wedge \dots \wedge C_{i-1}$ must also be a correct PCNF. To find the correct PCNF with i clauses, we can start from a correct PCNF containing $i - 1$ clauses with an extra empty clause added. The refinement operator can be applied again and again until good PCNFs are found.

7 Experiments

In this section we present some experiments which illustrate PCL and show that PCL can learn rules which can not be learned by existing systems that only learn single clauses.

Experiment 1 We considered a set of undirected graphs as positive examples. A possible example:

$r(a,b).$ $r(b,a).$ $r(a,c).$ $r(c,a).$
 $r(a,d).$ $r(d,a).$ $r(e,a).$ $r(a,e).$

Every graph had the property that each point was connected to at least one other point. PCL found this and also some other rules:

$$\forall x \forall y (r(x, y) \leftarrow r(y, x)), \quad \forall x \exists y (r(x, y) \leftarrow \text{point}(x))$$

Note that the last PCNF is made range restricted by adding a predicate *point*. PCL automatically makes PCNF formulas range restricted by using the language bias and the definitions of the domain predicates.

Experiment 2 We also did an experiment on some *bongard-like* examples mentioned at the beginning of last section. These are scenes of figures (in this case triangles and circles) which are related to each another. One example is

```
figure(a). figure(b). figure(c). figure(d),
in(a,b). in(c,b),
shape(a,triangle). shape(c,triangle). shape(b,circle). shape(d,circle).
```

The search space is large and many correct formulas are possible. This means that, even more than the case of Claudien, many trivial rules are found which do not give much new knowledge:

$$\begin{aligned} \exists x (\text{shape}(x, \text{triangle})), \quad \exists x \exists y (\text{in}(x, y)), \\ \exists y (\text{figure}(y) \wedge (\text{false} \leftarrow \text{shape}(y, \text{triangle}))). \end{aligned}$$

After the search continued for some time, more interesting results were given, such as: $\forall x \exists y (\text{shape}(y, \text{circle}) \wedge (\text{in}(x, y) \leftarrow \text{shape}(x, \text{triangle})))$.

8 Conclusion and Future Work

As we know, every closed formula is equivalent to a PCNF but not necessarily its Skolem standard form. Until now we consider in ILP almost exclusively conjunctions of universally quantified clauses, especially Horn clauses. To add expressiveness we should consider PCNF in general.

If we want to extend refinement operators from set of clauses to set of PCNF, we should first extend substitutions to PCNF. In this article we have defined the substitutions which specialize a given PCNF. Elementary substitutions and adding literals can be used to define a refinement operator ρ which is weakly complete. Notice that we have not used items 5 and 6 in ρ for weak completeness. In a set of formulas ordered by some kind of generalization, a refinement operator is *complete* if there is a refinement chain from ψ to ϕ whenever ψ is more general than ϕ . For example, item 5 is needed when we consider $\psi = \exists x p(x, x)$ and $\phi = \exists x \exists y p(x, y)$. We would like to know more about the search spaces where ρ is complete and the relation between item 5, 6 and the completeness.

This article lays a theoretical foundation for a system we would like to implement which generalizes the Claudien learning system. In fact, a simple system PCL is already implemented which deals with a finite search space of function free and range restricted PCNF.

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