Predicate Invention by Learning From Failures

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Abstract

Discovering novel high-level concepts is one of the most important steps needed for human-level AI. In inductive logic programming (ILP), discovering novel high-level concepts is known as predicate invention (PI). Although seen as crucial since the founding of ILP, PI is notoriously difficult and most ILP systems do not support it. In this paper, we introduce Poppi, an ILP system that formulates the PI problem as an answer set programming problem. Our experiments show that (i) PI can drastically improve learning performance when useful, (ii) PI is not too costly when unnecessary, and (iii) Poppi can substantially outperform existing ILP systems.

1 Introduction

Some of the greatest paradigm shifts in science come from the invention of new predicates, such as Galileo’s invention of acceleration and Joule’s invention of thermal energy [Russell and Norvig, 2010]. Russell [2019] argues that developing techniques to discover novel high-level concepts is one of the most important steps needed to reach human-level AI.

In inductive logic programming (ILP) [Muggleton, 1991], a form of logic-based machine learning, discovering novel high-level concepts is known as predicate invention (PI) [Stahl, 1995]. A classical example of PI is learning the definition of grandparent given only the relations mother and father. An ILP system without PI can learn the hypothesis:

\[
\text{grandparent}(A,B) \leftarrow \text{mother}(A,C), \text{mother}(C,B) \\
\text{grandparent}(A,B) \leftarrow \text{mother}(A,C), \text{father}(C,B) \\
\text{grandparent}(A,B) \leftarrow \text{father}(A,C), \text{mother}(C,B) \\
\text{grandparent}(A,B) \leftarrow \text{father}(A,C), \text{father}(C,B)
\]

By contrast, a system with PI can learn the hypothesis:

\[
\text{grandparent}(A,B) \leftarrow \text{inv}(A,C), \text{inv}(C,B) \\
\text{inv}(A,B) \leftarrow \text{mother}(A,B) \\
\text{inv}(A,B) \leftarrow \text{father}(A,B)
\]

The symbol inv is invented and can be understood as parent. Introducing this symbol makes the hypothesis smaller, both in the number of literals and clauses, which is beneficial because the search complexity of ILP is often a function of the size of the smallest solution [Cropper, 2019].

Although seen as crucial since the earliest days of ILP [Muggleton and Buntine, 1988] and repeatedly stated as a major challenge [Kok and Domingos, 2007; Muggleton et al., 2012; Kramer, 2020], most ILP systems do not support PI [Cropper et al., 2020]. As Kramer [1995] states, PI is difficult because it is unclear when and how we should invent a symbol, how many arguments should it have, what its types are, etc.

Interest in PI has resurfaced due to Metagol [Muggleton et al., 2015; Cropper and Muggleton, 2016], which uses metarules, second-order clauses, to reduce the complexity of PI by restricting the syntax of hypotheses. The major limitation of Metagol and other metarule-based approaches [Wang et al., 2015; Evans and Grefenstette, 2018; Kaminski et al., 2019; Hocquette and Muggleton, 2020] is the inherent need for metarules, which a user must provide. Given insufficient metarules, these approaches cannot learn any solution, let alone one with PI [Cropper and Tourret, 2020].

To overcome this limitation, we introduce a PI approach based on learning from failures (LFF) [Cropper and Morel, 2021], which frames the ILP problem as an answer set programming (ASP) problem [Gebser et al., 2012]. We build on LFF by framing the PI problem as an ASP problem. Compared to existing approaches, our approach does not need a user to manually provide metarules or specify the arity and argument types of an invented symbol [Law et al., 2014], i.e. our approach supports automatic PI. Moreover, our approach retains the benefits of LFF, notably scalability and the ability to learn recursive programs. Overall, our contributions are:

- We extend LFF to support predicate invention. We introduce a new type of redundancy constraint and show that it is sound with respect to optimal solutions.
- We introduce Poppi, a LFF implementation that supports automatic PI.
- We experimentally show that (i) PI can drastically improve learning performance when useful, (ii) PI is not too costly when unnecessary, and (iii) Poppi can substantially outperform existing ILP systems.
2 Related Work

Early work on PI was based on the idea of inverse resolution and W operators [Muggleton and Buntine, 1988]. Although these approaches could support PI, they never demonstrated completeness, partly because of the lack of a declarative bias to delimit the hypothesis space [Muggleton et al., 2015].

One PI approach is to use placeholders [Leban et al., 2008] to predefine invented symbols. However, this approach requires that a user manually specify the arity and argument types of an ‘invented’ symbol [Law et al., 2014], which rather defeats the point, or requires enumerating every possible symbol [Evans et al., 2021]. By contrast, POPPI does not need a user to manually pre-define predicates and can automatically infer argument types, i.e. POPPI supports automatic PI. INSPIRE [Schüller and Benz, 2018] also uses ASP for PI, but only learns single-clause non-recursive programs. By contrast, POPPI learns recursive multi-clause programs. PI can be performed by learning programs in a multi-task setting [Lin et al., 2014] or as a pre-/post-processing step [Dumancic and Blockeel, 2017; Cropper, 2019; Dumancic et al., 2019; Dumancic et al., 2021]. By contrast, POPPI performs PI whilst learning.

METAGOL uses metarules to restrict the syntax of hypotheses and drive PI. For instance, the chain metarule \( P(A, B) \leftarrow Q(A, C), R(C, B) \) allows METAGOL to induce programs such as \( f(A, B) \leftarrow \text{tail}(A,C), \text{tail}(C,B) \), which drops the first two elements from a list. To induce longer clauses, METAGOL chains clauses together using PI, such as the following program which drops the first four elements from a list:

\[
\begin{align*}
P = \{ & \ f(A, B) \leftarrow \text{inv}(A,C),\text{inv}(C,B) \\
& \ \text{inv}(A,B) \leftarrow \text{tail}(A,C),\text{tail}(C,B) \}
\end{align*}
\]

The major limitation of metarule-driven PI approaches [Wang et al., 2015; Evans and Grefenstette, 2018; Kaminski et al., 2019; Hocquette and Muggleton, 2020] is their inherent need for user-supplied metarules, which, in some cases, are impossible to provide [Cropper and Tourret, 2020]. POPPI overcomes this major limitation because it does not need metarules. Moreover, in Section 4, we show that POPPI subsumes METAGOL because it can replicate its search strategy.

POPPI builds on the LFF system POPPER, which works in three repeating stages: generate, test, and constrain. In the generate stage, POPPER builds a logic program that satisfies a set of hypothesis constraints. In the test stage, POPPER tests a program against the examples. A hypothesis fails when it is incomplete (does not entail all the positive examples) or inconsistent (entails a negative example). If a hypothesis fails, POPPER learns hypothesis constraints from the failure, which it then uses to restrict subsequent generate stages. It repeats this process until it finds a complete and consistent program. POPPI extends POPPER to support automatic PI.

3 Problem Setting

We now define PI and extend LFF to support PI. We assume familiarity with logic programming [Lloyd, 2012].

3.1 Predicate Invention

We focus on the ILP learning from entailment setting [Raedt, 2008].

**Definition 1 (ILP input).** An ILP input is a tuple \( (B, E^+, E^-, H) \), where \( B \) is a logic program denoting background knowledge, \( E^+ \) and \( E^- \) are sets of ground atoms which represent positive and negative examples respectively, and \( H \) is a hypothesis space (the set of all hypotheses).

In practice, the hypothesis space is restricted by a language bias, such as metarules or mode declarations. The ILP problem is to find a solution:

**Definition 2 (Solution).** Given an ILP input \( (B, E^+, E^-, H) \), the ILP problem is to return a hypothesis \( H \in H \) such that \( \forall e \in E^+, H \cup B \models e \) and \( \forall e \in E^-, H \cup B \not\models e \).

Muggleton [1994] and Stahl [1995] both provide definitions for PI, which we adapt. We denote the predicate signature (the set of all predicate symbols) of a logic program \( P \) as \( \text{ps}(P) \).

**Definition 3 (Predicate invention).** Let \( (B, E^+, E^-, H) \) be an ILP input and \( H \in H \). Then \( H \) contains an invented predicate symbol if and only if \( \text{ps}(H) \setminus \text{ps}(B \cup E^+ \cup E^-) \neq \emptyset \).

PI is necessary when needed to learn a solution:

**Definition 4 (Necessary predicate invention).** Let \( I = (B, E^+, E^-, H) \) be an ILP input. Then PI is necessary for \( I \) if no \( H \in H \) is a solution without PI.

PI is useful when it allows us to learn a better solution:

**Definition 5 (Useful predicate invention).** Let \( (B, E^+, E^-, H) \) be an ILP input and \( \text{cost} : H \rightarrow R \) be an arbitrary cost function. Then PI is useful when (i) there is a \( H \in H \) such that \( H \) is a solution with invented predicate symbols, and (ii) \( \forall H' \in H \), where \( H' \) is a solution, \( \text{cost}(H) \leq \text{cost}(H') \).

In this paper, we define the \( \text{cost}(H) \) to be the total number of literals in the logic program \( H \).

3.2 Learning From Failures

We extend LFF to support PI. LFF uses predicate declarations to restrict what predicate symbols may appear in a hypothesis. A predicate declaration is a ground atom of the form \( \text{head}_{\text{pred}}(p, a) \) or \( \text{body}_{\text{pred}}(p, a) \) where \( p \) is a predicate symbol of arity \( a \). Given a set of predicate declarations \( D \), a definite clause \( C \) is declaration consistent when (i) if \( p/m \) is the predicate in the head of \( C \), then \( \text{head}_{\text{pred}}(p, m) \) is in \( D \), and (ii) for all \( q/n \) predicate symbols in the body of \( C \), \( \text{body}_{\text{pred}}(q, n) \) is in \( D \). LFF uses hypothesis constraints to restrict the hypothesis space. Let \( \mathcal{L} \) be a language that defines hypotheses, i.e. a meta-language. Then a hypothesis constraint is a constraint expressed in \( \mathcal{L} \). Let \( C \) be a set of hypothesis constraints written in a language \( \mathcal{L} \). A set of definite clauses \( H \) is consistent with \( C \) if, when written in \( \mathcal{L} \), \( H \) does not violate any constraint in \( C \).

We define the LFF problem:

**Definition 6 (LFF input).** The LFF input is a tuple \((E^+, E^-, B, D, C)\) where \( E^+ \) and \( E^- \) are sets of ground
atoms denoting positive and negative examples respectively; 
B is a Horn program denoting background knowledge; D is 
a set of predicate declarations; and C is a set of hypothesis 
constraints.

A definite program is a hypothesis when it is consistent with 
both D and C. We denote the set of such hypotheses as \( \mathcal{H}_{D,C} \). 
We define a LFF solution:

**Definition 7 (LFF solution).** Given an input tuple 
\((E^+, E^-, B, D, C)\), a hypothesis \( H \in \mathcal{H}_{D,C} \) is a solution 
when \( H \) is complete (\( \forall e \in E^+, \ B \cup H \models e \)) and consistent 
(\( \forall e \in E^-, \ B \cup H \not\models e \)). 
If a hypothesis is not a solution then it is a failure or a 
failed hypothesis. A hypothesis is incomplete when \( \exists e \in E^+, \ H \cup B \not\models e \). A hypothesis is inconsistent when \( \exists e \in E^-, \ H \cup B \models e \). A hypothesis is totally incomplete 
when \( \forall e \in E^+, \ H \cup B \not\models e \). We define an optimal solution:

**Definition 8 (Optimal solution).** Given an input tuple 
\((E^+, E^-, B, D, C)\), a hypothesis \( H \in \mathcal{H}_{D,C} \) is optimal 
when (i) \( H \) is a solution, and (ii) \( \forall H' \in \mathcal{H}_{D,C} \), where \( H' \) is a solution, cost\((H) \leq \text{cost}(H')\).

3.3 Redundancy Constraints

The key idea of LFF is to learn hypothesis constraints from 
failed hypotheses. Cropper and Morel [2021] introduce constraints 
based on subsumption [Plotkin, 1971]. A clause \( C_1 \) 
subsumes a clause \( C_2 \) (\( C_1 \subseteq C_2 \)) if and only if there 
exists a substitution \( \theta \) such that \( C_1 \theta \subseteq C_2 \). A clausal theory 
\( T_1 \) subsumes a clausal theory \( T_2 \) (\( T_1 \subseteq T_2 \)) if and only if 
\( \forall C_2 \in T_2, \exists C_1 \in T_1 \) such that \( C_1 \subseteq C_2 \). A clausal 
theory \( T_1 \) is a specialisation of a clausal theory \( T_2 \) if and only if 
\( T_2 \not\subseteq T_1 \). A clausal theory \( T_1 \) is a generalisation of a 
clausal theory \( T_2 \) if and only if \( T_1 \subseteq T_2 \).

If a hypothesis \( H \) is incomplete, a specialisation constraint 
prunes specialisations of \( H \), as they are also guaranteed to 
be incomplete. Likewise, if a hypothesis \( H \) is inconsistent, a 
generalisation constraint prunes generalisations of \( H \), as 
they are also guaranteed to be inconsistent. Cropper and Morel 
[2021] show that generalisation and specialisation constraints 
are sound in that they never prune solutions from the hypothesis 
space. The authors also introduce a third type of constraint 
called an elimination constraint and show it is sound for op- 
timal solutions. If a hypothesis \( H \) is totally incomplete, then 
there is no need for \( H \) (or a specialisation of it) to appear in 
a complete and separable hypothesis. A separable hypothesis 
\( H \) is one where no predicate symbol in the head of a clause 
in \( H \) occurs in the body of a clause in \( H \). Elimination 
constraints are unsuitable for PI because an invented predicate 
should always appear in the body of a clause.

To overcome this limitation, we introduce redundancy con- 
straints. We adapt the standard notion of a dependency graph 
[Apt and Bol, 1994] of a program from predicates to clauses:

**Definition 9 (Dependency).** The dependency graph for 
the definite program \( P \) is a directed graph where the nodes are 
the clauses in \( P \). There is an edge between nodes \( C_1 \) and \( C_2 \) 
if the head predicate symbol of \( C_2 \) occurs in the body of \( C_1 \). 
We say \( C_1 \) depends on \( C_2 \) if there is a path from \( C_1 \) to \( C_2 \).

We require that each clause in a hypothesis is reachable from 
a target predicate clause (a clause that generalises the examples). 
We use the dependency relation to characterise when a 
program is at least as specific as another program:

**Definition 10 (Contained specialisation).** Let \( P \) and \( Q \) be 
definite programs and \( P' = \{ C \in Q \mid \exists D \in P, D \subseteq C \} \). A 
clause \( C \in P' \) P-specialises \( Q \) if (i) \( C \) does not depend on 
any clause in \( Q \setminus P' \), and (ii) no clause in \( Q \setminus P' \) depends on 
\( C \).

The idea is that part of \( Q \) cannot entail more than \( P \), as 
the clauses of \( Q \) on paths to \( C \) specialise \( P \), as we now illustrate:

**Example 1.** Let \( P = \{ C_1, C_2 \} \), \( C_1 = f(A,B) \leftarrow \) 
\( \text{inv}(A,C), \text{inv}(C,B), \) \( C_2 = \text{inv}(A,B) \leftarrow \text{tail}(A,C), \text{tail}(C,B), \) 
\( C_Q = f(A,B) \leftarrow \text{reverse}(A,B), \) and \( Q = P \cup \{ C_Q \} \). In \( Q \), neither 
\( C_2 \) nor \( C_Q \) depend on another, so \( C_2 \) P-specialises \( Q \). As \( C_2 \) cannot help \( Q \) entail more than \( P \) does, if \( P \) is a 
totally incomplete hypothesis then \( C_2 \) is redundant in \( Q \).

If the hypothesis \( P \) is totally incomplete and there is a clause 
that \( P \)-specialises the hypothesis \( Q \), we call \( P \) a redundant 
hypothesis. We show that redundant hypotheses are not opti- 
mal:

**Theorem 1 (Redundancy soundness).** Let 
\((E^+, E^-, B, D, C)\) be a LFF input, \((H_1, H_2) \in \mathcal{H}_{D,C}, \) 
and \( H_1 \) be totally incomplete. If \( H_2 \) has a clause that 
\( H_1 \)-specialises it, then \( H_2 \) is not an optimal solution.

The proof of Theorem 1 is in Appendix A. We call constraints 
that only prune redundant hypotheses redundancy constraints. 
We show that redundancy constraints prune more than elimination 
constraints:

**Theorem 2 (Redundancy effectiveness).** Let 
\((E^+, E^-, B, D, C)\) be a LFF input and \( H \in \mathcal{H}_{D,C} \) be 
totally incomplete. As (i) all separable hypotheses containing 
specialisations of \( H \) are redundant, and (ii) there exist 
\( H' \in \mathcal{H}_{D,C} \) that are redundant but not separable, redundancy 
constraints prune strictly more than elimination constraints.

**Proof.** For (i), let \( H^* \) be a separable hypothesis containing a 
specialisation of \( H \). As separability implies no clause of \( H^* \) 
depends on another, any clause of \( H^* \) specialising a clause of 
\( H \) is redundant. For (ii) Example 1 suffices, taking \( H = P \) 
and \( H' = Q \). Hypothesis \( Q \) is redundant but not separable.

4 POPPI

POPPI extends POPPER with a new PI module and the ability 
to learn redundancy constraints from failures. Due to space 
limitations, we cannot describe POPPER in detail, so we refer 
the reader to the original paper for a detailed explanation 
[Cropper and Morel, 2021]. POPPI works in three repeating 
stages: generate, test, and constrain, which we now describe.

**Generate**

POPPI takes as input (i) predicate declarations, (ii) hypothesis 
constraints, and (iii) bounds on the maximum number of variables, 
literals, and clauses in a hypothesis. POPPI returns an 
answer set which represents a definite program, if one exists. 
For instance, consider an answer set with the following head 
(\( b \_ \text{lit} \)) and body (\( b \_ \text{lit} \)) literals:
The first argument of each literal is the clause index, the second is the predicate symbol, the third is the arity, and the fourth is the literal variables, where 0 represents A, 1 represents B, etc. This answer set corresponds to the definite program:

```
last(A,B):- tail(A,C), empty(C), head(A,B).
last(A,B):- tail(A,C), last(C,B).
```

Figure 1 shows the base ASP program to generate programs. POPPI extends POPPER by allowing invented symbols (invented(P,A)) to appear in head and body literals.

POPPPI uses ASP constraints to ensure that a program is declaration consistent and obeys hypothesis constraints. For instance, to prune programs where the head literal appears in the body, POPPI enforces the constraint:

```
: - h_lit(C,P,A,Vs), b_lit(C,P,A,Vs).
```

By later adding learned hypothesis constraints, POPPI eliminates answer sets and thus prunes the hypothesis space.

```
head_p(P,A):- head_pred(P,A).
head_p(P,A):- invented(P,A).
body_p(P,A): body_pred(P,A).
body_p(P,A):- invented(P,A).
clause(0..N-1):- max_clauses(N).
{h_lit(C,P,A,Vs)}:- body_p(P,A), vars(A,Vs), clause(C).
```

Figure 1: Partial listing of the program generator in POPPI.

**PI Module.** POPPI builds on POPPER with a PI module, partially shown in Figure 2. Lines 1-3 show the ASP choice rules which allow POPPI to perform PI. POPPI automatically adds n – 1 choice rules to allow n – 1 invented symbols, where n is the maximum number of clauses allowed in a program. This module contains many constraints specific to PI to prune redundant programs. Lines 4-6 define an ordering over invented symbols, similar to METAGOL, and line 9 enforces this ordering. Lines 7-8 ensure that an invented symbol is in the head of a clause then it must also appear in the body of a clause (and vice-versa). Line 10 ensures that POPPI uses invented predicates in order, e.g. to prevent the symbol inv2 from appearing in a program if inv1 does not already appear. This module also includes code (omitted for brevity) to infer the argument types of an invented predicate by how it is used in the program and propagates the types through the program.

**Test and constrain**

The test stage of POPPI is identical to POPPER: POPPI transforms an answer set to a definite program (a Prolog program) and tests it against the training examples. If a hypothesis fails, then, in the constrain stage, POPPI derives ASP constraints which it adds to the generator program to prune answer sets and constrain subsequent hypothesis generation. For instance, suppose this hypothesis is inconsistent:

```
last(A,B):- reverse(A,C), head(C,B).
```

Then POPPI generates a generalisation constraint to prune generalisations of this hypothesis:

```
seen(C,id1):- h_lit(C,last,2,(V0,V1)), b_lit(C,reverse,2,(V0,V2)), b_lit(C,right,2,(V2,V1)).
```

POPPPI extends POPPER with redundancy constraints (Section 3.3). For instance, suppose this program is totally incomplete:

```
f(A,B):- inv1(A,C), right(C,B).
inv1(A,B):- right(A,C), right(C,B).
```

Whereas POPPER would only generate a specialisation constraint, POPPI additionally generates a redundancy constraint:

```
seen(C,id1):- h_lit(C,f,2,(V0,V1)), b_lit(C,inv1,2,(V0,V2)), b_lit(C,right,2,(V2,V1)).
```

Appendix B describes the algorithm POPPI uses to build redundancy constraints.

**Loop.** POPPI repeats the generate/test/constraint loop. To find an optimal solution, POPPI increases the number of literals allowed in a program when the hypothesis space is empty at a certain program size (e.g. when there are no more programs to generate). To improve efficiency, POPPI uses Clingo’s multi-shot solving [Gebser et al., 2019] to maintain state between the three stages and thus remember learned conflicts. This loop repeats until either (i) POPPI finds an optimal solution, or (ii) there are no more hypotheses to test.

**POPPPIMMIL** METAGOL needs metarules to define the hypothesis space and drive PI. POPPER can simulate metarules through hypothesis constraints [Cropper and Morel, 2021]. By supporting PI, POPPI subsumes METAGOL. In our experiments, we directly compare METAGOL against POPPI when given identical metarules, which we call POPPPIMMIL.

5 Experiments

Few papers empirically evaluate PI [Cropper, 2019; Hocquette and Muggleton, 2020] and none in a systematic manner. Therefore, our experiments try to answer the question:...
Q1 How beneficial is PI when it is useful?
To answer Q1, Experiments 5.1 and 5.2 compare ILP systems with and without PI on problems purposely designed to benefit from PI. Specifically, we compare (i) POPPI against POPPER, and (ii) METAGOL against METAGOL without the ability to reuse invented predicates, which we denote as METAGOL_{\neg}.

PI should improve performance when it is useful (Definition 5), but what about when it is unnecessary? In other words, can PI be harmful? To answer this question, our experiments try to answer the question:

Q2 How costly is PI when it is unnecessary?
To answer Q2, Experiment 5.3 compares the same systems on a problem that should not benefit from PI.

To test our claim that POPPI can go beyond existing systems that support PI, our experiments try to answer the question:

Q3 How well does POPPI perform against other ILP systems?
To answer Q3, we compare POPPI against POPPER. We also compare POPPI against METAGOL, which is the only system that supports automatic PI and learning recursive programs.

Settings. We use POPPI and POPPER with the same settings as Cropper and Morel [2021]: at most 6 variables in a clause, at most 5 body literals, and at most 3 clauses. METAGOL needs metarules. We consider two sets of metarules: with and without recursion, listed in Appendix C. POPPI_{MIL} uses the same metarules encoded as hypothesis constraints. We use a 3.8 GHz 8-Core Intel Core i7 with 32GB of ram. Note that all the ILP systems only use a single CPU.

5.1 Experiment 1 - Robot Planning
This experiment aims to answer Q1. We therefore use a problem where PI should be useful.

Materials. A robot is in a 100^2 grid world. An example is an atom f(x, y) where x and y are initial and final states respectively. A state describes the position of the robot. The problem is to learn a plan to move right k times. As BK, we provide the single dyadic predicate right, which moves the robot right one step.

Method. For each \(k\) in \{4, 8, 12, 16, 20, 24\}, we generate 10 positive training examples of the robot moving right \(k\) times and \(k-1\) negative training examples of the robot moving right \(i\) times for \(i = \ldots k - 1\). The target solution is a chain of \(k\) right actions. As the value \(k\) grows, PI should become more useful because a system can invent and reuse chains of actions. We repeat the experiment five times. We measure learning times and standard error. We set a learning timeout of two minutes.

Results. Figure 3 shows the results. Without recursion, METAGOL is the best performing system because it can chain invented predicate symbols, such as this program for when \(k = 16\), where each \(f_i\) is invented:

\[
\begin{align*}
f(A,B) & : - f_1(A,C), f_1(C,B). \\
f_1(A,B) & : - f_2(A,C), f_2(C,B). \\
f_2(A,B) & : - f_3(A,C), f_3(C,B). \\
f_3(A,B) & : - right(A,C), right(C,B). \\
\end{align*}
\]

This reuse allows Metagol (and POPPI_{MIL}) to move right \(2^n\) times using only \(n\) clauses, i.e. to move right \(k > 2\) times, METAGOL requires at most \(\ln(k)\) clauses. By contrast, METAGOL_{\neg} performs poorly because it cannot reuse invented symbols and to move right \(k > 2\) times requires \(k-1\) clauses.

POPPPI substantially outperforms POPPER. To move right \(k\) times, POPPER must learn a program with a single clause formed of \(k + 1\) literals. By contrast, POPPI can learn a more compact program, such as a program which requires only 10 literals to move right 16 times:

\[
\begin{align*}
f(A,B) & : - inv_1(A,C), inv_1(C,D), inv_1(D,E), inv_1(E,B). \\
inv_1(A,B) & : - right(A,C), right(C,D), right(D,E), right(E,B). \\
\end{align*}
\]

With recursion, METAGOL performs poorly because of its inefficient search algorithm. By contrast, POPPI and POPPI_{MIL} both perform well with recursion.

Overall, these results suggest that PI is extremely beneficial when useful (Q1) and that POPPI can drastically outperform existing systems (Q3).

5.2 Experiment 2 - List Transformation
This experiment aims to corroborate the results of Experiment 1 to answer Q1. We therefore use a problem where PI should be useful. This problem is modelled on the problems Rule et al. [2020] use to model human intelligence.

Materials. The task is to learn a program to find the \(kth\) element of a list. An example is an atom \(f(x, y)\), where \(x\) is a list of characters and \(y\) is a character. A list is a random permutation of all the ASCII lowercase letters. As BK, we provide the dyadic predicates head and tail.
Method. For each $k$ in $\{2, 4, 8, 10, 12, 14\}$, we generate 1 positive example where $y$ is the $k$th element of the list $x$. We generate a negative training example for every other element in the list. The target solution is a chain of $k-1$ tail relations followed by a head relation. As the value $k$ grows, PI should become more useful because a system can invent and reuse chains of actions. We repeat the experiment five times. We measure learning times and standard error. We set a learning timeout of two minutes.

Results. Figure 4 shows the results, which largely match those from Experiment 5.1 and again suggest that PI is extremely beneficial when useful (Q1) and that POPPI can drastically outperform existing systems (Q3).

5.3 Experiment 3 - Programming Puzzles

Experiments 1 and 2 clearly show that PI can drastically improve performance when it is useful (Q1). However, as we discussed at the start of Section 5, PI is not always useful. The main purpose of this experiment is to answer Q2. We therefore use problems where PI should not be useful.

Materials. We repeat the programming puzzles experiment from [Cropper and Morel, 2021]. The first column in Table 1 shows the problems. Note that these problems are extremely difficult for ILP systems and POPPER is the first system that can reliably learn solutions to them. We describe all the experimental materials in Appendix D.

Method. We generate 10 positive and 10 negative examples per problem. Each example is randomly generated from lists up to length 50 formed of integers from 1-100. We test on 1000 positive and 1000 negative randomly sampled examples. We measure predictive accuracy and learning time. We enforce a timeout of three minutes per task. We repeat the experiment five times and measure the mean and standard error.

Results. Table 1 shows that mean predictive accuracies. POPPER outperforms POPPI in all cases and a paired t-test confirms the significance at the $p < 0.01$ level, although the difference is always less than double. Overall, these results suggest that PI is not too costly when not useful (Q2). Moreover, as Table 1 shows, POPPI drastically outperforms METAGOL on all but three problems, where they both perform identically and helps answer (Q3).

| Name     | POPPI | POPPI\textsubscript{MIL} | POPPER | METAGOL |
|----------|-------|--------------------------|--------|---------|
| addhead  | 100 ± 0 | 50 ± 0 | 100 ± 0 | 50 ± 0 |
| droppk   | 100 ± 0 | 50 ± 0 | 100 ± 0 | 50 ± 0 |
| droplast | 100 ± 0 | 50 ± 0 | 100 ± 0 | 50 ± 0 |
| evens    | 100 ± 0 | 50 ± 0 | 100 ± 0 | 50 ± 0 |
| finddup  | 98 ± 0  | 80 ± 12 | 99 ± 0 | 50 ± 0 |
| last     | 100 ± 0 | 50 ± 0 | 100 ± 0 | 100 ± 0 |
| len      | 100 ± 0 | 50 ± 0 | 100 ± 0 | 50 ± 0 |
| member   | 100 ± 0 | 100 ± 0 | 100 ± 0 | 100 ± 0 |
| sorted   | 100 ± 0 | 50 ± 0 | 100 ± 0 | 50 ± 0 |
| threesame| 99 ± 0  | 50 ± 0 | 99 ± 0 | 99 ± 0 |

| Name     | POPPI | POPPI\textsubscript{MIL} | POPPER | METAGOL |
|----------|-------|--------------------------|--------|---------|
| addhead  | 1 ± 0 | 120 ± 0.1 | 0.4 ± 0 | 120 ± 0 |
| droppk   | 1 ± 0.1 | 0.1 ± 0 | 1 ± 0 | 0.2 ± 0 |
| droplast | 5 ± 1 | 120 ± 0.1 | 4 ± 0.8 | 120 ± 0 |
| evens    | 8 ± 0.5 | 0.7 ± 0 | 6 ± 0.2 | 120 ± 0 |
| finddup  | 91 ± 5 | 69 ± 22 | 48 ± 2 | 120 ± 0 |
| last     | 4 ± 0.2 | 120 ± 0.1 | 3 ± 0.3 | 0.6 ± 0.3 |
| len      | 25 ± 1 | 120 ± 0.1 | 16 ± 0.6 | 120 ± 0 |
| member   | 0.7 ± 0.1 | 0.2 ± 0 | 0.2 ± 0 | 0.3 ± 0 |
| sorted   | 32 ± 3 | 0.5 ± 0 | 35 ± 5 | 120 ± 0 |
| threesame| 0.2 ± 0 | 0.6 ± 0 | 0.2 ± 0 | 0.6 ± 0.2 |

Table 1: Programming puzzles predictive accuracies. We round accuracies to integer values. The error is standard error.

Table 2: Programming puzzles learning times. We round times over 1 second to the nearest second. The error is standard error.

6 Conclusions and Limitations

Although seen as key to human-level AI [Russell, 2019] and repeatedly stated as a major challenge, most ILP systems do not support PI, and those that do have severe limitations (Section 2). To overcome these limitations, we have extended LFF with redundancy constraints which are sound (Theorem 1) and more effective (Theorem 2) than existing constraints. We implemented our approach in the ILP system POPPI, which supports automatic PI, i.e., does not need metarules nor requires a user manually predefine invented symbols. We have experimentally shown that (i) PI can drastically improve learning performance when useful, (ii) PI is not too costly when unnecessary, and (iii) POPPI can substantially outperform existing ILP systems.

There are limitations for future work to address.

Inefficient PI. Although POPPI convincingly outperforms METAGOL, its PI technique is inefficient. For instance, in Experiment 5.1, when learning to move right eight times, POPPI considers this hypothesis:
We could address this issue by reasoning about unfolded hypotheses. From this failure, POPPI learns constraints to prune specialisations of it. However, POPPI will still consider logically equivalent hypotheses, such as:

\[
\begin{align*}
\text{f}(A,B) & \leftarrow \text{inv1}(A,C), \text{right}(C,D), \text{right}(D,B). \\
\text{inv1}(A,B) & \leftarrow \text{right}(A,C), \text{right}(C,B).
\end{align*}
\]

This hypothesis fails, as it only moves right four times. From this failure, POPPI learns constraints to prune specialisations of it. However, POPPI will still consider logically equivalent hypotheses, such as:

\[
\begin{align*}
\text{f}(A,B) & \leftarrow \text{right}(A,C), \text{inv1}(C,D), \text{right}(D,B). \\
\text{inv1}(A,B) & \leftarrow \text{right}(A,C), \text{right}(C,B).
\end{align*}
\]

We could address this issue by reasoning about unfolded hypotheses [Tamaki and Sato, 1984]. In general, we expect to make further substantial efficiency improvements in POPPI.

**Higher-arity invention.** METAGOL can only learn monadic and dyadic programs because of the restrictions imposed by metarules. Therefore, to perform a fair experimental comparison, our experiments only consider inventing monadic and dyadic predicates. POPPI can, however, invent predicates with arity greater than two. In future work, we want to apply POPPI to more general problems with higher-arity invention.

**References**

[Apt and Bol, 1994] Krzysztof R. Apt and Roland N. Bol. Logic programming and negation: A survey. *J. Log. Program.*, 1994.

[Cropper and Morel, 2021] Andrew Cropper and Rolf Morel. Learning programs by learning from failures. *Machine Learning*, 2021.

[Cropper and Muggleton, 2016] Andrew Cropper and Stephen H. Muggleton. Learning higher-order logic programs through abstraction and invention. In *IJCAI*, 2016.

[Cropper and Tourret, 2020] Andrew Cropper and Sophie Tourret. Logical reduction of metarules. *Machine Learning*, 2020.

[Cropper et al., 2020] Andrew Cropper, Sebastijan Dumancic, and Stephen H. Muggleton. Turning 30: New ideas in inductive logic programming. In *IJCAI*, 2020.

[Cropper, 2019] Andrew Cropper. Playgol: Learning programs through play. *IJCAI*, 2019.

[Dumancic and Blockeel, 2017] Sebastijan Dumancic and Hendrik Blockeel. Clustering-based relational unsupervised representation learning with an explicit distributed representation. In *IJCAI*, 2017.

[Dumancic et al., 2019] Sebastijan Dumancic, Tias Guns, Wannes Meert, and Hendrik Blockeel. Learning relational representations with auto-encoding logic programs. *IJCAI*, 2019.

[Dumancic et al., 2021] Sebastijan Dumancic, Tias Guns, and Andrew Cropper. Knowledge refactoring for inductive program synthesis. *AAAI*, 2021.

[Evans and Grefenstette, 2018] Richard Evans and Edward Grefenstette. Learning explanatory rules from noisy data. *JAIR*, 2018.

[Evans et al., 2021] Richard Evans, José Hernández-Orallo, Johannes Welbl, Pushmeet Kohli, and Marek Sget. Making sense of sensory input. *Artificial Intelligence*, 2021.

[Gebser et al., 2012] Martin Gebser, Roland Kaminski, Benjamin Kaufmann, and Torsten Schaub. *Answer Set Solving in Practice*. Morgan & Claypool Publishers, 2012.

[Gebser et al., 2019] Martin Gebser, Roland Kaminski, Benjamin Kaufmann, and Torsten Schaub. Multi-shot ASP solving with clingo. *TPLP*, 2019.

[Hocquette and Muggleton, 2020] Céline Hocquette and Stephen H. Muggleton. Complete bottom-up predicate invention in meta-interpretive learning. In *IJCAI*, 2020.

[Kaminski et al., 2019] Tobias Kaminski, Thomas Eiter, and Katsumi Inoue. Meta-interpretive learning using hex-programs. In *IJCAI*, 2019.

[Kok and Domingos, 2007] Stanley Kok and Pedro M. Domingos. Statistical predicate invention. In *ICML*, 2007.

[Kramer, 1995] Stefan Kramer. Predicate invention: A comprehensive view. *Technical report*, 1995.

[Kramer, 2020] Stefan Kramer. A brief history of learning symbolic higher-level representations from data (and a curious look forward). In *IJCAI*, 2020.

[Law et al., 2014] Mark Law, Alessandra Russo, and Kryzia Broda. Inductive learning of answer set programs. In *JELIA*, 2014.

[Leban et al., 2008] Gregor Leban, Jure Zabkar, and Ivan Bratko. An experiment in robot discovery with ILP. 2008.

[Lin et al., 2014] Dianhuan Lin, Eyal Dechter, Kevin Ellis, Joshua B. Tenenbaum, and Stephen Muggleton. Bias reformulation for one-shot function induction. In *ECAI*, 2014.

[Lloyd, 2012] John W Lloyd. *Foundations of logic programming*. Springer Science & Business Media, 2012.

[Muggleton and Buntine, 1988] Stephen Muggleton and Wray L. Buntine. Machine invention of first order predicates by inverting resolution. In *ICML*, 1988.

[Muggleton et al., 2012] Stephen Muggleton, Luc De Raedt, David Poole, Ivan Bratko, Peter A. Flach, Katsumi Inoue, and Ashwin Srinivasan. ILP turns 20 - biography and future challenges. *Machine Learning*, 2012.

[Muggleton et al., 2015] Stephen H. Muggleton, Dianhuan Lin, and Alireza Tamaddoni-Nezhad. Meta-interpretive learning of higher-order dyadic Datalog: predicate invention revisited. *Machine Learning*, 2015.

[Muggleton, 1991] Stephen Muggleton. Inductive logic programming. *New Generation Comput.*, 1991.

[Muggleton, 1994] Stephen Muggleton. Predicate invention and utilization. *J. Exp. Theor. Artif. Intell.*, 1994.

[Plotkin, 1971] G.D. Plotkin. *Automatic Methods of Inductive Inference*. PhD thesis, Edinburgh University, August 1971.

[Raedt, 2008] Luc De Raedt. *Logical and relational learning*. Cognitive Technologies. Springer, 2008.
We assign each hypothesis an identifier, e.g. h1. Suppose that H has N clauses. Then the head of the following seen program rule is true precisely when the program contains a specialisation of H:

\[
\text{seen}(\ldots) := \text{seen}(\ldots, c_1), \ldots, \text{seen}(\ldots, c_N).
\]

We then consider all predicates defined by H. When a predicate p depends on itself (is recursive), we say p is recursively called. For each predicate p of H that is not recursively called, we generate a constraint. For fixed p, let q1, ..., qM be all the predicates of H except p. Let #cls(P) denote the number of clauses defining predicate P in H. #rec_cls(p) denotes the number of recursive clauses of P. Each non-recursively called predicate of H then causes a redundancy constraint of the following shape to be generated:

\[
\begin{align*}
&-\text{seen}(h1), \\
&\text{num_clauses}(q1, #\text{cls}(q1)), \\
&\ldots, \\
&\text{num_clauses}(qM, #\text{cls}(qM)), \\
&\text{num_recursive}(p, #\text{rec_cls}(p)).
\end{align*}
\]

9 Appendix: Metarules

9.1 Experiments 5.1 and 5.2

Listing 1: Metarules without recursion.

\[
\begin{align*}
\text{metarule}([P,Q],[P,A,B],[[Q,A,B]]). \\
\text{metarule}([P,Q,R],[P,A,B],[[Q,A,B],[R,A]]). \\
\text{metarule}([P,Q,R],[P,A,B],[[Q,A,B],[R,B]]). \\
\text{metarule}([P,Q],[P,A],[[Q,A,B],[P,B]]). \\
\text{metarule}([P,Q,R],[P,A,B],[[Q,A,C],[R,C,B]]). \\
\end{align*}
\]

Listing 2: Metarules with recursion.

\[
\begin{align*}
\text{metarule}([P,Q],[P,A,B],[[Q,A,B]]). \\
\text{metarule}([P,Q,R],[P,A,B],[[Q,A,B],[R,A]]). \\
\text{metarule}([P,Q,R],[P,A,B],[[Q,A,B],[R,B]]). \\
\text{metarule}([P,Q],[P,A],[[Q,A,B],[P,B]]). \\
\text{metarule}([P,Q,R],[P,A,B],[[Q,A,C],[R,C,B]]). \\
\end{align*}
\]

9.2 Experiment 5.3

Listing 3: Metarules used in Experiment 5.3

\[
\begin{align*}
\text{metarule}([P,Q],[P,A],[[Q,A]]). \\
\text{metarule}([P,Q],[P,A],[[Q,A]]). \\
\text{metarule}([P,Q,R],[P,A,B],[[Q,A,B],[R,B]]). \\
\text{metarule}([P,Q],[P,A],[[Q,A,B],[P,B]]). \\
\text{metarule}([P,Q],[P,A,B],[[Q,A,B],[R,B]]). \\
\text{metarule}([P,Q],[P,A,B],[[Q,A,C],[P,C,B]]). \\
\end{align*}
\]

10 Appendix: Programming Puzzle

Experimental Details

We give each system the following dyadic relations head, tail, decrement, geq and the monadic relations empty, zero, one, even, and odd. We also include the dyadic relation increment in the len experiment. We had to remove this relation from the BK for the other experiments because when given this relation METAGOL runs into infinite recursion on almost every
problem and could not find any solutions. We also include member/2 in the find duplicate problem. We also include cons/3 in the addhead, dropk, and droplast experiments. We exclude this relation from the other experiments because METAGOL does not easily support triadic relations.

**POPI settings.** We set POPI to use at most five unique variables, at most five body literals, and at most two clauses. For each BK relation, we also provide both systems with simple types and argument directions (whether input or output). Because POPI can generate non-terminating Prolog programs, we set both systems to use a testing timeout of 0.1 seconds per example. If a program times out, we view it as a failure.