Heuristic Based Induction of Answer Set Programs
From Default theories to combinatorial problems

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Abstract Significant research has been conducted in recent years to extend Inductive Logic Programming (ILP) methods to induce Answer Set Programs (ASP). These methods perform an exhaustive search for the correct hypothesis by encoding an ILP problem instance as an ASP program. Exhaustive search, however, results in loss of scalability. In addition, the language bias employed in these methods is overly restrictive too. In this paper we extend our previous work on learning stratified answer set programs that have a single stable model to learning arbitrary (i.e., non-stratified) ones with multiple stable models. Our extended algorithm is a greedy FOIL-like algorithm, capable of inducing non-monotonic logic programs, examples of which includes programs for combinatorial problems such as graph-coloring and N-queens. To the best of our knowledge, this is the first heuristic-based ILP algorithm to induce answer set programs with multiple stable models.

Keywords Inductive Logic Programming · Machine Learning · Negation as Failure · Answer Set Programming

1 Introduction

Statistical machine learning methods produce models that are not comprehensible for humans because they are algebraic solutions to optimization problems such as risk minimization or data likelihood maximization. These methods do not produce any intuitive description of the learned model. Lack of intuitive descriptions makes it hard for users to understand and verify the underlying rules that govern the model. Also, these methods cannot produce a justification for a prediction they compute for a new data sample. Additionally, if prior knowledge (background knowledge) is extended in these methods, then the entire model needs to be re-learned. Finally, no distinction is made between exceptions and noisy data in these methods.

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Inductive Logic Programming [3], however, is one technique where the learned model is in the form of logic programming rules (Horn clauses) that are comprehensible to humans. It allows the background knowledge to be incrementally extended without requiring the entire model to be relearned. Meanwhile, the comprehensibility of symbolic rules makes it easier for users to understand and verify induced models and even edit them.

ILP learns theories in the form of Horn clause logic programs. Extending Horn clauses with negation as failure (NAF) results in more powerful applications becoming possible as inferences can be made even in absence of information. This extension of Horn clauses with NAF where the meaning is computed using the stable model semantics [5]—called Answer Set Programming[1]—has many powerful applications. Generalizing ILP to learning answer set programs also makes ILP more powerful. For a complete discussion on the necessity of NAF in ILP, we refer the reader to [15].

Once NAF semantics is allowed into ILP systems, they should be able to deal with multiple stable models which arise due to presence of mutually recursive rules involving negation (called even cycles) [1] such as:

\[ p :\neg q. \]
\[ q :\neg p. \]

Inducing answer set programs in presence of even cycles in the background knowledge has first been explored in [17], where the author describes the added expressiveness that results once background knowledge is allowed to have multiple stable models. Work by Otero [11] on induction of stable models formalizes induction of answer set programs with stable model semantics [5] such that in situations where \( B \cup H \) (\( B \) represents the background knowledge and \( H \) the hypothesis) has multiple stable models, it is just necessary to guarantee that each positive example is true in at least one stable model of \( B \cup H \). It also attempts to characterize inducing answer set programs from partial answer sets of \( B \cup H \) (the author calls them non-complete set of examples). These partial answer sets are treated as examples in the ILP problem. Otero also suggests that researchers should focus on learning answer set programs that model combinatorial and planning problems, but does not present any solution. Addressing the problem of learning such programs is the goal of our research presented in this paper.

In [15], Sakama introduces algorithms to induce a categorical logic program [2] given the answer set of the background knowledge and either positive or negative examples. Essentially, given a single answer set, Sakama tries to induce a program that has that answer set as a stable model. In [16], Sakama extends his work to learn from multiple answer sets. He introduces brave induction, where the learned hypothesis \( H \) is such that some of the answer sets of \( B \cup H \) cover the positive examples. The limitation of this work is that it accepts only one positive example as a conjunction of atoms. It does not take into account negative examples at all. Cautious induction, the counterpart of brave induction, is also too restricted as it can only induce atoms in the intersection of all stable models. Thus, neither brave induction nor cautious induction are able to express situations where something should hold in all or none of the stable models. An example of this limitation arises in the graph coloring problem where the following should hold in all answer sets: no two neighboring nodes in a graph should be painted the same color.

ASPAL [2] is the first ILP system to learn answer set programs by encoding ILP problems as ASP programs and having an ASP solver find the hypothesis. Its successor ILASP

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1 We use the term answer set programming in a generic sense to refer to normal logic programs, i.e., logic programs extended with NAF, whose semantics is given in terms of stable models [3].

2 A categorical logic program is an answer set program with at most one stable model.
is an ILP system capable of inducing hypotheses expressed as answer set programs too. ILASP defines a framework that subsumes brave/cautious induction and allows much broader class of problems relating to learning answer set programs to be handled by ILP. However, the algorithm exhaustively searches the space of possible clauses to find one that is consistent with all examples and background knowledge. To make this search feasible, it prohibits predicate invention, i.e., learning predicates other than the target predicate(s). Resorting to exhaustive search and not allowing predicate invention are weaknesses of ILASP that limit its applicability to many useful situations. Our research presented in this paper does not suffer from these problems.

XHAIL [14] is another ILP system capable of learning non-monotonic logic programs. It heavily incorporates abductive logic programming to search for hypotheses. It uses a similar language-bias as ILASP does, and thus suffers from the limitations similar to ILASP. It also does not support the notion of inducing answer set programs from partial answer sets.

All the systems discussed above, resort to an exhaustive search for the hypothesis. In contrast, traditional ILP systems (that only learn Horn clauses), use heuristics to guide their search. Use of heuristics allows these systems to avoid an exhaustive search. These systems usually start with the most general clauses and then specialize them. They are better suited for large-scale data-sets with noise, since the search can be easily guided by heuristics. FOIL [13] is a representative of such algorithms. However, handling negation in FOIL is somewhat problematic as we will soon show. Also, FOIL can not handle background knowledge with multiple stable models, nor it can induce answer set programs.

Recently we developed an algorithm called FOLD [18] to automate inductive learning of default theories represented as stratified answer set programs. FOLD (First Order Learner of Default rules) extends the FOIL algorithm and is able to learn answer set programs that represent the underlying knowledge very succinctly. However, FOLD is only limited to dealing with stratified answer set programs, i.e., mutually recursive rules through negation are not allowed in the background knowledge or the hypothesis. Thus, FOLD is incapable of handling cases where the background knowledge or the hypotheses admits multiple stable models. In this paper, we extend the FOLD algorithm to allow both the background knowledge and the hypothesis to have multiple stable models. The extended FOLD algorithm—called the XFOLD algorithm—is much more general than previously proposed methods.

This paper makes the following novel contributions: it presents the XFOLD algorithm, an extension of our previous FOLD algorithm, that can handle background knowledge with multiple stable models as well as allow inducing of hypotheses that have multiple stable models. To the best of our knowledge, XFOLD is the first heuristic based algorithm to induce such hypotheses. The XFOLD algorithm can learn ASP programs to solve combinatorial problems such as graph-coloring and N-queens. Because the XFOLD algorithm is based on heuristic search, it is also scalable. Lack of scalability is a major problem in previous approaches.

The rest of this paper is organized as follows: In section 2 we present the motivation of the FOLD algorithm by recalling some of the problems in FOIL algorithm. In section 3 we introduce the FOLD algorithm. In section 4 we present our extension to the FOLD algorithm, called XFOLD, to induce answer set programs with multiple stable models. In section 5 we show how XFOLD algorithm can induce programs for solving combinatorial problems. In section 6 we present related work while in section 7 we present our conclusions and future work.

We assume that the reader is familiar with answer set programming and stable model semantics. Books by Baral [1] and Gelfond and Kahl [4] are good sources of background material.
2 Background

In this section we describe our work on learning stratified answer set programs, i.e., learning hypothesis without cyclical rules using background knowledge that also does not have cyclical rules. The learning algorithm, called FOLD (First Order Learning of Default rules) [18], is itself an extension of the well known FOIL algorithm. FOIL is a top-down ILP algorithm which follows a sequential covering approach to induce a hypothesis. The FOIL algorithm is summarized in Algorithm 1. This algorithm repeatedly searches for clauses that score best with respect to a subset of positive and negative examples, a current hypothesis and a heuristic called information gain (IG). The FOIL algorithm learns a target predicate that has to be specified. Essentially, the target predicate appears as the head of the learned goal clause that FOIL aims to learn.

Algorithm 1 Overview of the FOIL algorithm

Input: goal, B, E⁺, E⁻
Output: Hypothesis H
1: Initialize \( H \leftarrow \emptyset \)
2: while not (stopping criterion) do
3: \( c \leftarrow \{ \text{goal} : \text{true}. \} \)
4: while not (stopping criterion) do
5: for all \( c' \in \rho(c) \) do
6: compute score \( (E^+, E^-, H \cup \{c'\}, B) \)
7: end for
8: let \( \hat{c} \) be the \( c' \in \rho(c) \) with the best score
9: \( c \leftarrow \hat{c} \)
10: end while
11: add \( \hat{c} \) to \( H \)
12: \( E^+ \leftarrow E^+ \setminus \text{covers}(\hat{c}, E^+, B) \)
13: end while

The inner loop searches for a clause with the highest information gain using a general-to-specific hill-climbing search. To specialize a given clause \( c \), a refinement operator \( \rho \) under \( \theta \)-subsumption [13] is employed. The most general clause is \( \{ p(X_1, \ldots, X_n) : \text{true}. \} \), where the predicate \( p/n \) is the target and each \( X_i \) is a variable. The refinement operator specializes the current clause \( \{ h : b_1, \ldots, b_n \} \). This is realized by adding a new literal \( l \) to the clause, which yields the following: \( \{ h : b_1, \ldots, b_n, l \} \). The heuristic based search uses information gain. In FOIL, information gain for a given clause is calculated as follows [8]:

\[
IG(L, R) = t \left( \log_2 \frac{p_1}{p_1 + n_1} - \log_2 \frac{p_0}{p_0 + n_0} \right)
\]

where \( L \) is the candidate literal to add to rule \( R \), \( p_0 \) is the number of positive bindings of \( R \), \( n_0 \) is the number of negative bindings of \( R \), \( p_1 \) is the number of positive bindings of \( R + L \), \( n_1 \) is the number of negative bindings of \( R + L \), \( t \) is the number of positive bindings of \( R \) also covered by \( R + L \).

FOIL handles negated literals in a naive way by adding the literal \( \text{not} L \) to the set of specialization candidate literals for any existing candidate \( L \). This approach leads to learning predicates that do not capture the concept accurately as shown in the following example:

Example 1 B, E⁺ are background knowledge and positive examples respectively under Closed World Assumption, and the target predicate is \( f(x) \).

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B: \[ \text{bird}(X) :- \text{penguin}(X). \]
\[ \text{bird}(\text{tweety}). \]
\[ \text{bird}(\text{et}). \]
\[ \text{cat}(\text{kitty}). \]
\[ \text{penguin}(\text{polly}). \]

\[ E^+ : \text{fly}(\text{tweety}). \]
\[ \text{fly}(\text{et}). \]

The FOIL algorithm would learn the following rule:

\[ \text{fly}(X) :- \text{not cat}(X), \text{not penguin}(X). \]

which does not yield a constructive definition, even though it covers all the positives (tweety is not a penguin and et is not a cat) and no negatives (neither cats nor penguins fly). In fact, the correct theory in this example is as follows: "Only birds fly but, among them there are exceptional ones who do not fly". It translates to the following logic programming rule:

\[ \text{fly}(X) :- \text{bird}(X), \text{not penguin}(X). \]

which FOIL fails to discover.

3 FOLD Algorithm

The intuition behind FOLD algorithm is to learn a concept in terms of a default and possibly multiple exceptions (and exceptions to exceptions, and so on). Thus, in the bird example given above, we would like to learn the rule that \( X \) flies if it is a bird and not a penguin, rather than that all non-cats and non-birds can fly. FOLD tries first to learn the default by specializing a general rule of the form \( \{\text{goal}(V_1, \ldots, V_n) :- \text{true}.\} \) with positive literals. As in FOIL, each specialization must rule out some already covered negative examples without decreasing the number of positive examples covered significantly. Unlike FOIL, no negative literal is used at this stage. Once the IG becomes zero, this process stops. At this point, if any negative example is still covered, they must be either noisy data or exceptions to the current hypothesis. Exceptions are separated from noise via distinguishable patterns in negative examples \[20\]. In other words, exceptions could be learned by calling the same algorithm recursively. This swapping of positive and negative examples, then recursively calling the algorithm can continue, so that we can learn exceptions to exceptions, and so on. Each time a rule is discovered for exceptions, a new predicate \( \text{ab}(V_1, \ldots, V_n) \) is introduced. To avoid name collisions, FOLD appends a unique number at the end of the string "ab" to guarantee the uniqueness of invented predicates. It turns out that the outlier data samples are covered neither as default nor as exceptions. If outliers are present, FOLD identifies and enumerates them to make sure that the algorithm converges.

Algorithm 2 shows a high level implementation of the FOLD algorithm. At lines 1-8, function FOLD, serves like the FOIL outer loop. At line 3, FOLD starts with the most general clause (e.g. \( \text{fly}(X) :- \text{true}. \)). At line 4, this clause is refined by calling the function SPECIALIZE. At lines 5-6, set of positive examples and set of discovered clauses are updated to reflect the newly discovered clause.

At lines 9-29, the function SPECIALIZE is shown. It serves like the FOIL inner loop. At line 12, by calling the function ADD_BEST_LITERAL the “best” positive literal is chosen and the best IG as well as the corresponding clause is returned. At lines 13-24, depending on the IG value, either the positive literal is accepted or the EXCEPTION function is called. If, at the very first iteration, IG becomes zero, then a clause that just enumerates the positive examples is produced. A flag called first_iteration is used to differentiate the first iteration. At lines 26-27, the sets of positive and negative examples are updated to reflect the changes
of the current clause. At line 19, the EXCEPTION function is called while swapping $E^+$ and $E^-$. At line 31, the "best" positive literal that covers more positive examples and fewer negative examples is selected. Again, note the current positive examples are really the negative examples and in the EXCEPTION function, we try to find the rule(s) governing the exception. At line 33, FOLD is recursively called to extract this rule(s). At line 34, a new ab predicate is introduced and at lines 35-36 it is associated with the body of the rule(s) found by the recurring FOLD function call at line 33. Finally, at line 38, default and exception are combined together to form a single clause.

The FOLD algorithm, once applied to Example 1 yields the following clauses:

\[
\begin{align*}
\text{fly}(X) &: \text{bird}(X), \neg \text{ab0}(X). \\
\text{ab0}(X) &: \text{penguin}(X).
\end{align*}
\]

Now, we illustrate how FOLD discovers the above set of clauses given $E^+ = \{\text{tweety, et}\}$ and $E^- = \{\text{polly, kitty}\}$ and the goal $\text{fly}(X)$. By calling FOLD, at line 2 while loop, the clause \{fly($X$) :- true.\} is specialized. Inside the SPECIALIZE function, at line 12, the literal $\text{bird}(X)$ is selected to add to the current clause, to get the clause $\hat{c} = \text{fly}(X) :- \text{bird}(X)$, which happens to have the greatest IG among $\{\text{bird, penguin, cat}\}$. Then, at lines 26-27 the following updates are performed: $E^+ = \{\}$, $E^- = \{\text{polly}\}$. A negative example $\text{polly}$, a penguin is still covered. In the next iteration, SPECIALIZE fails to introduce a positive literal to rule it out since the best IG in this case is zero. Therefore, the EXCEPTION function is called by swapping the $E^+$, $E^-$. Now, FOLD is recursively called to learn a rule for $E^+ = \{\text{polly}\}$, $E^- = \{\}$. The recursive call (line 33), returns \{fly($X$) :- penguin($X$)\} as the exception. At line 34, a new predicate $\text{ab0}$ is introduced and at lines 35-37 the clause \{ab0($X$) :- penguin($X$)\} is created and added to the set of invented abnormalities namely, AB. At line 38, the negated exception (i.e not $\text{ab0}(X)$) and the default rule's body (i.e $\text{bird}(X)$) are compiled together to form the clause \{fly($X$) :- \text{bird}(X), \neg \text{ab0}(X)\}.

Note, in two different cases enumerate function is called: i) At very first iteration of specialization if IG is zero for all the positive literals. ii) When the Exception routine fails to find a rule governing negative examples. Whichever is the case, corresponding samples are considered as noise. The following example shows a learned logic program in presence of noise. In particular, it shows how enumerate function works: It generates clauses in which the variables of the goal predicate can be unified with each member of a list of the examples for which no pattern exists.

**Example 2** Similar to Example 1 plus we have an extra positive example fly(jet) without any further information:

\[
\begin{align*}
B: & \quad \text{bird}(X) :- \text{penguin}(X). \\
& \quad \text{bird(tweety)}. \quad \text{bird(et)}. \\
& \quad \text{cat(kitty)}. \quad \text{penguin(polly)}. \\
E^+: & \quad \text{fly(tweety)}. \quad \text{fly(jet)}. \quad \text{fly(et)}.
\end{align*}
\]

FOLD algorithm on the Example 4.1 yields the following clauses:

\[
\begin{align*}
\text{fly}(X) &: \text{bird}(X), \neg \text{ab0}(X). \\
\text{fly}(X) &: \text{member}(X, [\text{jet}]). \\
\text{ab0}(X) &: \text{penguin}(X).
\end{align*}
\]
Algorithm 2 FOLD Algorithm

Input: \( \text{goal}, B, E^+, E^- \)
Output: 
\[ D = \{ c_1, \ldots, c_n \} \quad \text{\>} \quad \text{defaults' clauses} \]
\[ AB = \{ ab_1, \ldots, ab_m \} \quad \text{\>} \quad \text{exceptions/abnormal clauses} \]

1: \text{function FOLD}(E^+, E^-) \hfill \text{default initialization}
2: \text{while } (\text{size}(E^+)) > 0 \text{ do} \hfill \text{while loop}
3: \quad \hat{c} \leftarrow (\text{goal} : \text{true}) \hfill \text{goal initialization}
4: \quad \hat{c} \leftarrow \text{SPECIALIZE}(\hat{c}, E^+, E^-) \hfill \text{specialization}
5: \quad E^+ \leftarrow E^+ \setminus \text{covers}(\hat{c}, E^+, B) \hfill \text{update positive set}
6: \quad D \leftarrow D \cup \{ \hat{c} \} \hfill \text{add to defaults}
7: \text{end while} \hfill \text{end of while loop}
8: \text{end function} \hfill \text{return defaults}

9: \text{function SPECIALIZE}(c, E^+, E^-) \hfill \text{specialization function}
10: \quad \hat{c} \leftarrow \text{first iteration} \leftarrow \text{true} \hfill \text{initialize first iteration flag}
11: \text{while } (\text{size}(E^-)) > 0 \text{ do} \hfill \text{while loop}
12: \quad (c_{\text{def}}, \hat{IG}) \leftarrow \text{ADD}_\text{BEST}_\text{LITERAL}(c, E^+, E^-) \hfill \text{add best literal}
13: \quad \text{if } \hat{IG} > 0 \text{ then} \hfill \text{if condition}
14: \quad \quad \hat{c} \leftarrow c_{\text{def}} \hfill \text{add to defaults}
15: \quad \text{else} \hfill \text{else condition}
16: \quad \quad \text{if } \text{first iteration} \text{ then} \hfill \text{if first iteration}
17: \quad \quad \quad \hat{c} \leftarrow \text{enumerate}(c, E^+) \hfill \text{enumerate}
18: \quad \quad \text{else} \hfill \text{else condition}
19: \quad \quad \quad \hat{c} \leftarrow \text{EXCEPTION}(c, E^+, E^-) \hfill \text{exception}
20: \quad \quad \quad \text{if } \hat{c} = \text{null} \text{ then} \hfill \text{null check}
21: \quad \quad \quad \quad \hat{c} \leftarrow \text{enumerate}(c, E^+) \hfill \text{enumerate again}
22: \quad \quad \text{end if} \hfill \text{end of null check}
23: \quad \text{end if} \hfill \text{end of if condition}
24: \text{end if} \hfill \text{end of first iteration}
25: \quad \text{first iteration} \leftarrow \text{false} \hfill \text{reset iteration flag}
26: \quad E^+ \leftarrow E^+ \setminus \text{covers}(\hat{c}, E^+, B) \hfill \text{update positive set}
27: \quad E^- \leftarrow E^- \setminus \text{covers}(\hat{c}, E^-, B) \hfill \text{update negative set}
28: \text{end while} \hfill \text{end of while loop}
29: \text{end function} \hfill \text{return defaults}

30: \text{function EXCEPTION}(c_{\text{def}}, E^+, E^-) \hfill \text{exception function}
31: \quad \hat{IG} \leftarrow \text{ADD}_\text{BEST}_\text{LITERAL}(c, E^+, E^-) \hfill \text{add best literal}
32: \quad \text{if } \hat{IG} > 0 \text{ then} \hfill \text{if condition}
33: \quad \quad c_{\text{set}} \leftarrow \text{FOLD}(E^+, E^-) \hfill \text{add to defaults}
34: \quad \quad c_{\text{ab}} \leftarrow \text{generate next predicate()} \hfill \text{generate next predicate}
35: \quad \quad \text{for each } c \in c_{\text{set}} \text{ do} \hfill \text{for loop}
36: \quad \quad \quad AB \leftarrow AB \cup \{ c_{\text{ab}} : \text{bodyof}(c) \} \hfill \text{add to exceptions}
37: \quad \quad \text{end for} \hfill \text{end of for loop}
38: \quad \text{else} \hfill \text{else condition}
39: \quad \quad \hat{c} \leftarrow (\text{headof}(c_{\text{def}}) : \text{bodyof}(c), \text{not}(c_{\text{ab}})) \hfill \text{exception}
40: \quad \text{end if} \hfill \text{end of else condition}
41: \text{end function} \hfill \text{return defaults}

FOLD recognizes \textit{jet} as a noisy data. \textit{member/2} is a built-in logic programming predicate in that tests the membership of an atom in a list.

Sometimes, there are nested levels of exceptions. The following example shows how FOLD manages to learn the correct theory in presence of nested exceptions.

\textbf{Example 3} Birds and planes normally fly, except penguins and damaged planes that can’t. There are super penguins who can, exceptionally, fly.
### Table 1

In this experiment, we ran FOLD on each dataset and measured the accuracy using a 10-fold cross-validation and the results are compared against that of Aleph [19]. Aleph is a popular ILP system that has been widely used in prior work. To induce a clause, Aleph starts by building the most specific clause, which is called the “bottom clause”, that entails a seed example. Then, it uses a branch-and-bound algorithm to perform a general-to-specific heuristic search for a subset of literals from the bottom clause to form a more general rule. In most cases, our FOLD algorithm outperforms Aleph in terms of accuracy and succinctness of induced rules.

For instance, in UCI Labor-negotiations, which is a dataset of final settlements in labor negotiations in Canadian industry, the following hypothesis is induced by FOLD:

- good_contract(X) :- wage_inc_first_year(X,A), A > 2, not ab0(X).
- good_contract(X) :- holidays(X,A), A > 11.
- good_contract(X) :- health_plan_half_contribution(X), pension(X).
- ab0(X) :- no_longterm_disability_help(X).
- ab0(X) :- no_pension(X).

This hypothesis captures the highest priorities of employees in a good contract. Without having abnormality predicates, the hypothesis would have contained more clauses depending on the diversity of options on long term disability support and pension, whereas in default theory approach, as shown in this example, instead of covering examples with multiple clauses, a single clause is introduced as a default rule, and irrelevant predicates are excluded by abnormality predicates.

### 4 Induction of Answer Set Programs with Multiple Stable Models

In the previous section we assumed that the background knowledge $B$ is a normal logic program with one stable model and all examples belong to the only stable model of $B \cup H$. This would require the language bias not to allow even cycles which are responsible for generating multiple stable models.

In this section we extend our FOLD algorithm to learn normal logic programs that potentially have multiple stable models. The significance of Answer Set Programming paradigm...
| dataset    | size | ALEPH accuracy(%) | FOLD accuracy(%) | FOLD execution time(s) |
|------------|------|-------------------|------------------|------------------------|
| Credit-au  | 690  | 82                | 83               | 67                     |
| Credit-j   | 125  | 53                | 81               | 20                     |
| Credit-g   | 1000 | 70.9              | 78               | 87                     |
| Iris       | 150  | 85.9              | 95               | 1.3                    |
| Ecoli      | 336  | 91                | 90               | 6.1                    |
| Bridges    | 108  | 89                | 90               | 0.8                    |
| Labor      | 57   | 89                | 94               | 0.4                    |
| Acute(1)   | 34   | 100               | 100              | 0.3                    |
| Acute(2)   | 34   | 100               | 100              | 0.3                    |
| Mushroom   | 7724 | 100               | 100              | 11.4                   |

Table 1: FOLD evaluation on UCI benchmarks

is that it provides a declarative semantics under which each stable model is associated with one (alternative) solution to the problem described by the program. Typical problems of this kind are combinatorial problems, e.g., graph coloring and N-queens. In graph coloring, one should find different ways of coloring nodes of a graph without coloring two nodes connected by an edge with the same color. N-queen is the problem of placing N queens in a chessboard of size $N \times N$ so that no two queens attack each other.

In order to inductively learn such programs, the ILP problem definition needs to be revisited. In the new scenario, positive examples $e \in E^+$, may not hold in every model. Therefore, the ILP problem described in the background section would only allow learning of predicates that hold in all answer sets. This is too restrictive. Brave induction [16], in contrast, allows examples to hold only in some stable models of $B \cup H$. However, as stated in [6] and we will show using examples, this is not enough when it comes to learning global constraints (i.e., rules with empty head)\(^3\). Learning global constraints is essential because certain combinations may have to be excluded from all answer sets.

When $B \cup H$ has multiple stable models, there will be some instances of target predicate that would hold in all, none, or some of the stable models. Brave induction is not able to express situations in which a predicate should hold in all or none of the stable models. An example is a graph in which node 1 is colored red. In such a case, none of node 1’s neighbors should be colored red. If node 1 happens to have node 2 as a neighbor, brave induction is not able to express the fact that if the predicate $\text{red}(1)$ appears in any stable model of $B \cup H$, $\text{red}(2)$ should not. In [6], the authors propose a new paradigm called learning from partial answer sets that overcomes these limitations. We also adopt this paradigm in our work presented here. Next, we present our XFO LD algorithm.

**Definition 1** A partial interpretation $E$ is a pair $E = \langle E^{\text{inc}}, E^{\text{exc}} \rangle$ of sets of ground atoms called inclusions and exclusions, respectively. Let $A = \text{AS}(B \cup H)$ denote a stable model of $B \cup H$. A extends $\langle E^{\text{inc}}, E^{\text{exc}} \rangle$ if and only if $(E^{\text{inc}} \subseteq A) \land (E^{\text{exc}} \cap A = \emptyset)$.

**Example 4** Consider the following background knowledge about a group of friends some of whom are in conflict with others. The individuals in conflict will not attend a party together. Also, they cannot attend a party if they work at the time the party is held. We want our ILP

\[^3\text{Recall that in answer set programming, a constraint is expressed as a headless rule of the form } \text{:= } B,\]

\[^3\text{which states that } B \text{ must be false. A headless rule is really a short-form of rules of the form (called odd loops over negation } [\text{[}])]: p : = B, \text{ not } p.\]
algorithm to discover the rule(s) that will determine who will go to the party based on the set of partial interpretations provided.

\[ B: \text{conflict}(X,Y) :- \text{person}(X), \text{person}(Y), \text{conflict}(Y,X). \]
\[ \text{works}(X) :- \text{person}(X), \text{not \ off}(X). \]
\[ \text{off}(X) :- \text{person}(X), \text{not \ works}(X). \]
\[ \text{person}(p1). \text{person}(p2). \text{conflict}(p1,p4). \]
\[ \text{person}(p3). \text{person}(p4). \text{conflict}(p2,p3). \]

Some of the partial interpretations are as follows. The predicates g,w,o abbreviate goesToParty, works, off respectively:

\[ E_1 = \{\langle g(p1),o(p1),o(p2),w(p3),o(p4),w(p5)\rangle, \langle g(p3),g(p4)\rangle\} \]
\[ E_2 = \{\langle g(p3),g(p4),g(p5),o(p1),o(p2),o(p3),o(p4),o(p5)\rangle, \langle g(p1),g(p2)\rangle\} \]
\[ E_3 = \{\langle g(p1),g(p3),g(p5),o(p1),o(p2),o(p3),w(p4),o(p5)\rangle, \langle g(p2),g(p4)\rangle\} \]
\[ E_4 = \{\langle g(p2),g(p5),g(p5),w(p1),o(p2),w(p3),w(p4),o(p5)\rangle, \langle g(p1),g(p3),g(p4)\rangle\} \]

In the above example, each \( E_i \) for \( i = 1,2,3,4 \) is a partial interpretation and should be extended by at least one stable model of \( B \cup H \) for a learned hypothesis \( H \). For instance, let’s consider the hypothesis \( H_1 = \{\text{goesToParty}(X) :- \text{off}(X)\} \) for learning the target predicate \( \text{goesToParty}(X) \). By plugging the background knowledge, the non-target predicates in \( E_1 \), and the hypothesis \( H_1 \) into an ASP solver (CLASP [3] in our case), the stable model returned by the solver would contain \{\text{goesToParty}(p1), \text{goesToParty}(p2), \text{goesToParty}(p4)\}. It does not extend \( E_1 \). Although, \( E_1^{AS} \subseteq AS(B \cup H_1) \) but \( AS(B \cup H_1) \cap E_1^{AS} \neq \emptyset \). It should be noted that non-target predicates are treated as background knowledge upon calling ASP solver to compute the stable model of \( B \cup H \).

Definition 2 An XFOLD problem is defined as a tuple \( P = (B,L,E^+,E^-,T) \). \( B \) is a set program with potentially multiple stable models called the background knowledge. \( L \) is the language bias such that \( L = (M_b,M_h) \), where \( M_b \) (resp. \( M_h \)) are called the head (resp. body) mode declarations [10]. Each mode declaration \( m_b \in M_b \) (resp. \( m_h \in M_h \)) is a literal whose abstracted arguments are either variable \( v \) or constant \( c \). Type of a variable is a predicate defined in \( B \). The domain of each constant should be defined separately. The clause \( h :- b_1, \ldots, b_n, \text{not} \ c_1, \ldots, \text{not} \ c_m \) is in the search space if and only if: i) \( h \) is empty; ii) \( h \) is an atom compatible with a mode declaration in \( M_b \). Hypothesis \( h \) is said to be compatible with a mode declaration \( m \) if each instance of variable in \( m \) is replaced by a variable, and every constant takes a value from the associated domain. The set of candidate predicates in the greedy search algorithm are selected from \( M_b \cup M_h \).

The requirement of mode declarations in the XFOLD algorithm is due to a technicality: ASP solvers, need to ground the program, and for that matter, programmer should ensure that every variable is safe. A variable in head is safe if it occurs in a positive literal of body. XFOLD adds predicates required to ensure safety, but to keep our examples simple, we omit safety predicates in the paper. \( E^+ \) and \( E^- \) are sets of partial interpretations called positive and negative examples, respectively. \( T \in M_h \) is the target predicate’s name. Each XFOLD run learns a single target predicate. A hypothesis \( h \in L \) is an inductive solution of \( T \) if and only if:

1. \( \forall e^+ \in E^+ \exists A \in AS(B \cup H) \) such that \( A \) extends \( e^+ \)
2. \( \forall e^- \in E^- \nexists A \in AS(B \cup H) \) such that \( A \) extends \( e^- \)

The above definition adopted from [4] subsumes brave and cautious induction semantics [16]. Positive examples should be extended by at least one stable model of \( B \cup H \) (brave
Positive examples:

\[ E^+_1 = \{ \langle r(1), b(2), g(3), b(4) \rangle, \langle not b(1), not g(1), not r(2), not g(2), not r(3), not b(3), not r(4), not g(4) \rangle \} \]

\[ E^+_2 = \{ \langle b(1), r(2), g(3), r(4) \rangle, \langle not r(1), not g(1), not b(2), not g(2), not r(3), not b(3), not b(4), not g(4) \rangle \} \]

Negative examples:

\[ E^-_1 = \{ \langle r(1) \rangle, \langle not r(2) \rangle \} \]

\[ E^-_2 = \{ \langle r(1) \rangle, \langle not r(3) \rangle \} \]

Fig. 1: Partial interpretations as examples in graph coloring problem

The intuition behind the XFOLD algorithm is as follows: every positive example \( e \) that is a partial interpretation is considered as a separate learning problem. A partial score is computed for \( e \). Once all the positive examples are tested against a candidate clause, the overall score, i.e., the summation of all partial scores is stored as the score of current clause. Among all hypotheses, the one with highest overall score is chosen just like the single stable model case. For testing any given hypothesis \( h \), the background knowledge \( B \), all non-target predicates in \( E^{inc} \) and the hypothesis \( h \) are passed to the ASP solver as the input. The returned answer set is compared with the target predicates in \( E^{inc} \) and \( E^{exc} \). Next, the partial information gain score is computed. XFOLD chooses a clause with highest positive score (if one exists). Next, every partial interpretation is updated by removing the covered target predicates from \( E^{inc} \) and \( E^{exc} \). Once no target predicate in \( E^{exc} \) is covered, the internal loop finishes and the discovered rule(s) are added to the learned theory. Just like FOLD, if no literal with positive score exists, swapping occurs on each remaining partial interpretation and the XFOLD algorithm is recursively called. In this case, instead of introducing abnormality predicates, the negation symbol, \( \neg \), is prefixed to the current target predicate to indicate that the algorithm is now trying to learn the negation of concept being learned. It should also be noted that swapping examples is performed slightly differently due to the existence of partial interpretations. The summary of required changes in swapping of examples is as follows:

1. \( \forall e \in E_{inc} \) where \( e \) is and old target atom, \( e \) is restored
2. \( \forall e \in E_{inc} \) where \( e \) is and old target atom, \( \neg e \) is added to \( E_{exc} \)
3. \( \forall e \in E_{exc} \) where \( e \) is and old target atom, \( \neg e \) is added to \( E_{inc} \)
After iteration #1: \{\text{goesToParty}(X) : \text{off}(X)\}

\begin{align*}
E_1 &= \{\text{\text{off}(p_1)}, \text{\text{off}(p_2)}, \text{\text{off}(p_3)}, \text{\text{off}(p_4)}, \text{\text{off}(p_5)}\} \\
E_2 &= \{\text{\text{off}(p_1)}, \text{\text{off}(p_2)}, \text{\text{off}(p_3)}, \text{\text{off}(p_4)}, \text{\text{off}(p_5)}\} \\
E_3 &= \{\text{\text{off}(p_1)}, \text{\text{off}(p_2)}, \text{\text{off}(p_3)}, \text{\text{off}(p_4)}, \text{\text{off}(p_5)}\} \\
\end{align*}

After swapping \(E_{inc}, E_{esc}\)

\begin{align*}
E_1 &= \{\text{\text{off}(p_1)}, \text{\text{off}(p_2)}, \text{\text{off}(p_3)}, \text{\text{off}(p_4)}, \text{\text{off}(p_5)}\} \\
E_2 &= \{\text{\text{off}(p_1)}, \text{\text{off}(p_2)}, \text{\text{off}(p_3)}, \text{\text{off}(p_4)}, \text{\text{off}(p_5)}\} \\
E_3 &= \{\text{\text{off}(p_1)}, \text{\text{off}(p_2)}, \text{\text{off}(p_3)}, \text{\text{off}(p_4)}, \text{\text{off}(p_5)}\} \\
\end{align*}

Hypothesis = \{ \{\text{\text{off}(p_1)}, \text{\text{off}(p_2)}, \text{\text{off}(p_3)}, \text{\text{off}(p_4)}, \text{\text{off}(p_5)}\} \}

Fig. 2: Trace of XFold internal loop and recursive call on party example

4. \(T \leftarrow \neg T\). (Target predicate \(T\) now becomes its negation, \(\neg T\))

Figure 2 demonstrates execution of XFold for Example 3. At the end of first iteration, the predicate \(\text{off}(X)\) gets the highest score. \(E_4\) will be removed as it is already covered by the current hypothesis. In the second iteration, all candidate literals fail to get a positive score. Therefore, swapping occurs and algorithm tries to learn the predicate \(-\text{goesToParty}(X)\) as if it was an exception to the default case \{\text{\text{off}(X)} : \text{\text{off}(X)}\}. Since the new target predicate is \(-\text{\text{goesToParty}}(X)\), all ground atoms of \text{\text{goesToParty}} in \(E_{inc}\) are restored back. The old target atoms in \(E_{esc}\) are transformed to negated version and become members of \(E_{inc}\).

In Figure 2 after one iteration, \(E_4\) is removed because all target atoms in \(E_{inc}\) are already covered and targets atoms in \(E_{esc}\) are already excluded. After swapping, XFold is recursively called to learn \(-\text{\text{goesToParty}}\). After two iterations, since all examples are covered, the algorithm terminates.

In Example 3 we haven’t introduced any explicit negative example. Nevertheless, the algorithm was able to successfully find the cases in which the original target predicate does not hold (via learning \(-\text{\text{goesToParty}}(X)\) predicate). In general, it is not always feasible for the algorithm to figure out prohibited patterns without getting to see a very large number of positive examples.

5 Application: Combinatorial Problems

A well-known methodology for declarative problem solving is the generate and test methodology, whereby possible solutions to a problem are generated first, and then non-solutions are eliminated by testing. In Answer Set Programming, the generate part is encoded by enumerating the possibilities by introducing even cycles. The test part is realized by having constraints that would eliminate answer sets that violate the test conditions. ASP syntax allows rules of the form \(l[h_1, ..., h_k]\) such that \(0 \leq l \leq k\) and \(\forall i \in [1,k], h_i \in L\), where \(L\) is the language bias. This is a syntactic sugar for combination of even cycles and constraints, which is called choice rule in the literature [1, 4].
ILASP [6] directly searches for choice rules by including them in the search space. XFOLD, on the other hand, performs the search based on \( \theta \)-subsumption [12] and hence disallows search for choice rule hypotheses. Instead, it directly learns even cycles as well as constraints. This is advantageous as it allows for more sophisticated and flexible language bias.

It turns out that inducing the \textit{generate} part in a combinatorial problem such as graph-coloring requires an extra step compared to the FOLD algorithm. For instance, \texttt{red(X)} predicate has the following clause:

\[
\text{red}(X) :- \neg \text{blue}(X), \neg \text{green}(X).
\]

To enable XFOLD to induce such a rule, we adopted the “Mathews Correlation Coefficient” (MCC) [21] measure to perform the task of feature selection. MCC is calculated as follows:

\[
MCC = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}},
\]

This measure takes into account all the four terms TP (true positive), TN (true negative), FP (false positive) and FN (false negative) in the confusion matrix and is able to fairly assess the quality of classification even when the ratio of positive tuples to the negative tuples is not close to 1. The MCC values range from -1 to 1. A coefficient of +1 represents a perfect classification, 0 represents a classification that is no better than a random classifier, and -1 indicates total disagreement between the predicted and the actual labels. MCC cannot replace XFOLD heuristic score, i.e., information gain, because the latter tries to maximize the coverage of positive examples, while the former only maximally discriminates between the positives and negatives. Nevertheless, for the purpose of feature extraction among the negated literals which are disallowed in XFOLD algorithm, MCC can be applied quite effectively. For that matter, before running XFOLD algorithm, the MCC score of all candidate literals are computed. If a predicate scores “close” to +1, the predicate itself is added to the language bias. If it scores “close” to -1, its negation is added to the language bias. For example, in case of learning \texttt{red(X)}, after running the feature extraction on the graph given in Figure 1, XFOLD computes the scores -0.7, -0.5 for \texttt{green(X)} and \texttt{blue(X)}, respectively. Therefore, \{\neg \text{green(X)}, \neg \text{blue(X)}\} are appended to the list of candidate predicates. Now, after running the XFOLD algorithm, after two iterations of the inner loop, it would produce the following rule:

\[
\text{red}(X) :- \neg \text{green}(X), \neg \text{blue}(X).
\]

Corresponding rules for \texttt{green(X)} and \texttt{blue(X)} are learned in a similar manner. This essentially takes care of the \textit{generate} part of the combinatorial algorithm. In order to learn the \textit{test} part for graph coloring, we need the negative examples shown in Figure 1. It should be noted that in order to learn a constraint, we first learn a new target predicate which is the negation of the original one. Then we shift the negated predicate from the head to the body inverting its sign in the process. That is, we first learn a clause of the form

\[
-\text{\texttt{T}} \leftarrow \text{\texttt{b}}_1, \text{\texttt{b}}_2 \ldots \text{\texttt{b}}_n.
\]

which is then transformed into the constraint:

\[
\text{\texttt{b}}_1, \text{\texttt{b}}_2 \ldots \text{\texttt{b}}_n, \text{\texttt{T}}.
\]

Thus, the following steps should be taken to learn constraints from negative examples:

1. Add rule(s) induced for \textit{generate} part to B.
2. \( \forall e^+ \in E^+, e^- \in E^-, \text{if } e^\text{inc} \subseteq e^\text{exc} : \)
   - \( \text{if } e^\text{exc} \text{ is of the form } \{\neg p(V_1 \ldots V_m)\} \text{ then } e^\text{inc} + \leftarrow e^\text{inc} \cup \{\neg p(V_1 \ldots V_m)\} \)
   - \( \text{else } e^\text{inc} + \leftarrow e^\text{inc} \cup \{\neg p(V_1 \ldots V_m)\} \)
3. compute the contrapositive form of the rule(s) learned in generate part and remove the body predicates from the list of candidate predicates
4. run FOLD to learn \( p \)
5. shift \(-p\) from the head to the body for each rule returned by FOLD

The contrapositive of a statement has its antecedent and consequent inverted and flipped. For instance, the contrapositive of the clause \(
\{ \text{red}(X) :- \text{not green}(X), \text{not blue}(X) \} 
\) is shown in Figure 3.

The reason why step 3 is necessary is the following: running FOLD without eliminating the literals in contrapositive rule results in learning trivial clauses shown in Figure 3. However, as soon as those trivial choices are removed from search space, FOLD algorithm comes up with the next best hypothesis which is as follows:

\[-\text{red}(X) :- \text{edge}(X,Y), \text{red}(Y).\]

Shifting the predicate \(-\text{red}(X)\) to the body yields the following constraint:
As far as the generate part concerns, XFOLD algorithm would learn the following program:

\[
\begin{align*}
\text{red}(X) & : \neg \text{green}(X), \neg \text{blue}(X). \\
\text{green}(X) & : \neg \text{blue}(X), \neg \text{red}(X). \\
\text{blue}(X) & : \neg \text{green}(X), \neg \text{red}(X).
\end{align*}
\]

\[
\begin{align*}
& : \text{red}(X), \text{edge}(X,Y), \text{red}(Y). \\
& : \text{blue}(X), \text{edge}(X,Y), \text{blue}(Y). \\
& : \text{green}(X), \text{edge}(X,Y), \text{green}(Y).
\end{align*}
\]

As far as generate and test part concerns, XFOLD algorithm would learn the following program:

\[
\begin{align*}
q(X,Y) & : \neg \neg q(X,Y). \\
\neg q(X,Y) & : \neg q(X,Y).
\end{align*}
\]

The predicate \(-q(X,Y)\) is introduced by XFOLD algorithm as a result of swapping the examples and calling itself recursively. After computing the contrapositive form, \(q(X,Y)\) and \(-q(X,Y)\) are removed from the list of candidate predicates. Then based on the examples provided in Example 5, XFOLD would learn the following rules:

\[
\begin{align*}
\neg q(V_1,V_2) & : \neg \text{attack}_r(V_1,V_2,V_3,V_4). \\
\neg q(V_1,V_2) & : \neg \text{attack}_c(V_1,V_2,V_3,V_4). \\
\neg q(V_1,V_2) & : \neg \text{attack}_d(V_1,V_2,V_3,V_4).
\end{align*}
\]

After shifting the predicate \(-q(V_1,V_2)\) to the body, we get the following constraint:

\[
\begin{align*}
& : q(V_1,V_2), \text{attack}_r(V_1,V_2,V_3,V_4). \\
& : q(V_1,V_2), \text{attack}_c(V_1,V_2,V_3,V_4). \\
& : q(V_1,V_2), \text{attack}_d(V_1,V_2,V_3,V_4).
\end{align*}
\]

It should be noted that, since XFOLD is a sequential covering algorithm like FOIL, it takes three iterations before it can cover all examples which in turn becomes three constraints as shown above.
6 Related Work

Many researchers have tried to extend Horn ILP into richer non-monotonic logic formalisms. “Stable ILP” [17] was the first effort to explore the expressiveness of background knowledge with multiple stable models. A survey of extending Horn clause based ILP to non-monotonic logics can be found in [15]. In this paper Sakama also introduces algorithms to learn from the answer set of a categorical logic program. The algorithms learn from positive and negative examples separately and the approach also leads to redundant literals in the body of the induced clause as shown by Example 6.

Example 6 Consider the following background knowledge and positive example:

\[
B: \quad \text{bird}(X) :- \text{penguin}(X).
\]

\[
\text{bird(tweety)}, \quad \text{bird(et)}, \quad \text{bear(teddy)}, \quad \text{penguin(polly)}, \quad \text{cat(kitty)}.
\]

\[
E^+: \quad \text{fly(tweety)}.
\]

Sakama’s algorithm would induce the following clause:

\[
\text{fly}(X) :- \text{bird}(X), \neg \text{cat}(X), \neg \text{penguin}(X), \neg \text{bear}(X).
\]

The literals \(\neg \text{cat}(X), \neg \text{bear}(X)\) are redundant. The brave induction framework [16], although capable of learning ASP programs, only admits one positive example in the form of conjunction of literals. As we discussed, many problems, including programs for solving combinatorial problems, cannot be expressed without having a notion of a negative example. ILASP [6], introduces a framework that would allow to induce a hypothesis from multiple positive examples bravely (i.e., it uses brave induction), while it would exclude negative examples cautiously (i.e., it uses cautious induction). However, due to performing an exhaustive search on its predetermined language bias, ILASP is unable to scale up to large datasets or noisy datasets. It is not able to induce default theories with nested, or composite abnormality predicates to capture exceptions as shown in Example 7.

Example 7 A default theory with abnormality predicate represented as conjunction of two other predicates, namely \(s(X)\) and \(r(X)\).

\[
p(X) :- q(X), \neg \text{ab}(X).
\]

\[
\text{ab}(X) :- s(X), r(X).
\]

XHAIL [14] is an ILP system capable of learning non-monotonic logic programs. It relies heavily on abductive reasoning incorporated in a three-stage algorithm. It does not support inducing from multiple partial answer sets.

7 Conclusion and Future Work

In this paper we presented the first heuristic-based algorithm to inductively learn normal logic programs with multiple stable models. The advantage of this work over similar ILP systems such as ILASP [6] is that unlike these systems, XFOLD does not perform an exhaustive search to discover the “best” hypothesis. XFOLD adopts a greedy approach, guided by heuristics, that is scalable and noise resilient. Also, learning knowledge patterns in terms of defaults and exceptions produces more natural and intuitive results that correspond to
common sense reasoning employed by humans. We also showed how our algorithm could be applied to induce declarative logic programs that follow the generate and test paradigm for finding solutions to combinatorial problems such as graph-coloring and N-queens.

Our XFOLD algorithm has a number of novel features absent in other prior works: (i) it performs a heuristic search for learning hypotheses rather than an exhaustive search and thus is considerably more scalable; (ii) it admits predicate invention allowing us to learn a broader class of answer set programs that cannot be learned by other systems such as ASPAL, ILASP, and XHAIL; (iii) because of swapping of positive and negative examples, XFOLD is able to distinguish between exceptions and noise, producing more succinct hypotheses.

There are two main avenues for future work: (i) handling large datasets using methods similar to QuickFoil [21]. In QuickFoil, all the operations of FOIL are performed in a database engine. Such an implementation, along with pruning techniques and query optimization tricks can make the XFOLD training much faster; (ii) XFOLD learns function-free answer set programs. We plan to investigate extending the language bias towards accommodating functions.

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