Differentiable Inductive Logic Programming in High-Dimensional Space

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Abstract

Synthesizing large logic programs through symbolic Inductive Logic Programming (ILP) typically requires intermediate definitions. However, cluttering the hypothesis space with invented predicates typically degrades performance. In contrast, gradient descent provides an efficient way to find solutions within high-dimensional spaces; a property not fully exploited by neuro-symbolic ILP approaches. We propose extending the differentiable ILP framework by large-scale predicate invention, and thus exploiting the efficacy of gradient descent. We show that large-scale predicate invention is beneficial to inductive invariant synthesis and results in learning capabilities beyond existing neuro-symbolic ILP systems. Furthermore, we achieve these results without specifying the precise structure of the solution within the inductive bias.

1 Introduction

Neuro-symbolic ILP is quickly becoming one of the most important research domains in inductive synthesis (Cropper and Dumancic 2022). Such systems can aid explainability research by providing logical representations of what was learned and providing noise-handling capabilities to symbolic learners. Systems such as δILP can consistently learn solutions for many standard inductive synthesis problems (Evans and Grefenstette 2018; Shindo, Pfanschilling, and Dhami 2023). Nonetheless, searching through the hypothesis space remains a challenging task. To deal with this difficulty, inductive learners introduce problem-specific restrictions that reduce the size of the respective search space (Shindo, Nishino, and Yamamoto 2021; Sen et al. 2022); what is commonly referred to as language bias. While this is conducive to solving simple learning tasks, more complex synthesis tasks or tasks where the required language bias is not easily specifiable remain a formidable challenge.

Predicate Invention (PI) allows one to circumvent the issues associated with restricting the search space. However, in purely symbolic inductive synthesis, reliance on large-scale PI is avoided, as it is time- and space-wise too demanding (Muggleton et al. 2012), and has only been used effectively in very restricted settings (Muggleton 2023).

This paper presents an approach based on differentiable ILP (Evans and Grefenstette 2018), an influential approach to neuro-symbolic inductive synthesis, amenable to large-scale predicate invention. We show that a few changes to the original architecture is enough to train models using a reduced language bias that tests with significantly higher success rate. Our extension synthesizes a user-provided number of invented predicates during the learning process. Large-scale PI is either intractable for most systems due to memory requirements or results in a performance drop as it clutters the hypothesis space. In contrast, gradient descent methods generally benefit from large search spaces (high dimensionality). Thus, we propose introducing a large number of invented predicates to improve performance. We evaluate the approach on several standard ILP tasks (many derived from (Evans and Grefenstette 2018)), including several which existing neuro-symbolic ILP systems find to be a significant challenge (see Hypothesis 1).

Solutions found by our extension of δILP, in contrast to the usual ILP solutions, include large numbers of invented predicates. We posit the usefulness of large-scale PI for synthesizing complex logic programs. While adding many invented predicates can be seen as a duplication of the search space and, therefore, equivalent to multiple initializations of existing neuro-symbolic ILP systems, we demonstrate that our extension of δILP easily outperforms the re-initialization approach on a particularly challenging task (see Hypothesis 2). We compare to the most relevant existing approach, δILP (presented in (Evans and Grefenstette 2018)).

Unlike the experiments presented in (Evans and Grefenstette 2018), which specify the solution’s precise structure, we assume a generic shape for all predicate definitions. Thus, our experiments force the learner to find both the correct predicates to reference within an invented predicate’s definition and the structure of the definition. In this experimental setting, our approach is on par with δILP and, for challenging tasks, outperforms it. In particular, we outperform δILP on tasks deemed difficult in (Evans and Grefenstette 2018) such as \(0 \equiv X \mod 3\) and \(0 \equiv X \mod 5\).

Furthermore, we propose an adjusted measure of task difficulty. In (Evans and Grefenstette 2018), the authors proposed the number of intensional predicates as a measure of learning complexity. While our results do not contradict this assertion, it is more precise to focus on predicates that relate two universal variables through an existentially quantified variable; our system illustrates this by solving \(0 \equiv X \mod 5\)
(requiring four intensional predicates) consistently, but performing poorly on the seemingly simpler task \( Y = X + 4 \) needing only two intensional predicates (Hypothesis 3). Improving our understanding of task difficulty will aid future investigations.

In this paper, we present (i) an extension of \( \delta \)ILP capable of large-scale predicate invention, (ii) we experimentally show that our extension outperforms \( \delta \)ILP on challenging tasks when language bias is reduced, (iii) we experimentally show that large-scale predicate invention differs from weight re-initialization, (iv) we propose a novel criterion for task complexity and experimentally validate it.

## 2 Related Work

We briefly introduce Inductive logic programming (Cropper and Dumancic 2022), cover aspects of \( \delta \)ILP (Evans and Grefenstette 2018) directly relevant to our increase in dimensionality, and compare our approach to related systems inspired by \( \delta \)ILP. We assume familiarity with basic logic and logic programming; see (Raedt 2008).

### 2.1 Inductive Logic Programming (ILP)

ILP is traditionally a form of symbolic machine learning whose goal is to derive explanatory hypotheses from sets of examples (denoted \( E^+ \) and \( E^- \)) together with background knowledge (denoted \( BK \)). Investigations often represent explanatory hypotheses as logic programs of some form (Cropper and Morel 2021; Cropper and Muggleton 2016; Law, Russo, and Broda 2014; Purgal, Cerna, and Kaliszky 2022; Quinlan 1990). A benefit of this approach is that only a few examples are typically needed to learn an explanatory hypothesis (Dai et al. 2017).

The most common learning paradigm implemented within ILP systems is learning from entailment (Raedt 2008). The systems referenced above, including \( \delta \)ILP, use this paradigm which is succinctly stated as follows: A hypothesis \( H \) explains \( E^+ \) and \( E^- \) through the \( BK \), if

\[
\forall e \in E^+, BK \land H \models e \quad \text{and} \quad \forall e \in E^-, BK \land H \not\models e
\]

Essentially, the hypothesis, together with the background knowledge, entails all the positive examples and none of the negative examples. In addition to the learning paradigm, one must consider how to search through the hypothesis space, the set of logic programs constructible using definitions from the \( BK \) together with the predicates provided as examples. Many approaches exploit subsumption (\( \leq_{sub} \)), which has the following property in relation to entailment: \( H_1 \leq_{sub} H_2 \Rightarrow H_1 \models H_2 \) where \( H_1 \) and \( H_2 \) are plausible hypotheses. Subsumption provides a measure of specificity between hypotheses and, thus, is used to measure progress.

The FOIL (Quinlan 1990) approach (top-down) iteratively builds logic programs using this principle. Bottom-up approaches, i.e. Progol (Muggleton 1995), build the subsumptively most specific clause for each positive example and use FOIL to extend more general clauses towards it.

The ILP system Metagol (Cropper and Muggleton 2016) implements the meta-learning approach to search. It uses second-order Horn templates to restrict and search the hypothesis space. An example template would be \( P(x, y):-Q(x, z), R(z, y) \) where \( P, Q, \) and \( R \) are variables ranging over predicate symbols. This approach motivated the template representation used by \( \delta \)ILP and our work.

### 2.2 Differentiable ILP

Given that \( \delta \)ILP plays an integral role in our work, we go into some detail concerning the system architecture. However, while we strive to make this paper as self-contained as possible, due to space constraints, we cannot cover all aspects of this earlier work, and thus we refer the reader to (Evans and Grefenstette 2018) for more details.

The \( \delta \)ILP system provides a framework for differentiable learning from entailment ILP. Logic programs are represented by vectors whose components encode whether a particular code fragment is likely to be part of the solution. Such programs are “executed” in fuzzy logic, using a weighted average of code fragments. The hypothesis space consists of all possible combinations of these code fragments captured by user-provided templates, a particular generalization of metarules (Cropper and Muggleton 2016). In our setting metarules take the following form:

**Definition 1** (\( V \)-Metarule). Let \( x, y, z_1, z_2, z_3, z_4 \) be first-order variables, \( V \) a set of first-order variables such that \( x, y \in V \) and \( z_1, z_2, z_3, z_4 \notin V \), and \( P, Q, R \) second-order variables ranging over predicate symbols. Then \( P(x, y):-Q(z_1, z_2), R(z_3, z_4) \) is a \( V \)-metarule.

Unlike standard metarules, \( V \)-Metarules can have various instances.

**Definition 2** (\( V \)-Metarule Instance). Let \( M = P(x, y):-Q_1(x_1, x_2), R_1(x_3, x_4) \) be a \( V \)-Metarule. Then \( P(x, y):-Q_1(y_1, y_2), R_1(y_3, y_4) \) is an Instance of \( M \) if \( y_1, y_2, y_3, y_4 \in V \).

Essentially \( V \)-metarules are a generalization of metarules allowing for different variable configurations. A \( (V, p) \)-template is defined using \( V \)-Metarules as follows:

**Definition 3** (\( V \)-template). Let \( p \) be a predicate symbol, \( M = P(x, y):-Q_1(x_1, x_2), R_1(x_3, x_4) \) and \( M' = P'(x, y):-Q_2(x_1, x_2), R_2(x_3, x_4) \) be \( V \)-metarules. Then the \( (V, p) \)-template constructed from \( M \) and \( M' \) is the pair of clauses \( (M' \rightarrow p), M'(\{P' \rightarrow p\}) \).

An instance of a \((V, p)\)-template \((M_1, M_2)\) is the pair \((M_1', M_2')\) where \( M_1' \) and \( M_2' \) are \( V \)-Metarule Instances of \( M_1 \) and \( M_2 \), respectively.

An instantiation of a \((V, p)\)-template \((M_1, M_2)\) is \((M_1', M_2')\) where \((M_1', M_2')\) is an instance of \((M_1, M_2)\) and \( \sigma \) maps the second-order variables to predicate symbols.

In (Evans and Grefenstette 2018), additional restrictions were put on the instantiations of the second-order variables to simplify the hypothesis space for harder tasks. The authors designed the templates to allow precise descriptions of the solution structure, thus simplifying the search. We took a more general approach allowing us to define templates uniformly. This results in a larger hypothesis space and, thus, a more challenging experimental setting.

**Example 1.** Consider a \( (\{x, y, z\}, p) \)-template. possible instances of the contained \((\{x, y, z\}, p)\)-metarules include

\[ p(x, y):-Q_1(x, y), R_1(x, y) \quad p(x, y):-Q_2(x, z), R_2(x, z) \]
A program fitting this template would be the following:
\[ p(x, y) : - \text{succ}(x, y) \quad p(x, y) : - \text{succ}(x, z), p(x, z) \]
where \( R_2 \) maps to \( p \) and \( Q_1, Q_1, R_1, \) and \( Q_2 \) map to \( \text{succ} \).

Templates are generalizable to higher-arity predicates: learning such predicates is theoretically challenging for this ILP setting (Muggleton, Lin, and Tamaddoni-Nezhad 2015). It is common practice to restrict learning to dyadic predicates. Reducing template complexity is important when introducing many templates (up to 150). From now on, by template, we mean \((V, p)\)-template.

As input, \( \delta \text{ILP} \) requires a set of templates \( T \) (using pairwise distinct symbols, \( p_1, \ldots, p_n \)) and \( BK \). From this, it derives a satisfiability problem where each disjunctive clause \( C_{i,j} \) denotes the range of possible choices for clause \( j \) given template \( t \in T \), i.e. over all instantiations of \( t \). The logical models satisfying this formula denote logic programs modulo the clauses derivable using the template instantiated by the \( BK \) and the symbols \( p_1, \ldots, p_n \). Switching from a discrete semantics over \( \{0, 1\} \) to a continuous semantics allows the use of differentiable logical operators when implementing differentiable deduction. Solving ILP tasks, in this setting, is reduced to minimizing loss through gradient descent.

\( \delta \text{ILP} \) uses \( E^+ \) and \( E^- \) as training data for a binary classifier to learn a model attributing \text{true} or \text{false} to ground instances of predicates. This model implements the conditional probability \( p(\lambda | \omega, W, T, L, BK) \), where \( \lambda \in \{\text{true}, \text{false}\} \), \( \alpha \) is a ground instance, \( W \) a set of weights, \( T \) the templates, and \( L \) the symbolic language used to describe the problem containing a finite set of atoms.

Each \( \{(x, y, z), p_i\} \)-template \((t_1, t_2) \in T \) is associated with a weight matrix whose shape is \( d_1 \times d_2 \) where \( d_i \) denotes the number of clauses constructible using the \( BK \) and \( L \) modulo the constraints of \( t_j \). The number of weights may be roughly approximated (\textit{quintic}) in terms of the number of templates (considering possible instances and the four second-order variables to instantiate). The weights denote \( \delta \text{ILP}'s \) confidence in an instantiation of a template being part of the solution; so-called \textit{per template} assignment. We provide a detailed discussion of weight assignment in Section 3.

\( \delta \text{ILP} \) implements differentiable inferencing by providing each clause \( c \) with a function \( f_c : [0, 1]^m \rightarrow [0, 1]^m \) whose domain and range are values of grounded instantiations of templates. Note, \( m \) is not the number of templates; rather, it is the number of groundings of each template, a much larger number dependent on the \( BK \), language bias, and the atoms of the symbolic language \( L \). Consider a template \((t_1, t_2)\) admitting the clause pair \((c_1, c_2)\), and let the current valuation be \( \mathcal{V}_i \) and \( g : [0, 1] \times [0, 1] \rightarrow [0, 1] \) a function computing \( \lor\)-clausal (disjunction between clauses). Assuming we have a definition of \( f_c \), then \( g(f_c(\mathcal{V}_i), f_{c_2}(\mathcal{V}_i)) \) denotes one step of \textit{forwards-chaining}. Computing the weighted average over all clausal combinations admitted by \((t_1, t_2)\), using the \text{softmax} of the weights, and finally performing \( \lor\)-\textit{step} (disjunction between inference steps) between their sums, in addition to \( \mathcal{V}_i \), results in \( \mathcal{V}_{i+1} \). This process is repeated \( n \) times (the number of forward-chaining steps), where \( \mathcal{V}_0 \) is derived from the \( BK \).

The above construction still depends on a precise definition of \( f_c \). Let \( c_g = p(x, y) : -Q_1(y_1, y_2), Q_2(y_3, y_4) \)
where \( y_1, y_2, y_3, y_4 \in \{x, y, z\} \). We want to collect all ground predicates \( p_g \) for which a substitution \( \theta \) into \( Q_1, Q_2, y_1, y_2, y_3, y_4 \) exists such that \( p_g \in \{Q_1(y_1, y_2)\theta, Q_2(y_3, y_4)\theta\} \). These ground predicates are then paired with the appropriate grounding of the left-hand side of \( c_g \). The result of this process can be reshaped into a tensor emphasizing which pairs of ground predicates derive various instantiations of \( p(x_1, x_2) \). In the case of existential variables, there is one pair per atom in the language. Pairing this tensor with some valuation \( \mathcal{E}_i \) allows one to compute \( \land\)-\textit{literal} (conjunction between literals of a clause) between predicate pairs. As a final step, we compute \( \lor\)-\textit{exists} (disjunction between variants of literals with existential variables) between the variants and thus complete computation of the tensor required for a step of \textit{forward-chaining}.

Four operations parameterize the above process for conjunction and disjunction. We leave discussion to section 4.

### 2.3 Related Approaches
To the best of our knowledge, three recent investigations are related to \( \delta \text{ILP} \) and build on the architecture. The \textit{Logical Neural Network} (LNN) (Sen et al. 2022) uses a similar template, but only to learn non-recursive \textit{chain rules}, i.e. of the form \( p_0(X, Y) : -p_1(X, Z_1), \ldots, p_n(Z_n, Y) \); this is simulatable using \( \delta \text{ILP} \) templates, especially for the short rules presented by the authors. They introduced particular parameterized, differentiable, logical operators optimizable for ILP.

Another system motivated by \( \delta \text{ILP} \) is \textit{cILP} (Shindo, Pfanschilling, and Dhami 2023). The authors focused on learning logic programs that recognize visual scenes rather than general ILP tasks. The authors restricted the \( BK \) to predicates explaining aspects of the visual scenes used for evaluation. To build clauses, the authors start from a set of initial clauses and use a \textit{top-k beam search} to iteratively extend the body of the clauses based on evaluation with respect to \( E^+ \).

In this setting, predicate invention and recursive definitions are not considered. Additionally, learning a relation between two variables is not considered.

### Feed-Forward Neural-Symbolic Learner (Cunnington et al. 2023)
\( \delta \text{ILP} \) does not directly build on the \( \delta \text{ILP} \) architecture but provides an alternative approach to one of the problems the \( \delta \text{ILP} \) investigation addressed, namely developing a neural-symbolic architecture that can provide symbolic rules when presented with noisy input. In this work (Cunnington et al. 2023), rather than softening implication and working with fuzzy versions of logical operators, compose the \textit{Inductive answer set programming} learners \textit{ILASP} (Law, Russo, and Broda 2014) and \textit{FASL} (Law et al. 2020) with various pre-trained neural architectures for classification tasks.

This data is then transformed into a weighted knowledge for the symbolic learner. While this work is to some extent relevant to the investigation outlined in this paper, we focus on improving the differentiable implication mechanism developed by the authors of \( \delta \text{ILP} \) rather than completely replacing it. Furthermore, the authors focus on tasks with simpler logical structure, similar to the approach taken by \textit{cILP}.

Earlier investigations, such as \textit{NeuralILP} (Yang, Yang,
and Cohen 2017), experimented with various T-norms, and part of the investigation reported in (Evans and Grefenstette 2018) studied their influence on learning. The authors leave scaling their approach to larger, possibly recursive programs as future work, a limitation addressed herein.

In (Shindo, Nishino, and Yamamoto 2021), the authors built upon δILP but further restricted templating to add a simple term language (at most term depth 1). Thus, even under the severe restriction of at most one body literal per clause, they can learn predicates for list append and delete. Nonetheless, scalability remains an issue. Neural Logical Machines (Dong et al. 2019), in a limited sense, addressed the scalability issue. The authors modeled propositional formulas using multi-layer perceptrons wired together to form a circuit. This circuit is then trained on many (10000s) instances of a particular ILP task. While the trained model was accurate, interpretability is an issue, as it is unclear how to extract a symbolic expression. Our approach provides logic programs as output, similar to δILP.

Some related systems loosely related to our work are Logical Tensor Networks (Donadello, Serafini, and d’Avila Garcez 2017), Lifted Relational Neural Networks (Sourek et al. 2017), Neural theorem prover (Minervini et al. 2020), and DeepProbLog (Manhaeve et al. 2021). While some, such as Neural theorem prover, can learn rules, it also suffers from scaling issues. Overall, these systems were not designed to address learning in an ILP setting. Concerning the explainability aspects of systems similar to δILP, one notable mention is Logic Explained Networks (Ciravegna et al. 2023), which adapts the input format of a neural learner to derive explanations from the output. Though, the problem they tackle is only loosely connected to our work.

3 Contributions

The number of weights used by δILP is approximately quintic in the number of templates used, thus incurring a significant memory footprint (See Section 2.2). This issue is further exacerbated as computing evaluations requires grounding the hypothesis space. As a result, experiments performed in (Evans and Grefenstette 2018) use task-specific templates precisely defining the structure of the solution; this is evident in their experiments as certain tasks, i.e. the even predicate (See Figure 1), list multiple results, with different templating. These restrictions result in only a few of the many possible solutions being present in the search space. Furthermore, this language bias greatly influences the success rate of δILP on tasks such as length; the authors report low loss in 92.5% of all runs, which significantly differs from our reduced language bias experiments, i.e. 0% correct solutions and 0% achieving low loss.

To achieve low loss, in addition to the chosen language bias, δILP’s authors assign weights per template resulting in a large vector of learnable parameters, see Section 4. This seems to imply high dimensionality; however, softmax is applied to v during differentiable inferencing and thus transforms v into a distribution, effectively reducing its dimensionality.

Our investigation aims to: (i) increase the dimensionality of the search space while maintaining the efficacy of the differentiable inferencing, and (ii) minimize the bias required for effective learning. We proceed by adding many \( \{x,y,z,p\}\)-templates (each with a unique symbol p) as discussed in subsection 2.2; this largely reduces the biases towards solutions of a particular shape. Nonetheless, given the significant number of weights required, large-scale PI remains highly intractable. Thus, we amend how weights are assigned to templates (See Section 4).

Assigning weights per template is the main source of the significant memory footprint. The authors discuss this design choice in Appendix F of (Evans and Grefenstette 2018). In this Appendix, the authors describe assignment per clause, i.e. the weight denotes the likelihood of a given instantiation of a metarule instance occurring within an instantiation of a template. This approach was abandoned as it was “incapable of escaping local minima on harder tasks”. Assigning weights per clause results in roughly a quadratic reduction in the number of assigned weights.

In our work, we assign weights per literal, i.e. the weight denotes the likelihood of a given literal occurring within an instantiation of a template. Assignment per literal results in another roughly quadratic reduction in the number of assigned weights. We refer to our system as δILP\(_2\).

We observed that the most challenging tasks require learning a binary relation whose solution requires using a third (non-argument) variable, an additional existential variable. This observation differs from the observations presented in (Evans and Grefenstette 2018) where complexity was measured purely in terms of the number of intensional predicates required. For example, consider \( 0 = X \mod 5 \)-hard and \( Y = X + 4 \); our approach solves the former 61% of the time and the latter 4% of the time. Note, \( 0 = X \mod 5 \)-hard requires four intensional predicates while \( Y = X + 4 \) requires two, yet unlike \( 0 = X \mod 5 \)-hard, both predicates relate two variables through a third non-argument variable.

We test δILP\(_2\) and support our observation through experimentally testing the following hypotheses (see Section 5):

- **Hypothesis 1:** Differentiable ILP benefits from increasing the number of templates used during training.
- **Hypothesis 2:** The benefit suggested by hypothesis 1 is not solely due to the relationship between increasing the number of templates and training a multitude of times with a task-specific number of templates.
- **Hypothesis 3:** Learning binary predicates that use existential quantification remains a challenge regardless of the weight assignment approach.

4 Methodology

We now outline the methodological differences between our implementations of differentiable inferencing and δILP; We (i) assign weights per literal, (ii) use slightly different logical operators, (iii) use more precise measures of training outcomes, and (iv) use a slightly different method of batching examples. We cover these differences below.

**Weight assignment** To exploit the benefits of large-scale PI, we need to reduce the large memory footprint incurred by δILP’s weight assignment approach, per template assignment. We distinguish three types of weight assignment:
per template: weight encodes the likelihood that a pair of clauses is the correct choice for the given template.

per clause: weight encodes the likelihood that a clause occurs in the correct choice of clauses for the given template.

per literal: weight encodes the likelihood a literal occurs in one of the correct clauses for the given template.

Per literal assignment is the coarsest of the three but also has the least memory footprint thus allowing for large-scale PI. Our system, $\delta$ILP$_2$, implements per Literal assignment.

**T-norm for fuzzy logic** Differentiable inferencing (Section 2) requires four differentiable logic operators. The choice of these operators greatly impacts overall performance. The Author’s of $\delta$ILP experimented with various t-norms, continuous versions of classical conjunction (Esteva and Godo 2001), from which continuous versions of other logical operators are derived. The standard t-norms are $\max (x \land y \equiv \max\{x, y\})$, product ($x \land y \equiv x \cdot y$) and Łukasiewicz ($x \land y \equiv \max\{x + y - 1, 0\}$). For simplicity, we refer to all operators derived from a t-norm by the conjunctive operator, i.e. $x \lor y \equiv \min\{x, y\}$ is referred to as $\max$ when discussing the chosen t-norm.

| Operator | $\delta$ILP | $\delta$ILP$_2$ |
|----------|-------------|----------------|
| $\land$-Literal | product | product |
| $\lor$-Exists | max | max |
| $\lor$-Clausal | max | max |
| $\lor$-Step | product | max |

When computing many inference steps, product produces vanishingly small gradients. Large programs require more inferencing, see Figure 3, thus, we use $\max$ for $\lor$-step.

**Batch probability** We require computing values for all predicates over all combinations of atoms, thus motivating an alternative approach to typical mini-batching. Instead of parameterization by batch size, we use a batch probability – the likelihood of an example contributing to gradient computation. When computing the loss, the example sets $E^+$ and $E^-$ equally contribute. Regardless of the chosen examples, the loss is balanced (divided by the number of examples contributing). If batching results in no examples from $E^+$ ($E^-$), we set that half of the loss to 0 (with 0 gradient). Performance degrades when the batch probability is near 0.0 or 1.0. In all our experiments, we used the value of 0.5.

### 4.1 Considered outcomes

The experiments outlined in section 5 (See Table 1 & 2) allow for five possible outcomes: Correct on Test (C), Fuzzily Correct on Test (FT), Fuzzily Correct on Training (CT), Correct on Training (F), and FAIL. We differentiate between test and training to cover the possibility of overfitting and differentiate between correct and fuzzy to cover the possibility of learning programs only correct using fuzzy logic.

**Overfitting** $\delta$ILP avoids overfitting as the search space is restricted enough to exclude overfitting programs. However, this method is no longer viable when 100s of templates are used. For example, when learning even, it is possible, when training with enough invented predicates, to remember all even numbers provided in $E^+$. Thus, we add a validation step testing our solutions on unseen data (i.e. numbers up to 20 after training on numbers up to 10). Given the types of tasks we evaluated and the structure of the resulting model, a relatively large number of unseen examples is enough to validate. Learning over-fitting solutions for large, unseen input is highly unlikely as the programs would be very large. During experimentation, we observed that $\delta$ILP$_2$ rarely overfits, even when it clearly could. A plausible explanation is that shorter, precise solutions have a higher frequency in the search space.

**Fuzzy solutions** Another class of solutions observed in both our and the earlier experimental design is the class of fuzzy solutions; that is, programs that made correct predictions using fuzzy logic, but made incorrect predictions when evaluated using classical logic (using the predicates with the highest weight). Typically, fuzzy solutions are worse at generalizing – they are correct when tested using the training parameters (for example, inference steps) and break on unseen input. Entirely correct solutions for even are translatable into a program correct for all natural numbers, while a fuzzy solution fails to generalize beyond the training set.

### 5 Experiments

We compare $\delta$ILP$_2$ (per Literal) to $\delta$ILP (per Template) on tasks presented in (Evans and Grefenstette 2018)$^1$ plus additional tasks to experimentally test Hypothesis 2 & 3. The tasks are separated into four domains, numeric, list, ancestors, and graphs. Results are shown in Table 1 & 2. Tasks annotated by easy contain extra background knowledge simplifying the learning process, while hard versions do not use the extra background knowledge. Concerning experimental parameters, we ran $\delta$ILP$_2$ using 150 templates to produce Table 1. For $\delta$ILP, we ran it with the precise number of templates needed to solve the task. Using more templates was infeasible for many tasks due to the large memory foot-

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$^1$Section 5 and Appendix G of (Evans and Grefenstette 2018).
Table 1: Per Literal results: difference computed with respect to Table 2. Significance computed using t-test and $p < e^{-4}$. We use $\dagger$ to denote differences that are not significant. The arity of the learned predicate comes after the name, i.e. even has arity 1 and length has arity 2. Problems marked with a * should be significantly easier for per template as the entire hypothesis space fits in one weight matrix.

| Task                  | C   | F   | CT  | FT  | diff C | diff CT |
|-----------------------|-----|-----|-----|-----|--------|---------|
| predecessor/2         | 100 | 100 | 100 | 100 | +2% $\dagger$ | +2% $\dagger$ |
| even/1                | 92  | 99  | 92  | 99  | +32%   | +32% $\dagger$ |
| $(X \leq Y)/2^*$      | 30  | 31  | 35  | 38  | -70%   | -65%     |
| $(0=X \mod 3)/1$      | 91  | 97  | 91  | 97  | +91%   | +91% $\dagger$ |
| $(0=X \mod 5)/1$-easy | 77  | 80  | 97  | 100 | +77%   | +97%     |
| $(0=X \mod 5)/1$-hard | 61  | 65  | 61  | 65  | +61%   | +65%     |
| $(Y=X+2)/2$           | 99  | 100 | 99  | 100 | -1% $\dagger$ | +1% $\dagger$ |
| $(Y=X+4)/2$           | 4   | 12  | 5   | 13  | +4% $\dagger$ | +5% $\dagger$ |
| member/2*             | 17  | 19  | 37  | 43  | -67%   | -67%     |
| length/2              | 25  | 26  | 31  | 38  | +25%   | +31%     |
| grandparent/2         | 38  | 38  | 92  | 94  | +38%   | +89%     |
| undirected_edge/2     | 94  | 94  | 100 | 100 | +75%   | +81%     |
| adjacent_to_red/1     | 94  | 99  | 94  | 99  | +48%   | +48%     |
| two_children/1        | 74  | 100 | 74  | 100 | +13%   | +13%     |
| graph_colouring/1     | 83  | 85  | 96  | 100 | -15%   | -2% $\dagger$ |
| connectedness/2*      | 40  | 41  | 98  | 99  | +16%   | +74%     |
| cyclic/1              | 19  | 19  | 90  | 100 | +18%   | +89%     |

Figure 2: Learning $0 = X \mod 3$ (A) and $X \leq Y$ (B) varying the number of templates (X-axis). The Y-axis is the proportion of solutions in each category.

Table 2: Per Template result. Due to significant memory requirements, neither $(0=X \mod 5)$ task fits in GPU memory (46GB). Problems annotated with * are easy for Per template as the hypothesis space fits in one weight matrix.

| Task                  | C   | F   | CT  | FT  |
|-----------------------|-----|-----|-----|-----|
| predecessor/2         | 98  | 100 | 98  | 100 |
| even/1                | 70  | 94  | 70  | 94  |
| $(X \leq Y)/2^*$      | 100 | 100 | 100 | 100 |
| $(0=X \mod 3)/1$      | 0   | 0   | 0   | 0   |
| $(0=X \mod 5)/1$-easy | 0   | 0   | 0   | 0   |
| $(0=X \mod 5)/1$-hard | 0   | 0   | 0   | 0   |
| $(Y=X+2)/2$           | 100 | 100 | 100 | 100 |
| $(Y=X+4)/2$           | 0   | 0   | 0   | 0   |
| member/2*             | 84  | 100 | 84  | 100 |
| length/2              | 0   | 0   | 0   | 0   |
| grandparent/2         | 0   | 0   | 3   | 3   |
| undirected_edge/2     | 19  | 100 | 19  | 100 |
| adjacent_to_red/1     | 46  | 90  | 46  | 90  |
| two_children/1        | 61  | 100 | 61  | 100 |
| graph_colouring/1     | 98  | 100 | 98  | 100 |
| connectedness/2*      | 24  | 100 | 24  | 100 |
| cyclic/1              | 0   | 0   | 1   | 1   |

5.1 Hypothesis 1

Figure 2 illustrates the proportion of runs within each of our five categories (C, FT, CT, F, FAIL). As the number of templates increases, the proportion of the runs categorized as correct and generalizing increases. This pattern emerges even for tasks that remain hard to learn. Thus Figure 2 clearly provides strong evidence supporting Hypothesis 1.

When comparing with δILP, out of the 17 tasks we tested δILP and δILP$_2$ on, δILP$_2$ showed improved performance on 13 tasks, and the improved performance was statistically significant for 12 of these tasks. Of the four remaining tasks, δILP showed a statistically significant performance difference on two, namely $X \leq Y$ and member. Both benefit from per template assignment as the entire search space fits into one weight matrix. Thus, δILP is essentially performing brute force search. While one would expect the same issue to occur for connectedness, there are fewer solutions to member and $X \leq Y$ in the search space than in the case of connectedness; it is a more general concept. Thus, even when δILP has an advantage, δILP$_2$ outperforms it when training on more complex learning tasks.

Notably, δILP$_2$ outperforms δILP on many challenging tasks. For example, $0=X \mod 5$ cannot be solved by δILP in our experimental setting. In (Evans and Grefenstette 2018), low loss was attained only 14% of the time when +2 and +3 where added to the BK (Evans and Grefenstette 2018). In contrast, we achieved a 61% success rate on this task even when the BK contained only successor and zero; for the dependency graphs of a solution learned, see Figure 3.

5.2 Hypothesis 2

To illustrate that large-scale predicate invention is not equivalent to re-initialization of weights, we ran δILP$_2$ on the $0=X \mod 6$ while varying the numbers of templates used during training (results shown in Table 3). Note, $0=X \mod 6$...
| task       | C  | F  | CT | FT    |
|------------|----|----|----|-------|
| 3 templates | 0% | 0.02% | 0% | 0.02% |
| 5 templates | 0.11% | 0.13% | 0.11% | 0.14% |
| 50 templates | 60% | 65% | 60% | 65% |

Table 3: δILP<sub>2</sub> learning \( 0 = X \mod 6 \). Ran 10k times for 3 and 5 templates and 100 times for 50.

Figure 3: Template dependency graph of a correct program learned by δILP<sub>2</sub> for the \( (0 = X \mod 5) \)-hard task.

is slightly more challenging than \( 0 = X \mod 5 \) and thus aids in illustrating the effect of larger-scale predicate invention.

According to Table 3, when training with three templates (minimum required), we would need to run δILP<sub>2</sub> 5000 times to achieve a similar probability of success (finding a fuzzily correct solution) as a single 50 predicate run.

When using five invented predicates, which is minimum required to avoid constructing binary predicates (see Hypothesis 3), we would need to run δILP<sub>2</sub> 750 times to achieve a similar probability of success (finding a fuzzily correct solution) as a single 50 predicate run.

These results do not necessarily imply that using more predicates is always beneficial over doing multiple runs; however, they show that repeated training with intermediary weight re-initialization is not a sufficient explanation of the observed benefits of large-scale predicate invention.

5.3 Hypothesis 3

In Table 1 & 2, one can observe that some tasks requiring the system to learn a relatively simple program (i.e. length) are more challenging than tasks such as \( 0 = X \mod 6 \) that require learning a much larger program.

As stated above, we hypothesize this is due to propagating the gradient through an existential quantification. This results in difficulties when learning predicates that relate two universal variables through an existentially quantified variable. The difficulty increases with the number of such predicates required to solve the task.

We introduced an additional task explicitly designed to test this hypothesis: \( Y = X + 4 \). This task requires only one more predicate than \( Y = X + 2 \), yet the success rate drops significantly with respect to \( Y = X + 2 \) (from 99% to 4%). For \( 0 = X \mod 2 \) (even) and \( 0 = X \mod 5 \), the change is not as steep (from 92% to 61%).

Thus, the number of relational predicate definitions that a given task requires learning is a more precise measure of complexity than the number of intensional predicates.

6 Conclusion & Future Work

The main contribution of this work (Hypothesis 1) is providing strong evidence that additional templating (beyond what is necessary) improves performance. Verification of this hypothesis used δILP<sub>2</sub>, our modified version δILP. We performed our experiments using reduced language bias compared to the experiments presented in (Evans and Grefenstette 2018). Furthermore, we used the same generic template for all predicate definitions learned by the system. This choice makes some tasks significantly more difficult. Additionally, we verified that the performance gains were not simply due to properties shared with weight re-initialization when using a task-specific number of templates during the learning process (Hypothesis 2).

During experimentation, we noticed that the difficulty of the task did not correlate well with the number of intensional predicates needed to solve it but rather with the arity and the necessity of an existential variable. Therefore, we tested this conjecture using the tasks \( Y = X + 2 \) and \( Y = X + 4 \). While both systems solve \( Y = X + 2 \), performance drastically drops for \( Y = X + 4 \), which only requires learning two invented predicates. Note, \( 0 = X \mod 5 \) requires learning four invented predicates and is easily solved by δILP<sub>2</sub>. This observation highlights the challenging tasks for such inductive synthesis approaches (Hypothesis 3) and suggests a direction for future investigation.

As a continuation of our investigation, we plan to integrate ILP with Deep Neural Networks as a hybrid system that is trainable end-to-end through backpropagation. The Authors of δILP presented the first steps in (Evans and Grefenstette 2018). One can imagine the development of a network inferring a discrete set of objects in an image (Carion et al. 2020), or integration with Transformer-based (Vaswani et al. 2017) language models that produce atoms δILP can process. This research direction can lead to a network that responds to natural language queries based on a datalog database.

We also consider further optimization of inferencing within δILP<sub>2</sub>. By stochastically using only a fraction of all clauses matching a template, similar to the REINFORCE algorithm (Williams 1992), there is the potential to save a significant amount of computation time and memory. Thus, we can further exploit the benefits of large-scale predicate invention and solve more complex tasks. A similar idea would be decomposing a program into several small parts and learning by gradient descent using a different programming paradigm, such as functional programming.

Finally, we can improve our approach by adding an auxiliary loss. Such loss could range from measuring the used program size (to promote smaller, more general solutions) to using a language model to guide the search toward something that looks like a solution.

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References

Carion, N.; Massa, F.; Synnaeve, G.; Usunier, N.; Kirillov, A.; and Zagoruyko, S. 2020. End-to-End Object Detection with Transformers. CoRR, abs/2005.12872.

Cravegna, G.; Barbiero, P.; Giannini, F.; Gori, M.; Liò, P.; Maggini, M.; and Melacci, S. 2023. Logic Explained Networks. Artif. Intell., 314: 103822.

Cropp, A.; and Dumancic, S. 2022. Inductive Logic Programming At 30: A New Introduction. J. Artif. Intell. Res., 74: 765–850.

Cropp, A.; and Morel, R. 2021. Learning programs by learning from failures. Mach. Learn., 110(4): 801–856.

Cropp, A.; and Muggleton, S. 2016. Metagol System. github.com/metagol/metagol.

Cunnington, D.; Law, M.; Lobo, J.; and Russo, A. 2023. FFNSL: Feed-Forward Neural-Symbolic Learner. Mach. Learn., 112(2): 515–569.

Dai, W.; Muggleton, S. H.; Wen, J.; Tamaddoni-Nezhad, A.; and Zhou, Z. 2017. Logical Vision: One-Shot Meta-Interpretive Learning from Real Images. In Lachieze, N., and Vrain, C., eds., ILP 2017, volume 10759 of LNCS, 46–62. Springer.

Donadello, I.; Serafini, L.; and d’Avila Garcez, A. S. 2017. Logic Tensor Networks for Semantic Image Interpretation. In Sierra, C., ed., Proceedings of the Twenty-Sixth International Joint Conference on Artificial Intelligence, IJCAI 2017, Melbourne, Australia, August 19-25, 2017, 1596–1602. ijcai.org.

Dong, H.; Mao, J.; Lin, T.; Wang, C.; Li, L.; and Zhou, D. 2019. Neural Logic Machines. In 7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019. OpenReview.net.

Esteva, F.; and Gordo, L. 2001. Monoidal t-norm based logic:towards a logic for left-continuous t-norms. Fuzzy Sets and Systems, 124(3): 271–288. Fuzzy Logic.

Evans, R.; and Grefenstette, E. 2018. Learning explanatory rules from noisy data. Journal of Artificial Intelligence Research, 61: 1–64.

Law, M.; Russo, A.; Bertino, E.; Broda, K.; and Lobo, J. 2020. FastLAS: Scalable Inductive Logic Programming Incorporating Domain-Specific Optimisation Criteria. In The Thirty-Fourth AAAI Conference on Artificial Intelligence, AAAI 2020. The Thirty-Second Innovative Applications of Artificial Intelligence Conference, IAAI 2020, The Tenth AAAI Symposium on Educational Advances in Artificial Intelligence, EAAI 2020, New York, NY, USA, February 7-12, 2020, 2877–2885. AAAI Press.

Law, M.; Russo, A.; and Broda, K. 2014. Inductive Learning of Answer Set Programs. In Proceedings of Logics in Artificial Intelligence, 311–325. Springer.

Manhaeve, R.; Dumancic, S.; Kimmig, A.; Demeester, T.; and Raedt, L. D. 2021. Neural probabilistic logic programming in DeepProbLog. Artif. Intell., 298: 103504.

Minervini, P.; Bosnjak, M.; Rocktäschel, T.; Riedel, S.; and Grefenstette, E. 2020. Differentiable Reasoning on Large Knowledge Bases and Natural Language. In The Thirty-Fourth AAAI Conference on Artificial Intelligence, AAAI 2020. The Thirty-Second Innovative Applications of Artificial Intelligence Conference, IAAI 2020, The Tenth AAAI Symposium on Educational Advances in Artificial Intelligence, EAAI 2020, New York, NY, USA, February 7-12, 2020, 5182–5190. AAAI Press.

Muggleton, S. 1995. Inverse Entailment and Progol. New Generation Computing, 13(3&4): 245–286.

Muggleton, S. H. 2023. Supplementary material from “Hypothesizing an algorithm from one example: the role of specificity”.

Muggleton, S. H.; Lin, D.; and Tamaddoni-Nezhad, A. 2015. Meta-interpretive learning of higher-order dyadic datalog: predicate invention revisited. Mach. Learn., 100(1): 49–73.

Muggleton, S. H.; Raedt, L. D.; Poole, D.; Bratko, I.; Flach, P. A.; Inoue, K.; and Srinivasan, A. 2012. ILP turns 20 - Biography and future challenges. Mach. Learn., 86(1): 3–23.

Paszke, A.; Gross, S.; Massa, F.; Lerer, A.; Bradbury, J.; Chanan, G.; Killeen, T.; Lin, Z.; Gimelshein, N.; Antiga, L.; Desmaison, A.; Kopf, A.; Yang, E.; DeVito, Z.; Raison, M.; Tejani, A.; Chilamkurthy, S.; Steiner, B.; Fang, L.; Bai, J.; and Chintala, S. 2019. PyTorch: An Imperative Style, High-Performance Deep Learning Library. In Wallach, H.; Larochelle, H.; Beygelzimer, A.; d’Alché-Buc, F.; Fox, E.; and Garnett, R., eds., Advances in Neural Information Processing Systems 32, 8024–8035. Curran Associates, Inc.

Purgal, S. J.; Cerna, D. M.; and Kaliszyk, C. 2022. Learning Higher-Order Logic Programs From Failures. In Raedt, L. D., ed., Proceedings of the Thirty-First International Joint Conference on Artificial Intelligence, IJCAI 2022, Vienna, Austria, 23-29 July 2022, 2726–2733. ijcai.org.

Quinlan, J. R. 1990. Learning Logical Definitions from Relations. Mach. Learn., 5: 239–266.

Raedt, L. D. 2008. Logical and relational learning. Cognitive Technologies. Springer. ISBN 978-3-540-20040-6.

Sen, P.; de Carvalho, B. W. S. R.; Riegel, R.; and Gray, A. G. 2022. Neuro-Symbolic Inductive Logic Programming with Logical Neural Networks. In Thirty-Sixth AAAI Conference on Artificial Intelligence, AAAI 2022, Thirty-Fourth Conference on Innovative Applications of Artificial Intelligence, IAAI 2022, The Twelveth Symposium on Educational Advances in Artificial Intelligence, EAAI 2022 Virtual Event, February 22 - March 1, 2022, 8212–8219. AAAI Press.

Shindo, H.; Nishino, M.; and Yamamoto, A. 2021. Differentiable Inductive Logic Programming for Structured Examples. In Thirty-Fifth AAAI Conference on Artificial Intelligence, AAAI 2021, Thirty-Third Conference on Innovative Applications of Artificial Intelligence, IAAI 2021, The Eleventh Symposium on Educational Advances in Artificial Intelligence, EAAI 2021 Virtual Event, February 2-9, 2021, 5034–5041. AAAI Press.
Shindo, H.; Pfanschilling, V.; and Dhami, D. 2023. αILP: thinking visual scenes as differentiable logic programs. *Machine Learning*.

Sourek, G.; Svatos, M.; Zelezný, F.; Schockaert, S.; and Kuzelka, O. 2017. Stacked Structure Learning for Lifted Relational Neural Networks. In Lachiche, N.; and Vrain, C., eds., *Inductive Logic Programming - 27th International Conference, ILP 2017, Orléans, France, September 4-6, 2017, Revised Selected Papers*, volume 10759 of *Lecture Notes in Computer Science*, 140–151. Springer.

Vaswani, A.; Shazeer, N.; Parmar, N.; Uszkoreit, J.; Jones, L.; Gomez, A. N.; Kaiser, L.; and Polosukhin, I. 2017. Attention Is All You Need. *CoRR*, abs/1706.03762.

Williams, R. J. 1992. Simple Statistical Gradient-Following Algorithms for Connectionist Reinforcement Learning. *Mach. Learn.*, 8: 229–256.

Yang, F.; Yang, Z.; and Cohen, W. W. 2017. Differentiable Learning of Logical Rules for Knowledge Base Reasoning. In Guyon, I.; von Luxburg, U.; Bengio, S.; Wallach, H. M.; Fergus, R.; Vishwanathan, S. V. N.; and Garnett, R., eds., *Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, December 4-9, 2017, Long Beach, CA, USA*, 2319–2328.