Neuro-Symbolic Inductive Logic Programming with Logical Neural Networks

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Abstract
Recent work on neuro-symbolic inductive logic programming has led to promising approaches that can learn explanatory rules from noisy, real-world data. While some proposals approximate logical operators with differentiable operators from fuzzy or real-valued logic that are parameter-free thus diminishing their capacity to fit the data, other approaches are only loosely based on logic making it difficult to interpret the learned “rules”. In this paper, we propose learning rules with the recently proposed logical neural networks (LNN). Compared to others, LNNs offer strong connection to classical Boolean logic thus allowing for precise interpretation of learned rules while harboring parameters that can be trained with gradient-based optimization to effectively fit the data. We extend LNNs to induce rules in first-order logic. Our experiments on standard benchmarking tasks confirm that LNN rules are highly interpretable and can achieve comparable or higher accuracy due to their flexible parameterization.

1 Introduction
Inductive logic programming (ILP) (Muggleton 1996) has been of long-standing interest where the goal is to learn logical rules from labeled data. Since rules are explicitly symbolic, they provide certain advantages over black box models. For instance, learned rules can be inspected, understood and verified forming a convenient means of storing learned knowledge. Consequently, a number of approaches have been proposed to address ILP including, but not limited to, statistical relational learning (Getoor and Taskar 2007) and more recently, neuro-symbolic methods.

Since logical operators such as conjunction and disjunction are not differentiable, one issue that most neuro-symbolic ILP techniques have to address is how to learn rules using gradient-based optimization. A popular solution is to employ extensions from fuzzy or real-valued logic that are either differentiable or have subgradients available. For instance, NeuralLP (Yang, Yang, and Cohen 2017) substitutes logical conjunction with product t-norm \( (x \land y \equiv xy) \) and logic tensor networks (Donadello, Serafini, and d’Avila Garcez 2017) with Łukasiewicz t-norm \( (x \land y \equiv \max(0, x + y - 1)) \). In an interesting experiment, Evans and Grefenstette (2018) show that among the various options, product t-norm seems to lead to the best ILP result. This indicates that the learning approach, rather than the user, should be in charge of substituting logical connectives besides learning the rules themselves. Neural logic machine (NLM) (Dong et al. 2019) achieves this but at the cost of interpretability. More precisely, it models propositional formulae (consisting of conjunctions, disjunctions and/or negations) with multi-layer perceptrons (MLP). Once trained, it may not be possible to interpret NLM as rules since there exists no standard translation from MLP to logic. What is needed is an extension of classical logic with ties strong enough to be amenable to interpretation and can learn not only rules but also the logical connectives using gradient-based optimization.

In this paper, we propose ILP with the recently proposed logical neural networks (LNN) (Riegel et al. 2020). Instead of forcing the user to choose a function that mimics a logical connective, LNNs employ constraints to ensure that neurons behave like conjunctions or disjunctions. By decoupling neuron activation from the mechanism to ensure that it behaves like a logical connective, LNNs offer tremendous flexibility in how to parameterize neurons thus ensuring that they fit the data better while maintaining close connections with classical Boolean logic which, in turn, facilitates principled interpretation. We propose first-order extensions of LNNs that can tackle ILP. Since vanilla backpropagation is insufficient for constraint optimization, we propose flexible learning algorithms capable of handling a variety of (linear) inequality and equality constraints. We experiment with diverse benchmarks for ILP including gridworld and knowledge base completion (KBC) that call for learning of different kinds of rules and show how our approach can tackle both effectively. In fact, our KBC results represents a 4-16% relative improvement (in terms of mean reciprocal rank) upon the current best rule-based KBC results on popular KBC benchmarks. Additional, we show that joint learning of rules and logical connectives leads to LNN rules that are easier to interpret vs. other neuro-symbolic ILP approaches.

2 Related Work
\( \partial \text{ILP} \) (Evans and Grefenstette 2018) is another neuro-symbolic ILP technique whose main parameter is a tensor with one cell per candidate logic program. Since the number of candidates is exponential in both the number of available predicates and the number of constituent rules in the program, \( \partial \text{ILP} \)’s complexity is exponential making it impractical for anything but the smallest learning task.
To reign in the complexity, \( \partial \text{ILP} \) asks the user to specify the ILP task using a template consisting of two rules each containing a maximum of two predicates. In reality, most neuro-symbolic ILP approaches ask the user to specify a template. NeuralLP’s (Yang, Yung, and Cohen [2017]) template is meant for link prediction in incomplete knowledge bases (sometimes called open path or chain rule) which only includes binary predicates and is of the form \( T(X_1, X_n) \leftarrow R_1(X_1, X_2) \land R_2(X_2, X_3) \land \ldots \land R_{n-1}(X_{n-1}, X_n) \) positing that the head predicate \( T(X_1, X_n) \) can be modeled as a path from \( X_1 \) to \( X_n \). NLM (Dong et al. [2019]) is restricted to learning rules where the head and body predicates each contain the same set of variables. For instance, to model the rule learned using rules where the head and body predicates each contain the same set of variables.

In accordance with our knowledge, none of these learn rules to address ILP. Logical neural networks (LNN) (Riegel et al. 2020) allow the use of almost any parameterized function as a logical connector. Logical neural networks (LNN) (Riegel et al. 2020) allow the use of almost any parameterized function as a logical connector. Logical neural networks (LNN) (Riegel et al. 2020) allow the use of almost any parameterized function as a logical connector.

Neural theorem provers (NTP) (Rocktäschel and Riedel 2017) generalize the notion of unification by embedding logical constants into a high-dimensional latent space. NTPs can achieve ILP by learning the embedding for the unknown predicate which forms part of the rule, and subsequently comparing with embeddings of known predicates. NTPs can have difficulty scaling to real-world tasks since the decision to unify two constants is no longer Boolean-valued leading to an explosion of proof paths that need to be explored. To improve scalability, recent proposals either greedily choose (GNTP (Minervini et al. 2020a)) or learn to choose (CTP (Minervini et al. 2020b)) most promising proof paths. We compare against CTP in Section 5.

Lifted relational neural networks (LRNN) (Sourek et al. 2017) model conjunctions using (generalized) sigmoid but fix certain parameters to ensure that it behaves similar to Łukasiewicz t-norm. This limits how well LRNN can model the data, which is contrary to our goal as stated in the previous section. While other combinations of logic and neural networks exist, e.g., logic tensor networks (Donadello, Seragnoli, and d’Avila Garcez 2017), ReILNN (Kazemi and Poole 2018), DeepProbLog (Manhaeve et al. 2018), to the best of our knowledge, none of these learn rules to address ILP.

3 Generalized Propositional Logic with Logical Neural Networks

Logical neural networks (LNN) (Riegel et al. 2020) allow the use of almost any parameterized function as a logical connector. We illustrate how LNNs generalize conjunction (\( \wedge \)). Let 0 denote false and 1 denote true. Let \( a, b \in \{0, 1\} \) and \( x, y \in [0, 1] \) denote Boolean-valued and continuous-valued variables, respectively. While Boolean logic defines the output of \( \wedge \) when \( x, y \) attain the extremities of their permissible domains (shown in Figure 1(a)), to fully define real-valued logic’s \( \wedge \) we need to also extend its definition to \( x, y \in (0, 1) \).

![Figure 1](image_url)\(^{1}\)

\( a \wedge b = 0 \) if \( b - w_1 (1-x) - w_2 (1-y) < 0 \)
\( 1 \) if \( b - w_1 (1-x) - w_2 (1-y) > 1 \)
\( \beta - w_1 (1-x) - w_2 (1-y) \) otherwise

where \( \beta, w_1, w_2 \) denote learnable parameters subject to the following constraints translated from above:

LNN-\( \wedge(1-\alpha, 1; \beta, w_1, w_2) = \beta - w_1 \alpha \leq 1 - \alpha \)

LNN-\( \wedge(1, 1-\alpha; \beta, w_1, w_2) = \beta - w_2 \alpha \leq 1 - \alpha \)

LNN-\( \wedge(\alpha, 1-\alpha; \beta, w_1, w_2) = \beta - (w_1 + w_2)(1-\alpha) \geq \alpha \)

To ensure that LNN-\( \wedge \) is monotonically increasing, we also need to enforce non-negativity of \( w_1, w_2 \). It is easy to extend LNN-\( \wedge \) to an \( n \)-ary conjunction (\( n \geq 2 \)):

\[
\text{LNN-} \wedge(\alpha_1, \ldots, \alpha_n; \beta, w_1, w_2) \equiv \text{relu}_1(\beta - w^T(1-x))
\]

subject to:
\[
\begin{align*}
w_0 &\geq 0, \beta - \alpha w &\leq (1-\alpha)1 \\
\beta - (1-\alpha)1 &\geq \alpha
\end{align*}
\]

\(^{1}\)We remove the upper and lower clamps since they do not apply in the active region of the constraints.
where \( \text{relu}(x) \) denotes \( \max(0, \min(1,x)) \) (Krizhevsky 2010) and, \( x, w \) and 1 denote vectors of continuous-valued inputs, weights, and 1s, respectively.

Note that, Figure 1 (b) does not enforce constraints on \( 1 - \alpha < x, y < \alpha \). Essentially, \( \alpha \) acts as a tunable knob that controls the size of this unconstrained region where we can learn LNN operators without impedance which is an arguably better approach than choosing a parameter-less \( t \)-norm that would arbitrarily interporate from Boolean-logic’s \& to real-valued logic’s \& to real-valued logic’s \& to real-valued logic’s \& to real-valued logic’s \&.

Following previous work (Yang, Yang, and Cohen 2017; Evans and Grefenstette 2018; Dong et al. 2019), we also utilize program templates expressed in higher-order logic to be fed by the user to guide the learning in the right direction. Our definition of a program template draws inspiration from meta-interpretive learning (Muggleton et al. 2014). In contrast to previous work on neuro-symbolic AI however, our definition of a program template is more general and includes as special cases the templates utilized by Evans and Grefenstette (considers only rules whose body contains up to 2 predicates), Yang, Yang, and Cohen (considers only binary predicates) and Dong et al. (considers only rules whose head includes all variables contained in the body). After introducing our logic program template, we then describe how to combine it with data to construct a neural network that may then be trained to learn the logic program of interest.

Let \( \text{pred}(X_1, \ldots, X_n) \) denote an \( n \)-ary predicate which returns true (1) or false (0) for every possible joint assignment of \( X_1, \ldots, X_n \) to constants in the knowledge base. The main construct in first-order logic (FOL) is a rule or clause:

\[
h \leftarrow b_1 \land b_2 \land \ldots \land b_m
\]

where \( b_1, \ldots, b_m \) denote predicates in its body and \( h \) denotes the head predicate. If the conjunction of all predicates in the body is true then the head is also true. The head \( h \) in a clause may contain fewer logical variables than the body \( b_1, \ldots, b_m \) which means that there must exist an assignment to the missing variables in the head for it to hold. More precisely, if \( B = b_1, \ldots, b_n \) denotes the body and is defined over logical variables \( Y \) then \( h(X) \), such that \( X \subseteq Y \), is true if \( \exists Y \setminus X : B(Y) \) is true. Assignments that lead to the predicate being true are also called facts.

Figure 3 (a) introduces a toy knowledge base (KB) which will serve as a running example. The KB contains three binary predicates, each containing their respective facts along with a unique identifier for easy reference. Thus, \( A(X, Y) \)'s facts are \( A(1,2) \) (denoted \( a_1 \)) and \( A(1,5) \) (denoted \( a_2 \)). Figure 3 (b) shows a template for learning \( R(X, Z) \) with three crucial pieces of information: 1) the first predicate in its body \( P \) is binary and while we do not know the identity of this predicate we know its domain \( \text{Dom}(P) \) is \( \{A, B\} \) to keep the example simple, the second predicate in the body \( Q \) has a singleton domain (\( \{C\} \)), and lastly 3) the second argument in the first predicate should be equal to the first argument in the second predicate indicated by repeated use of \( Y \). Figure 3 (b) (bottom) expresses the same template as a tree where \( P(X, Y) \) and \( Q(Y, Z) \) are annotated with their respective domains forming children of \( R(X, Z) \) whose label \& indicates that the predicates in its body are to be conjuncted together.

Figure 3 (c) shows a more complex template that disjuncts \( R(X, Z) \) with \( O(X, Z) \), such that \( \text{Dom}(O) = \{A, B\} \), to produce \( S(X, Z) \). Figure 3 (d) shows generated facts (with unknown truth-values) that can be possibly produced when this template is combined with the KB from Figure 3 (a). \( P, Q \) and \( O \) contain the union of all facts included in the predicates in their respective domains. Since \( p_1 \) and \( q_1 \) are the only two facts that agree on value of \( Y \), \( PQ \), the predicate produced by the body of \( R \), contains only one generated fact. \( R \) is obtained by dropping \( Y \), which is then united with \( O \) to produce \( S \). By comparing generated facts in \( S \) with labels in the training data, it is possible to learn a full program which in this case constitutes learning: 1) which predicates to replace \( P, Q \) and \( O \) with, and 2) the logical connectives, \( \text{LNN-\&} \) and \( \text{LNN-\lor} \), used to model \( R \) and \( S \) with, respectively. We next state a more formal problem definition.

Figure 2: (a) Lukasiewicz \( t \)-norm vs. (b) Product \( t \)-norm vs. \( \text{LNN-\&} \) with (c) \( \alpha = 0.7 \), (d) \( \alpha = 0.9 \). (e) \( \text{LNN-\lor} (\alpha = 0.7) \).
Figure 3: (a) A toy KB. (b) An example rule template (top) and its tree form (bottom). (c) A more complex program template. (d) Generated facts for our running example.

Let \( T = (V, E, L) \) denote a tree-structured program template where \( V \) denotes the set of nodes, \( E \) denotes the set of edges and \( L \) denotes a mapping from \( V \) to node labels. \( L \) maps \( T \)'s leaves to the corresponding domain of predicates in the KB. In the worst case, the domain can be the subset of predicates in the KB that agrees with the arity of the leaf. \( L \) maps internal nodes to a logical operator \( \{ \land, \lor, \neg \} \). The ILP task can then be stated as, given \( T \), a knowledge base KB, and truth-values corresponding to generated facts in the root of \( T \), to learn all logical connectives involved along with selecting predicates for each leaf in \( T \).

In the remainder of this section, we describe how to achieve the above ILP task given ground truth values for generated facts belonging to the root of the template. Let \( \psi(v) \) denote the truth value associated with (generated) fact \( v \). Our strategy is to build a neural network that connects the truth values of generated facts from the root of the template to other (generated) facts in its lineage right down to the facts in the base KB whose truth values are defined to be \( 0 \). The whole neural network can then be trained end-to-end using backpropagation. Let \( V(X) \) denote any node in \( T \) whose predicate is defined over variables \( X \) and whose children in \( T \) is denoted by \( N(V) \). Also, let \( V(x) \) denote a fact obtained by the substitution \( X = x \) and \( F(V) \) denote all facts of \( V \).

### 4.1 Combining Base Facts

Let \( V(X) \) denote a leaf in \( T \) with domain \( \mathcal{L}(V) \) then \( \mathcal{F}(V) \) is given by \( \bigcup_{P \in \mathcal{L}(V)} \mathcal{F}(P) \). Computing \( \psi(V(X = x)) \) corresponding to \( X = x \) requires truth values of all facts corresponding to the same substitution. We provide two options that associate parameters with predicates in \( \mathcal{L}(V) \): 1) attention (Yang, Yang, and Cohen 2017) and 2) our proposed LNN-pred operator:

1. \( \psi(V(x)) = \sum_{P \in \mathcal{L}(V)} w_P \psi(P(x)) \)
2. \( \psi(V(x)) = 1 - \text{relul}\left(\beta - \sum_{P \in \mathcal{L}(V)} w_P \psi(P(x))\right) \)

where \( \beta, w_P \) denote learnable parameters. One issue with attention is that it may lack sparsity assigning a majority of predicates in \( \mathcal{L}(V) \) non-zero weights thus hampering interpretability. To address this, we propose an alternate parameterization, LNN-pred, that is a simpler version of LNN-v and lacks all constraints except for non-negativity of \( w_P \) (since we do not require disjunctive semantics). As an example, the lower left corner of Figure 4 shows how to compute \( \psi(p_1) \) from \( \psi(a_1), \psi(b_1) \) since \( a_1, b_1 \) form the lineage for \( p_1 \) (Figure 3). Here, \( \beta, w_1 \) denote LNN-pred’s parameters.

### 4.2 Combining Facts with Conjunction

We handle conjunctions in two steps: 1) first construct the result of the body of the clause, and then 2) construct the head, dropping variables if needed. Let \( V(Y) \) in \( T \) be such that \( \mathcal{L}(V) = \land \) and \( \mathcal{N}(V) \) denote its children. Also, let \( I(X) \) denote the intermediate predicate produced from the body of \( V(Y) \) potentially containing additional variables such that \( X \supseteq Y \). We use LNN-\land to compute \( \psi(I(x)) \):

\[
\psi(I(x)) = \text{relul}\left(\beta - \sum_{P \in \mathcal{N}(V)} w_P (1 - \psi(P(x_{\text{var}(P)})))\right)
\]

where \( \text{var}(P) \) denotes predicate \( P \)'s arguments and \( x_{\text{var}} \) denotes the substitution restricted to variables in var. When \( X \supseteq Y \), multiple facts from \( \mathcal{F}(I) \) may combine to produce a fact in \( V(Y) \) and we use \( \text{maxout} \) for this:

\[
\psi(V(y)) = \text{maxout} \{ \psi(I(x)) \mid x_Y = y, I(X) \in \mathcal{F}(I) \}
\]

where \( \text{maxout} \{ x_1, \ldots \} \) (Goodfellow et al. 2013) returns the maximum of the set. Figure 4 shows how \( \psi(p_{12}) \) is computed from \( \psi(p_{1}), \psi(q_{1}) \) where \( \beta_2, w_2 \) denotes LNN-\land’s parameters. Since \( p_{12} \) is the only intermediate fact leading to \( r_1 \), we do not need \( \text{maxout} \) in this case. However, if that was not the case, Figure 4 shows how \( \text{maxout} \) would appear.

### 4.3 Combining Facts with Disjunction

Given \( V(X) \) in \( T \) such that \( \mathcal{L}(V) = \lor \), \( \psi(V(x)) \) can be computed using LNN-\lor:

\[
\psi(V(x)) = 1 - \text{relul}\left(\beta - \sum_{P \in \mathcal{N}(V)} w_P \psi(P(x))\right)
\]

In Figure 4 shows how \( \psi(s_1) \) is computed from \( \psi(r_1) \) and \( \psi(o_2) \) where \( \beta_4, w_4 \) denotes LNN-\lor’s parameters.

### 4.4 Other Operations and Extensions

Implementing negation is more involved since it requires that we consider assignments that \emph{may} lead to facts in \( V \) but are
Learning Constrained Activations

Frerix, Nießner, and Cremers (2020) recently showed how to handle a system of linear inequality constraints of the form \( Az \leq b \) where \( A \) denotes a matrix containing coefficients in the constraints, \( z \) denotes the parameters (in our case, some concatenation of \( \beta \) and \( w \)), and \( b \) denotes the constants in the constraints. We begin with the Minkowski-Weyl theorem:

**Theorem 4.1.** A set \( C = \{ z \mid Az \leq b \} \) is a convex polyhedron if and only if:

\[
C = \{ \sum \mu \lambda \mid \mu, \lambda \geq 0, 1^\top \lambda = 1 \}
\]

where \( \Sigma \) and \( \Gamma \) contain a finite number of rays and vertices, respectively.

which states that there exists a translation from \( A, b \) to \( \Sigma, \Gamma \) obtained via the double-description method (Motzkin et al. 1953). Assuming we can generate non-negative vectors \( \mu, \lambda \) and additionally ensure that \( \lambda \) sums to 1, then one can access a point \( z = [\beta, w]^\top \) from the feasible set \( C \) by computing \( \Sigma \mu + \Gamma \lambda \). Sampling vectors \( \mu, \lambda \) can be achieved, for instance, by using relu (Nair and Hinton 2010) and softmax:

\[
\mu = \max(0, \hat{\mu}) \quad \lambda = \frac{\exp(\hat{\lambda})}{Z}, \quad Z = 1^\top \exp(\hat{\lambda})
\]

Additionally, these operations can be easily included into any neural network as additional layers. For instance, Figure 4 contains in dashed boxes the above set of layers needed to generate \( w_i, \beta_i \), \( i = 1, \ldots, 4 \). The resulting neural network is self-contained, and can be trained by vanilla backpropagation end-to-end thus ensuring that the learned LNN parameters satisfy their respective constraints.

5 Experiments

Our experiments compare ILP with LNN against other neuro-symbolic ILP approaches on standard benchmarks. We evaluate rules in terms of application-specific goodness metrics and interpretability.

5.1 Gridworld

The goal in Gridworld is to learn rules that can help an agent move across an \( N \times N \) regular grid. Some of the cells on the grid are deemed obstacles that the agent cannot step onto, and the agent’s goal is to arrive at the cell which has been deemed the destination.

**Predicates, Template and Rewards:** We include two kinds of base predicates to describe the grid 1) \( \text{HasObstacle-dir}(X,Y) \) is true if the cell next to \( X, Y \) in direction \( \text{dir} \) contains an obstacle, 2) \( \text{HasTarget-dir}(X,Y) \) is true if the destination lies in direction \( \text{dir} \) from cell \( X, Y \). There are four directions, North, South, East, and West, and including their negated counterparts, \( \neg \text{HasObstacle-dir}(X,Y) \) and \( \neg \text{HasTarget-dir}(X,Y) \), brings the total number of base predicates to 8. The template is \( S(X,Y) \leftarrow P(X,Y) \land Q(X,Y) \) where \( P \)’s domain includes all \( \text{HasObstacle-dir} \) predicates and their negated counterparts, and \( Q \)’s domain includes all \( \text{HasTarget-dir} \) predicates and their negated counterparts. We set \( a = 0.8 \) and use a simple reward mechanism: +1 for moving towards the destination, -1 for moving
away, and -2 for stepping on an obstacle. The learning objective is to maximize rewards on randomly generated $5 \times 5$ grids with 3 obstacles sampled uniformly at random. We test the learned rules on grids with 12 obstacles.

**Results:** We compare our approach based on LNN-pred and LNN-$\land$ against NeuralLP which uses attention and product t-norm. Figure 5 (a) shows mean rewards averaged across all cells of 50 test grids produced by the learned rules on the y-axis vs. number of training grids observed on the x-axis. NeuralLP requires a lot more grids before it can learn the desired rules whereas we learn almost perfect rules after observing as few as 20 training grids. Essentially, in comparison to product t-norm, due to the extra learnable parameters in LNN-$\land$, we can learn with fewer learning iterations. Figure 5 (b) shows the weights for the LNN rule for $\text{GoSouth}(X,Y)$ on the edges and biases in parenthesis. This rule allows the agent to go South if 1) target is in that direction and, 2) there is no obstacle to the immediate South of the current cell. Despite the leaves of the template containing 8 predicates each in their respective domains, the learned LNN-preds are quite sparse and thus highly interpretable. The left LNN-pred assigns 1 non-zero weight to $\neg \text{HasObstacleSouth}$ out of all HasObstacle-$\text{dir}$ predicates and their negated counterparts, and the right LNN-pred assigns 1 non-zero weight to HasTargetSouth out of all HasTarget-$\text{dir}$ predicates and their negated counterparts. This may be due to the use of $\text{relu}$ in LNN-pred whose sparsity-inducing properties have been noted before (Krizhevsky 2010). In Figure 5 (c), we also plot $\text{GoSouth}(X,Y)$’s learned LNN-$\land$.

### 5.2 Knowledge Base Completion

Knowledge base completion (KBC) is a standard benchmark for ILP. We experiment with publicly available KBC datasets Kinship, UMLS (Kok and Domingos 2007), WN18RR (Dettmers et al. 2018), and FB15K-237 (Toutanova and Chen 2015) (see Table 1 for statistics). We compare against a host of rule-based KBC approaches: NeuralLP (Yang, Yang, and Cohen 2017), DRUM (Sadeghian et al. 2019), CTP (Minervi et al. 2020b), which is an improvement on neural theorem provers (Rocktäschel and Riedel 2017), and the recently proposed RNNLogic (Qu et al. 2021).

**Task Description and Template:** A popular abstraction of the KBC task is to complete edges or triples missing from the knowledge graph (KG). More precisely, given a query $\langle h, r, ? \rangle$, where $h$ denotes a source vertex and $r$ denotes a relation from the KG, most KBC approaches provide a ranked list of destination vertices. Most of the aforementioned rule-based KBC approaches exclusively focus on learning chain FOL rules as discussed in Section 2. There are at least two prevalent approaches to learn chain rules for KBC. The first approach (Yang, Yang, and Cohen 2017, Sadeghian et al. 2019) represents each predicate in the body as a mixture of relations present in the KG, and subsequently combines these via a conjunction operator. Figure 3 (c)’s template captures this where the subtree rooted at $R$ defines chain rules of length 2 predicates and $O$ captures length 1 thus enabling learning of chain rules capturing multi-hop paths of length up to 2. The only change we need to make to this template is to include all relations in the KG into the domains of the leaves. It is also easy to extend the template to learn longer chain rules. A different approach, pioneered by MINERVA (Das et al. 2018) and RNNLogic (Qu et al. 2021), is to define the chain rule as a mixture over all possible paths that can exist in the KG. This latter approach leads to more effective KBC and thus we report results by expressing it in our LNN framework as follows: 1) Express each possible multi-hop path as a base relation, and 2) Use one LNN-pred operator to express a mixture over all multi-hop paths.

**Metrics and Methodology:** We learn a chain rule per relation present in the KG. Following previous work (Yang, Yang, and Cohen 2017), we also add inverse relations to the KG which switches the source and destination vertices. We also include inverse triples into our test set. We compute filtered ranks for destinations (Bordes et al. 2013), which removes all true triples ranked above, and compute the following metrics based on Sun et al. (2020)’s suggestions. Let $n$ denote the number of destinations that have a score strictly greater than

| Name   | Vertices | Predicates | Facts | Queries |
|--------|----------|------------|-------|---------|
| UMLS   | 135      | 49         | 5216  | 661     |
| Kinship| 104      | 26         | 10686 | 1074    |
| WN18RR | 40945    | 11         | 86835 | 3134    |
| FB15K-237 | 14505 | 237       | 272115 | 20466  |

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2 All available at [github.com/shehzaadzd/MINERVA](https://github.com/shehzaadzd/MINERVA)
3 We compare with rules-only RNNLogic ("w/o embed."), since using embeddings is out of scope of this work.


Table 2: KBC Results: Bold font denotes best in row. CTP does not scale to WN18RR, FB15K-237. * indicates results copied from original paper.

|            | NeuralLP | DRUM | CTP    | RNNLogic | Ours    |
|------------|----------|------|--------|----------|---------|
| Hits@10    | 89.1     | 86.1 | 93.9   | 91.1     | 98.4    |
| MRR        |          |      |        |          |         |
|            | 48.8     | 40.0 | 70.3   | 64.5     | 81.9    |
| Hits@10    | 93.0     | 97.9 | 97.0   | 91.1     | 99.4    |
| MRR        |          |      |        |          |         |
|            | 55.3     | 61.8 | 80.1   | 71.0     | 90.0    |
| Hits@10    | 50.2     | 52.1 | −      | 53.1*    | 55.5    |
| MRR        |          |      |        |          |         |
|            | 43.3     | 44.6 | −      | 47.5*    | 49.7    |
| MRR        | 33.7     | 34.8 | −      | 45.5*    | 47.3    |
|            | 32.8     | 33.1 | −      | 44.5*    | 47.0    |
| MRR        | 19.8     | 20.0 | −      | 31.5*    | 34.2    |
|            | 17.4     | 17.5 | −      | 28.6*    | 30.7    |

where \( \delta(\cdot) \) denotes the Dirac delta function. For each method, we report averages across all test set triples. We learn chain \( \delta \)s where \( n \) terms of multi-hop path, this looks like: \( \sum_{r=n+1}^{m} \frac{1}{r} \). Hits@K = \( \frac{1}{m} \sum_{r=n+1}^{m} \delta(r \leq K) \)

Table 3: Learned rules from FB15K-237.

1) \( \text{person}_\text{language}(P, L) \leftarrow \text{nationality}(P, N) \land \text{spoken_in}(L, N) \)
2) \( \text{film}_\text{country}(F, L) \leftarrow \text{film}_\text{country}(F, C) \land \text{spoken_in}(L, C) \)
3) \( \text{tv_program}_\text{language}(P, L) \leftarrow \text{country_of_tv_program}(P, N) \land \text{official_language}(N, L) \)
4) \( \text{burial_place}(P, L) \leftarrow \text{nationality}(P, N) \land \text{located_in}(L, N) \)
5) \( \text{tv_program}_\text{actor}(P, A) \leftarrow \text{tv_program}_\text{country}(P, N) \land \text{actor}(A, L) \land \text{located_in}(L, N) \)
6) \( \text{film}_\text{release}_\text{region}(F, R) \leftarrow \text{film}_\text{crew}(F, P) \land \text{film}_\text{release}(F, L) \land \text{located_in}(L, R) \)
7) \( \text{marriage}_\text{location}(P, L) \leftarrow \text{marriage}_\text{location}(P, L) \land \text{location}_\text{adjoins}(L', L) \)

other relations that can be utilized to infer language such as the \text{official_language} spoken in a country. Rule 3 uses this relation to infer the language spoken in a TV program by first exploiting knowledge of its country of origin. Rules 5, 6 and 7 are longer rules containing 3 relations each in their body. Rule 5 infers a TV program’s country by first exploiting knowledge of one of its actor’s birth place and then determining which country the birth place belongs to. Rule 6 is similar but uses a film crew member’s marriage location instead to infer the region where the film was released. Lastly, Rule 7 infers the marriage location of a celebrity by exploiting knowledge of where their friends got married.

Additional KBC Results: Due to space constraints, in Appendix B we report results on the Countries dataset \cite{Bouchard2015} for which ground truth rules are known. On Countries, our KBC accuracy is comparable to other approaches and the learned LNN rules formed a close match with the ground truth rules specified in \cite{Nickel2016}.

6 Conclusion

Our experiments show that learning rules and logical connectives jointly is not only possible but leads to more accurate rules than other neuro-symbolic ILP approaches. Templates provide a flexible way to express a wide range of ILP tasks. The templates used for Gridworld and KBC are distinct, yet we outperformed baselines in both cases. LNN rules use weights sparingly and are eminently interpretable while LNN operators’ constraint formulation ensures close ties to classical logic’s precise semantics compared to other approaches (e.g., NLM). While our neural network requires grounding the KB, our approach is still scalable enough to tackle the larger KBC benchmarks whereas others are not (e.g., CTP). In terms of future work, we aim to combine the ideas presented here with embedding of predicates and constants in a high-dimensional latent space to hopefully further improve performance. We would also like to extend our approach to learn more general Prolog-style rules.

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**A Implementation Details for KBC Experiments**

Given a training knowledge graph $\mathcal{G} = (\mathcal{V}, \mathcal{R}, \mathcal{E})$ whose vertices are given by $\mathcal{V}$, edges are given by $\mathcal{E}$ and relations are given by $\mathcal{R}$, we learn a chain FOL rule for each $r \in \mathcal{R}$ independently. Each edge in $\mathcal{E}$ is given by a triple $(h, r, t)$ where $h, t \in \mathcal{V}$ denote source and destination vertices, and $r \in \mathcal{R}$ denotes a relation. Following previous work (Yang and Cohen 2017), we also add inverse relations. In other words, for each $r \in \mathcal{R}$ we introduce a new relation $r^{-1}$ by adding for each $(h, r, t) \in \mathcal{E}$ a new triple $(t, r^{-1}, h)$ to $\mathcal{G}$. Learning to predict destinations for a given relation $r$ in the augmented set of relations is essentially a binary classification task where $(h, r, t) \in \mathcal{E}$ and $(\hat{h}, r, \hat{t}) \notin \mathcal{E}, \forall h, t \in \mathcal{V}$, denote positive and negative examples, respectively.

**Training Algorithm & Hyperparameter Settings:** In each iteration, we sample uniformly at random a mini-batch of positive triples $B^+$ from $(h, r, t) \in \mathcal{E}$ and negative triples $B^-$ from $(\hat{h}, r, \hat{t}) \notin \mathcal{E}, \forall h, t \in \mathcal{V}$, such that $|B^+| = |B^-|$ to minimize the following loss:

$$\sum_{(h, r, t) \in B^+} \max\{0, \text{score}(h', t') - \text{score}(h, t) + \gamma\}$$

where $\gamma$ denotes the margin hyperparameter. We use Adagrad (\?) with step size $\in \{0.1, 1.0\}$, margin $\gamma \in \{0.1, 0.5, 1.0, 2.0\}$ and batch size $|B^+| = |B^-| = 8$. We use the validation set to perform hyperparameter tuning and
learn rules of length up to 4 for FB15K-237, 5 for WN18RR, and 3 for Kinship, UMLS.

B Additional KBC Experiments

Besides the experiments presented in Section 5, we also experiment with the Countries dataset [Bouchard, Singh, and Trouillon2015] which contains 272 vertices, 1108 facts and 2 predicates locatedIn(X, Y) (abbreviated locIn) and neighborOf(X, Y) (abbreviated ngbrOf). Following previous work [Das et al.2018], we report area under the precision-recall curve (AUC-PR).

Nickel, Rosasco, and Poggio (2016) permute the facts in this dataset to pose 3 learning tasks \{S1, S2, S3\} each corresponding to learning a different rule. S1 and S2’s rules contain 2 predicates in their bodies, whereas S3’s body contains 3. We use \(S(X, Z) \leftarrow P(X, Y) \land Q(Y, Z)\) as template for S1 and S2, and \(S(X, Z) \leftarrow P(X, W) \land Q(W, Y) \land O(Y, Z)\) for S3, where \(\text{Dom}(P) = \text{Dom}(Q) = \text{Dom}(O) = \{\text{locIn}, \text{ngbrOf}\}\). We compare against NeuralLP [Yang, Yang, and Cohen 2017], neural theorem provers (NTP-\(\lambda\)) [Rocktäschel and Riedel 2017], conditional theorem provers (CTP) [Minervini et al. 2020b] and neural logic machines (NLM) [Dong et al. 2019].

Table 4 reports averages across 3 runs. The NLM implementation we report results with is quite pessimistic almost never predicting a link. All other approaches achieve perfect AUC-PR on S1. We outperform NeuralLP on S2 and NTP shows high variance on S3 perhaps due to its excessive parameterization (NTP learns embeddings for predicates and vertices). CTP performs well on the first two tasks but fails on S3. To find out why, we take a close look at the learned rules next.

![Figure 6: LNN-rule (left) vs. NeuralLP’s (5) rules (top right) vs. CTP’s rule (bottom right) for Countries-S3.](image)

|       | NLM | NTP-\(\lambda\) | CTP | NeuralLP | Ours |
|-------|-----|-----------------|-----|-----------|------|
| S1    | 58.06 ± 2.4 | 100 ± 0 | 99.6 ± 0.5 | 100 ± 0 | 100 ± 0 |
| S2    | 40.57 ± 5.3 | 93.04 ± 0.4 | 92.4 ± 1.7 | 75.1 ± 0.3 | 92.3 ± 0 |
| S3    | 53.37 ± 2.8 | 77.26 ± 17.0 | 55.4 ± 3.5 | 92.2 ± 0.2 | 91.3 ± 0 |

The goal in S2 and S3 (Countries) is to learn the following rules (Nickel, Rosasco, and Poggio 2016):

(S2) \(\text{locIn}(X, Z) \leftarrow \text{ngbrOf}(X, Y) \land \text{locIn}(Y, Z)\)

(S3) \(\text{locIn}(X, Z) \leftarrow \text{ngbrOf}(W, Y) \land \text{ngbrOf}(W, Y) \land \text{locIn}(Y, Z)\)

We compare the rules learned by our approach, NeuralLP and CTP for Countries-S3. NeuralLP produces a weighted list of 5 rules (see Figure 6, top right, weights omitted) none of which capture the correct rule shown above. CTP learns that \text{ngbrOf} is a symmetric relation [Minervini et al. 2020b] which makes sense (Figure 6, bottom right). Unfortunately however, all facts that need to be proved in the test set of Countries-S3 pertain to \text{locIn} predicate which explains why CTP’s AUC-PR for Countries-S3 is so poor (Table 4).

In contrast, the learned LNN-rule shown in Figure 6 (left) is a near perfect translation of the correct logical rule into real-valued logic. Note that, the leftmost and middle LNN-preds place a large weight on \text{ngbrOf} vs. a small weight on \text{locIn} while the rightmost LNN-pred does the opposite, which lines up perfectly with the rule to be learned.

We also compared the rules learned for S2. Just as in the case of S3, for S2, the learned LNN-rule’s (shown in Figure 7) left LNN-pred places a large weight on \text{ngbrOf} while placing a small weight on \text{locIn} whereas the right LNN-pred does the opposite, closely matching the correct FOL rule shown above. The list of rules learned by NeuralLP (weight depicted in parenthesis) is shown below:

\(\text{locIn}(X, Z) \leftarrow \text{locIn}(X, Y) \land \text{ngbrOf}(Z, Y)\)
\(\text{locIn}(X, Z) \leftarrow \text{locIn}(X, Y) \land \text{ngbrOf}(Y, Z)\)
\(\text{locIn}(X, Z) \leftarrow \text{locIn}(X, Y) \land \text{locIn}(Z, Y)\)
\(\text{locIn}(X, Z) \leftarrow \text{locIn}(X, Y) \land \text{locIn}(Y, Z)\)

none of which match the correct rule to be learned for S2. CTP learns the following rule [Minervini et al. 2020b]:

![Figure 7: LNN rule learned from Countries-S2](image)
\[
\text{ngbr0f}(X, Z) \leftarrow \text{ngbr0f}(X, Y) \land \text{locIn}(Y, Z)
\]

Not only does this rule not match the correct rule to be learned, it is also not very useful from the perspective of proving facts in the test set which pertain to predicate \text{locIn} exclusively.