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Directed Graph Networks for Logical Entailment

Michael Rawson and Giles Reger

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Directed Graph Networks for Logical Reasoning

Michael Rawson and Giles Reger

University of Manchester, UK
michael@rawsons.uk, giles.reger@manchester.ac.uk

Abstract

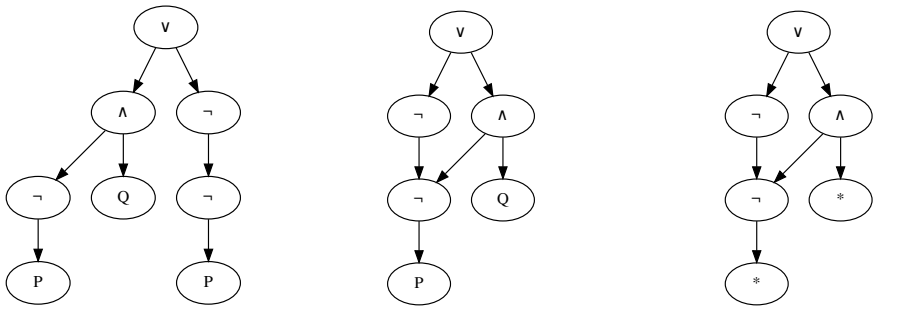
We introduce a neural model for approximate logical reasoning based upon learned bi-directional graph convolutions on directed syntax graphs. The model avoids inflexible inductive bias found in some previous work on this domain, while still producing competitive results on a benchmark propositional entailment dataset. We further demonstrate the generality of our work in a first-order context with a premise selection task. Such models have applications for learned functions of logical data, such as in guiding theorem provers.

1 Introduction

Neural networks are ubiquitous in tasks in which features must be extracted from unstructured data — tasks such as computer vision, or natural language processing. However, learning in a similar way from data that are already highly-structured is only beginning to be studied, but is sorely needed in fields such as program synthesis or automated reasoning. We approach this area from guidance of automatic theorem provers for first-order logic: an undecidable setting that nevertheless might benefit from heuristic guidance, as strategies for a subset of "useful problems" can be learned this way. It should be noted that we do not aim to *solve* known computationally-hard or undecidable problems with this approach, merely approximate these functions for practical purposes. In this work we explore the use of neural models for heuristic tasks on logical data, first in a propositional context, then progressing to a first-order setting.

Propositional Task and Dataset Evans et al. [3] introduce a dataset for studying the ability of neural networks to perform tasks which are "primarily or purely *about* sequence structure". The dataset consists of tuples of the form (A, B, y) where A and B are propositional formulae and y is the binary output variable. The task is to predict logical entailment: whether or not $A \models B$ holds in classical propositional logic. A and B use only propositional variables and the connectives $\{\neg, \wedge, \vee, \Rightarrow\}$ with the usual semantics. The dataset provides training, validation and test sets, with the test set split into several categories: "easy", "hard", "big", "massive" and "exam". The "massive" set is of particular interest to us as it contains larger entailment problems, more similar in size to those found in real-world problems.

Previous Approaches *PossibleWorldNet* is introduced alongside this dataset as a possible solution to the task: an unusual neural network architecture making use of algorithmic assistance in generating repeated random "worlds" to test the truth of the entailment in that world, in a similar way to model-based heuristic SAT solving. This approach performs exceptionally well, but does suffer from inflexibility: it is unclear how this model would perform on harder tasks without a finite number of possible worlds, or tasks where model-based heuristics don't perform as well. Tending instead toward a purely-neural approach, Chvalovský introduces TopDownNet [1], a recursively-evaluated neural network with impressive results on this dataset. Graphical representations have been used with some success for logical tasks: Olšák et al. introduce a model based on message-passing networks working on hypergraphs [14], while Paliwal et



(a) syntax tree (b) DAG - named (c) DAG - nameless

Figure 1: Producing a DAG representation of $(\neg P \wedge Q) \vee \neg\neg P$.

al [15] use undirected graph convolutions for a higher-order task. An interesting effort related to the propositional task is that of NeuroSAT [20], a neural network that learns to solve SAT problems presented in conjunctive normal form.

Graph Neural Networks Graphs have historically proven difficult for learning algorithms of various varieties, mostly due to a very rich structure. However, recent advances [12] have produced a family of methods generally known as *Graph Neural Networks*, with *graph convolutions* as a central technique. These are simple, efficient networks practically useful for many tasks operating on graph data.

Contributions Our main contribution is a neural model working directly on logical syntax that performs well on benchmark datasets, while remaining subjectively simple and flexible. Input representations retain all relevant information required to reconstruct a logically-equivalent input. To achieve this we utilise a bi-directional convolution operator working over directed graphs and experiment with different architectures to accommodate this approach. Strong performance is shown on the propositional entailment dataset discussed above. Progressing to first-order logic, we also demonstrate a lossless first-order encoding method and investigate the performance of an identical network architecture.

2 Input Encoding

Directed acyclic graphs (DAGs) are a natural, lossless representation for most types of logical formulae the authors are aware of; including modal, first-order and higher-order logics, as well as other structural data such as type systems or parsed natural language. A formula-graph is formed by taking a syntax tree and merging common sub-trees, followed by mapping distinct named nodes to nameless nodes that remain distinct: an example is shown in Figure 1. Such graphs have previously been used for problems such as premise selection [24] or search guidance of automatic theorem provers [18]. It should be noted that the acyclic property of these graphs does not seem to be particularly important — it just so happens that convenient representations happen to be acyclic. This representation has several desirable properties:

Table 1: Encoding Statistics

	valid	easy	hard	big	massive	exam
mean node count	23.5	23.7	47.5	51.4	80.2	9.1
maximum node count	37	39	65	86	102	13
standard deviation	4.6	4.7	5.9	11.0	6.7	2.1
mean symbol count	5.2	5.3	5.8	5.2	18.5	2.4

Compact size. Sufficiently de-duplicated syntax DAGs have little to no redundancy, and in pathological cases syntax trees are made exponentially smaller.

Shared processing of redundant terms. Common sub-trees are mapped to the same DAG node, so models that work on the DAG can identify common sub-terms trivially.

Bounded number of node labels. By use of nameless nodes, a finite number of different node labels are found in any DAG. This allows for simple node representations and does not require a separate textual embedding network, although this can be employed.

Natural representation of bound variables. Representing bound variables such as those found in first-order logic can be difficult [17] — this representation side-steps most, if not all, of these issues and naturally encodes α-equivalence.

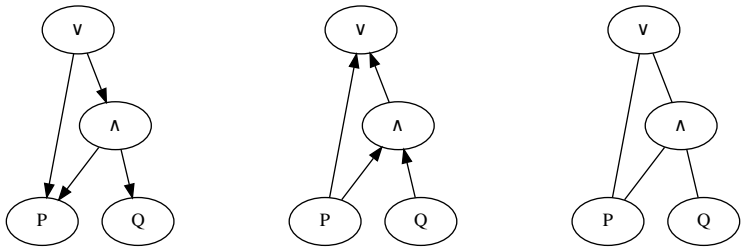
One drawback of such DAGs as a representation for logical formulae is that they lack ordering among node children: with a naïve encoding, the representation for $A \Rightarrow B$ is the same as $B \Rightarrow A$, but the two are clearly not equivalent in general. The same problem also arises with first-order terms: $f(c, x)$ is indistinguishable from $f(x, c)$ [24]. However, this problem can be removed by use of auxiliary nodes and edges such that an ordering can be retrieved, as shown in Section 5. For the propositional dataset, the classical equivalence $A \Rightarrow B \equiv \neg A \vee B$ is used to rewrite formulae, avoiding ordering issues. We also recast the entailment problem $A \models B$ as a satisfiability problem: is $A \wedge \neg B$ unsatisfiable? These methods reduce the total number of node labels used (4 in total — one for propositional variables, and one for each of $\{\neg, \wedge, \vee\}$), and allow the network to re-use learned embeddings and filters for the existing operators.

3 Model

We introduce and motivate a novel neural architecture for learning based on DAG representations of logical formulae. Unusual neural structures were found to be useful, and are described first, before these blocks are then combined into the model architecture.

3.1 Bi-directional Graph Convolutions

We assume the input DAG is a graph $(\mathbf{X}, \mathbf{A})$ where $\mathbf{X}$ is the node feature matrix and A is the directed graph adjacency matrix. Various graph convolution operators [25] (denoted $\text{conv}(\mathbf{X}, \mathbf{A})$ here as an arbitrary operator) have enjoyed recent success. These generalise the trainable convolution operators found in image-processing networks to work on graphs, by allowing each layer of the network to produce an output node per input node based on the input node's existing data and that of neighbouring nodes connected with *incoming* edges. This can be seen as passing messages around the graph: with k convolution layers, a conceptual "message" may



(a) top-down only (b) bottom-up only (c) undirected

Figure 2: Information flow in a formula DAG representing $P \wedge Q \vee P$.

propagate k hops across the graph. Here, we use the standard convolutional layer found in Graph Convolutional Networks [12]. This operator suffers from a shortcoming (illustrated in Figure 2) on DAGs such as those used here: information will only pass in one direction through the DAG, as messages propagate only along incoming edges. Unidirectional messages are not necessarily a problem: bottom-up schemes such as TreeRNNs [23] exist, Chvalovský uses a top-down approach [1], and cyclic edges are another possible solution. However, to play to the strengths of the graphical approach the ideal would have messages passed in both directions, with messages from incoming and outgoing edges dealt with separately. It is possible to simply make the input graph undirected, but this approach discards much of the crucial encoded structure and was not found to perform much better than chance on the propositional task. Instead, a bi-directional convolution is one possible solution:

$$\text{biconv}(\mathbf{X}, \mathbf{A}) = \text{conv}(\mathbf{X}, \mathbf{A}) \| \text{conv}(\mathbf{X}, \mathbf{A}^\mathsf{T})$$

where the $\|$ operator denotes feature concatenation. By convolving in both edge directions and concatenating the node-level features produced, information may flow through the graph in either direction while retaining edge direction information. A concern with the use of bi-directional convolution in deep networks is that each unidirectional convolution must decrease the size of output features by a factor of at least 2 in order to avoid exponential blowup in the size of feature vectors as the graph propagates through the network. Due to the use of a *DenseNet*-style block with feature reduction built-in, this was not an issue here.

3.2 *DenseNet*-style blocks

Recent trends in deep learning for image processing suggest that including shorter "skip" connections between earlier stages and later stages in a deep convolutional network can be beneficial [8]. DenseNets [9] take this to a logical extreme, introducing direct connections from any layer in a block to all subsequent layers. We found a graphical analogue of this style of architecture very useful. Suppose that $\mathbf{X}_{i-1}$ is the input of some convolutional layer H_i. Then, by analogy with DenseNets, H_i should also be given the outputs of previous layers as input:

$$\mathbf{X}_i = H_i\left(\mathbf{X}_0 \| \mathbf{X}_1 \| \ldots \| \mathbf{X}_{i-1}, \mathbf{A}\right)$$

However, in later layers this node-level input vector becomes very large for a computationally-expensive convolutional layer such as H_i. DenseNets also include measures designed to reduce

the size of inputs to convolutional layers, such as 1×1 convolutions. We include an analogous "compression" fully-connected layer h, which reduces the input size before convolution by allowing the network to project relevant node features from previous layers:

$$\mathbf{X}_i = H_i \left(h \left(\mathbf{X}_0 \| \mathbf{X}_1 \| \dots \| \mathbf{X}_{i-1} \right), \mathbf{A} \right)$$

3.3 Graph Isomorphism Networks and Pooling

It has been shown that the standard graph convolution layer is incapable of distinguishing some types of graph. Since logical reasoning is almost entirely about graph structure and is known to be computationally hard, it was expected that the more-powerful Graph Isomorphism Networks [25] would produce better results, but this was not found to be the case. Similarly, localised pooling is well-known to be useful in image processing tasks, and its graphical analogues such as top-k pooling [5] and edge contraction pooling [2] also perform well on some benchmark tasks. These also appear useful here, perhaps corresponding to the human approach of simplifying sub-formulae. However, these were also not found to be useful, possibly due to the lack of redundancy in formula graphs. Further investigations into integrating these powerful methods is left as future work.

3.4 Architecture

A simplistic neural architecture is described. Batch normalisation (BN) [10] is utilised before convolutional and fully-connected layers, and rectified linear units (ReLU) [13] are used as nonlinearities throughout, except for the embedding layer (no activation) and the output layer.

Embedding. An embedding layer maps one-hot input node features into node features of the size used in convolutional layers.

Dense Block. DenseNet-style convolutional layers follow, including the fully-connected network so that each layer consists ReLU-BN-FC-ReLU-BN-BiConv. Only one block is used, with each layer using all previous layers' outputs.

Global Average Pooling. At this point the graph is collapsed via whole-graph average pooling into a single vector. Passing forward outputs from all layers in the dense block to be pooled was found to stabilise and accelerate training significantly.

Output Layer. A fully-connected layer produces the final classification output.

A relatively large number of convolutional layers — 48 — are included in the dense block, for both theoretical and practical reasons. Theoretically, if information from one part of the graph must be passed to another some distance away in order to determine entailment or otherwise, then a greater number of layers can prevent the network running out of "hops" to transmit this information. Practically, more layers were found to perform better, particularly on the larger test categories, confirming the theoretical intuition. In principle there is no limit to the number of layers that might be gainfully included.

4 Experimental Setup and Results

Source code for an implementation using the PyTorch Geometric [4] extension library for PyTorch [16] is available[1].

[1] https://github.com/MichaelRawson/gnn-entailment

Table 2: Network and Training Hyper-Parameters

network		**training**	
input features	4	batch size	64
convolutional features	16	momentum	0.9
convolutional layers	48	weight decay	0.0001
		initial min. learning rate	0.01
		initial max. learning rate	0.1
		learning rate decay factor	0.99995
		learning rate cycle length	8000

Table 3: Propositional Entailment Accuracy

model	**valid**	**easy**	**hard**	**big**	**massive**	**exam**
PossibleWorldNet	98.7	98.6	**96.7**	**93.9**	73.4	96.0
TopDownNet	95.5	95.9	83.2	81.6	83.6	96.0
Contribution	**99.4**	**99.3**	91.2	88.3	**89.2**	**97.0**

Training Training setup generally follows that suggested for DenseNets [9]: the network is trained using stochastic gradient descent with Nesterov momentum [22] and weight decay, with the suggested parameters. Parameter initialisation uses PyTorch's defaults: "Xavier" initialisation [6] for convolutional weights and "He" initialisation [7] for fully-connected weights. A cyclic learning rate [21] was found to be useful for this model — we applied a learning rate schedule ("`exp_range`" in PyTorch) in which the learning rate cycles between minimum and maximum learning rates over a certain number of minibatches, while these extremes themselves decay over time. Training continued until validation loss ceased to improve. See Table 2 for training parameter details.

Augmentation No data augmentation is used as the dataset is relatively large already, and further it is unclear what augmentation would be applied: the "symbolic vocabulary permutation" approach [3] is not applicable here due to the nameless representation, but randomly altering the structure of the graph does not seem useful as it could well change the value of y unintentionally. One could imagine a *semantic* augmentation in which A is made stronger or B weaker — this would produce data augmentation without invalidating the value of y.

Reproducibility Results are reproducible, but with caveats. Training runs performed on a CPU are fully deterministic, but tediously slow. Conversely, training runs performed on a GPU are not fully deterministic[2], but are significantly accelerated. The results reported here are obtained with a GPU, but produce very similar results on repeated runs in practice. This is a significant limitation of this work that we hope to address if and when a suitable deterministic implementation becomes available.

[2] An unfortunate consequence of GPU-accelerated "scatter" operations. See https://pytorch.org/docs/stable/notes/randomness.html

Results Experimental results are shown in Table 3. Results reported from PossibleWorldNet and TopDownNet ($d = 1024$) are also included verbatim, without reproduction, for comparison. Test scores of the best-performing model on each data split are highlighted. Results show that our model is competitive on the test categories, both with algorithmically-assisted approaches (PossibleWorldNet), and with the a pure neural approach (TopDownNet). The model significantly outperforms on the "massive" test category.

Discussion We conjecture that our model generalises to some degree the approach taken with TopDownNet. In our model arbitrary message-passing schemes within the entire DAG are permitted, rather than TopDownNet's strict top-down/recurrent approach, which may go some way to explaining the difference in performance. However, the relationship with PossibleWorldNet is less clear-cut, and this is reflected in results: PossibleWorldNet remains unbeaten on the "hard" and "big" categories, but is surpassed on all others.

5 First-Order Logic

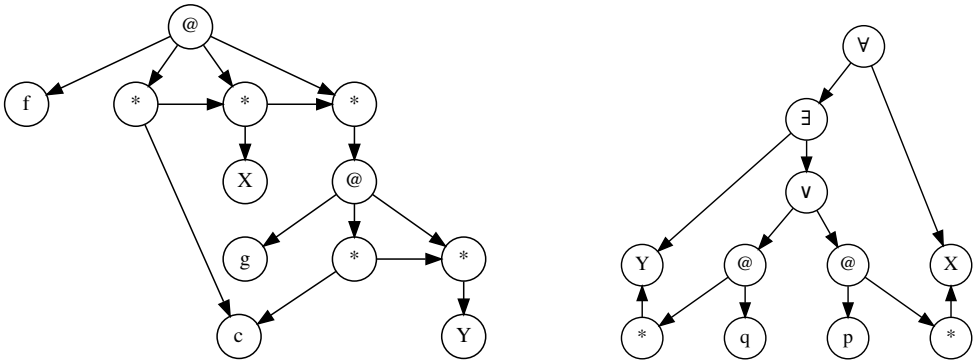
We demonstrate the flexibility and generality of our approach by also applying the same model without further adaptation or tuning to a different dataset expressed in first-order logic.

Dataset We employ the Mizar/DeepMath premise-selection dataset [11] used in the evaluation of the hypergraph model of Olšák et al. The task is to predict whether or not a given premise is required for a given conjecture, both expressed in full first-order logic. Unfortunately, we cannot produce a direct comparison as formulae are clausified in their work, which we do not attempt and simply encode the whole formula as presented. It is unclear to what extent clausification helps or hinders machine learning approaches.

Representation A similar representation to that in the propositional case is used here. However, argument order in function and predicate application must be preserved in order to maintain a lossless representation. This is achieved by use of an auxiliary "argument node" for each argument in an application, connected by edges indicating the order of arguments, shown in Figure 3. Quantifier nodes have two children: the variable which they bind, and the subformula in which the variable is bound. More space-efficient or otherwise performant graph representations are a possibility left as future work. 17 node types are used in total.

Training and Results We used an identical configuration as with the propositional case: it is possible that with some tuning better performance can be produced. We do however note that using fewer layers, (down to around 24 — half of the original number) did not seem to hurt performance for this benchmark and significantly reduced computation requirements and memory usage. Data was split at the conjecture level into 29,144 training conjectures, 3252 testing conjectures, and a validation set of 128. The model achieves a classification accuracy around 76% on the unseen test set.

Discussion On this task the network does not reach the state of the art. However, without tuning we consider this a good result: the network architecture is able to perform without much adaptation on more complex tasks expressed in different logics.



(a) $f\,(c, X, g\,(c, Y))$ (b) $\forall x.\exists y.P(x) \vee Q(y)$

Figure 3: First-order graph encodings, showing (a) argument ordering and (b) variable binding.

6 Conclusions and Future Work

We explore directed-graph representations and a new architecture for logical approximation tasks and show that they have a number of advantages — notably simplicity — and good performance characteristics. The approach can work over many different logics in principle, and practical experiment suggests this is true in practice. The network does not utilise any algorithmic assistance as PossibleWorldNet does, yet achieves competitive performance — this allows the network to process similar tasks which do not have a useful concept of "possible worlds". Combining this work with the best of other approaches, such as using the densely-connected network architecture with hypergraph methods, is a promising direction.

In some applications, such as guiding automatic theorem provers, network prediction throughput is crucial. High-performance automatic theorem prover internals typically use a graphical representation [19], so graphs are a natural choice for these structures. Additionally, graph neural networks parallelise [4] somewhat more naturally than previous approaches such as TreeNets, suggesting that this style of network may be more applicable to these domains.

Much future work is possible. No systematic effort has been made to tune network hyperparameters or overall architecture yet. In particular, we suspect that multiple dense blocks might use fewer parameters or perform better than one large block. Other convolution methods and the conspicuous absence of local pooling may also be investigated. We aim to apply some variation of this work to guidance scenarios for first-order provers in the medium-term.

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