Learning to Reason in Large Theories without Imitation

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Abstract

Automated theorem proving in large theories can be learned via reinforcement learning over an indefinitely growing action space. In order to select actions, one performs nearest neighbor lookups in the knowledge base to find premises to be applied. Here we address the exploration for reinforcement learning in this space. Approaches (like $\epsilon$-greedy strategy) that sample actions uniformly do not scale to this scenario as most actions lead to dead ends and unsuccessful proofs which are not useful for training our models. In this paper, we compare approaches that select premises using randomly initialized similarity measures and mixing them with the proposals of the learned model. We evaluate these on the HOList benchmark for tactics based higher order theorem proving. We implement an automated theorem prover named DeepHOL-Zero that does not use any of the human proofs and show that our improved exploration method manages to expand the training set continuously. DeepHOL-Zero outperforms the best theorem prover trained by imitation learning alone.

1 Introduction

Automated theorem proving is a challenging domain to learn by reinforcement learning: self-play known from two player games like in Silver et al. [2017] is not applicable in this setup, the reward is very sparse as successful proofs are hard to come by and create. In addition, the knowledge base of applicable statements increases indefinitely which makes the action space unbounded as one needs to select from an increasingly large corpus of possible premises to be applied at every step of the proof. All these issues made it seem essential to start with imitation learning and use the resulting models as a useful starting point for further training by reinforcement learning. However, the apparent necessity of imitation learning has multiple major drawbacks:

- Efficient exploration is critical for the performance of reinforcement approaches in general. Utilizing imitation learning is just a way to delay the study of such methods and can cover up some of the deficiencies of existing systems. Trying to learn without imitation learning allows for addressing the question of exploration head on and benchmarking different approaches more quickly and directly.
- Theorem proving on a new proof assistant would require a creation of training data from existing human proofs, which is a significant technical hurdle as it involves a complicated instrumentation of the assistant and carefully logging all important tactic applications with their parameters. Doing so is a cumbersome, technically complex task.
- The long term vision of auto-formalization requires the exploration of new mathematical areas automatically, a lot of them not having significant amount of (or any) human proofs, so imitation learning is not even an option in those cases.
- Open ended improvement and super-human performance would require exploration that can go beyond the level achieved by existing human formalizations.
Therefore, we are interested in studying various approaches of improving the exploration in a reinforcement learning scenario for automated theorem proving. For our experiments we have used the HOList environment and benchmark for higher order theorem proving by Bansal et al. [2019]. This benchmark is based on the core and complex analysis libraries of the proof assistant HOL Light by Harrison [1996]. Their setup is based on a linear ordering of those theorems. When attempting to prove a theorem, it allows for using all previous theorems and definitions in the ordering of the theorem database, but not the later ones.

The HOList environment enables testing AI methods for tactic based reasoning on higher order logic. The provided DeepHOL prover comes with a set of predefined tactics that can be applied at any point of the proof search. The complicating factor is that tactics can refer to definitions and theorems that have been proved already. This means that the action space is continuously expanding. In fact the most important tactic application – the “rewrite” tactic – performs a search in the current goal for a term to be rewritten by some of the equations provided for the tactic parameters.

Premise selection – the selection of theorems and definitions to be applied in tactic applications – is crucial for good performance of the theorem prover. The HOList baseline solution by Bansal et al. [2019] is based on a ranking network to select a small number of parameters for the tactic application. Running the baseline solution without imitation learning can cause two kinds of problems:

- The randomly initialized ranking model does not start with a useful similarity metric and therefore only few theorems close and they do not provide enough signal to bootstrap the learning of a good similarity metric. This is verified by our first baseline experiment.
- Even during the later stages of learning, we do not explore enough alternative options and after a while, we just do not find any new proofs to learn from. This makes the reinforcement learning level off quickly because of not finding enough new proofs.

To address the above issues, we propose the following solutions. They are based on the assumption that premises need to have a certain amount of similarity with the goal statement to be useful and applicable.

- We apply a random similarity metric that is useful from the very beginning. Here we tested two randomized variants of bag-of-word based embeddings and the cosine similarity between the learned embeddings of the goal and the premise. In the latter case, for increased exploration, we perturb the scores further by a Gaussian noise.
- During reinforcement learning, when generating the parameter lists for the tactic applications, we mix in a random selection of the most similar set of premises that have a high similarity score with the subgoal to be proved. Note however that this subset is chosen randomly, besides taking an anyways randomized similarity metric.

In addition to improved exploration, we learn to avoid unsuccessful branches by generating additional training data from failed tactic applications.

### 1.1 Related Work

Reinforcement learning without imitation learning has been successful for computer games (cf. Mnih et al. [2013]) and it was demonstrated later in Silver et al. [2017] that imitation learning was not necessary for complex games like chess and go. This has been an inspiration for our work.

Premise selection has been an active research topic in the domain of automated theorem proving. For an early review see Blanchette et al. [2016]. More recent works include Alama et al. [2014], Blanchette et al. [2016], Kaliszyk and Urban [2015] and Wang et al. [2017]. Neural networks were first applied to premise selection for automated theorem proving in Alemi et al. [2016].

There are a few automated theorem provers that based on reinforcement learning: Whalen [2016], Kaliszyk et al. [2018] and Zombori et al. [2019], but premise selection tends to be done by ad-hoc, hand engineered mechanisms. None of those try to do theorem proving without any imitation learning or improve exploration for premise selection in large theories.
Figure 1: Two-tower neural architecture for ranking actions.

2 Details

Our baseline solution is the DeepHOL theorem prover as given in Bansal et al. [2019]. They give two related approaches: one is based on pure imitation learning and another employs a combination of imitation learning and reinforcement learning. Both of them were tested on the complex analysis benchmark dataset of HOList. This benchmark consists of 10200 theorems in the training set and 3225 theorems in the validation set. The approach presented in this paper uses reinforcement learning alone on the same training set and will be compared with both solutions from Bansal et al. [2019].

We also keep the same prover algorithm with the same hyperparameters as used in Bansal et al. [2019]. This means that we do a breadth first search in which our policy network generates tactic application (operations) that can fail, prove the goal or generate a set of new subgoals. In the latter case, proving all of the newly generated subgoals constitutes a proof for the original subgoal.

2.1 Model Architecture

In order to be able to do ablation analyses, we have decided to utilize the same model architectures that were used and open sourced in Bansal et al. [2019]. This allows us to isolate the effects of improved exploration from that of the architectures and other changes to the training methodology and compare our results to the results presented there. The architecture is given in Figure 1, in which both combiner networks are non-causal WaveNet towers (cf. Van Den Oord et al. [2016]) without weight sharing. In order to compute a score for the usefulness of a given premise as a tactic parameter for a given subgoal, we compute separate embedding vectors for the subgoal and the premise to be scored. Then, the concatenation of these two vectors is fed into a combiner network which consists of a few fully connected layers followed by a linear output to compute logit that measures the usefulness of the premise.

2.2 Exploration Approaches

In the DeepHOL prover, whenever a subgoal is selected for a new proof attempt, some tactics are selected by the policy network and are given a set of tactic parameters, which is commonly a set of premises that needs to be proved. (In other cases terms generated from scratch could be passed to the tactics, but in its current form DeepHOL never generates such terms). In general, we need to select these statements from all preceding theorems and definitions in our theorem database. The number of premises from which we can choose can exceed 20000 in the HOList benchmark. However, tactics are engineered to cope with only a few of them. In fact, human proofs tend to have one or two tactic parameters typically. In our setup, we limit the number of parameters passed to any tactic application to 32 as higher numbers tend to result in timeouts and memory problems.

A crucial observation is that selecting and passing more premises than necessary is less detrimental to the overall performance than not passing theorems that are essential for processing the subgoal. There are two ways that extra premises might become harmful:

- By increasing the search space of the tactic application to the extent that the tactic just times out.
- By being applicable to the subgoal statement and rewriting it in a way that makes it harder or impossible to prove. (Note that tactics may create new subgoals that are not true).
In the first case, we have the freedom to introduce more parameters than necessary by having a generous enough timeout for the tactic applications. However, once the tactic application is successfully applied, we prune all those theorem parameters that did not affect the result of the tactic application. More dangerous is the second failure mode, but it is much less common given that it is much less frequent that useless premises are applicable.

The above considerations suggest that for exploration we should mix in extra premises in addition to a set of tactics already ranked highly by our policy network. While this slows down the proof search, those premises that turn out to be useless will be pruned away in the parameter pruning phase, as described in Bansal et al. [2019], and no positive training data will be generated for them.

The main question remains on how to generate this set of additional tactic parameters in a manner that increases exploration but does not introduce too many useless tactic parameters.

Here we explore multiple approaches. In each of our approaches we use epsilon greedy strategy for tactic selection with the same annealing schedule of decaying \( \epsilon \) from 1 to 0.1 in the first 20 rounds of the reinforcement loop.

Our most simple baseline solution starts with a randomly initialized policy network without any additional changes to the premise selection.

Our next baseline takes a seed dataset by performing one round of proving with a premise selection network that scores the premises by their cosine similarity between their embeddings that was produced by a randomly initialized embedding network. That is, the premises \( p_i \) are ranked by closeness to a given goal \( g \) according to \( s(N(g), N(p_i)) \), where \( s(x, y) \) is given by \( \langle x, y \rangle / \|x\|\|y\| \), where \( N \) is a randomly initialized WaveNet model.

Then we tested two methods for adding an exploration element to training of our reinforcement learning loop by mixing in new elements to the proposed set of premises. Formally, we select a union \( P_1 \cup P_2 \) of the subsets of the premises in which \( P_1 \) is selected as the top-\( k_1 \) top-scoring premises as ranked by our policy network, but \( P_2 \) is selected by one of the following methods:

**PET:** Using the the premise-embedding tower (PET) \( P \) of the policy network, we compute the cosine similarity \( s_i = s(P(g), P(p_i)) \) between goal \( g \) and each possible (preceding) premise \( p_i \) in the theorem database. After selecting \( P'_2 \), the top-\( k'_2 \) in this ranking (\( k'_2 \) was selected to be 100 in our experiment), we rerank \( P'_2 \) by perturbing the similarity between the elements by adding \( \nu_i \) to each cosine similarity \( s_i \), where \( \nu_i \) is sampled from a Gaussian noise with mean 0 and stddev 0.2 for each premise \( p_i \) independently. Then \( P_2 \) is selected to be the top \( k_2 \) highest scoring elements of \( P'_2 \) with respect to \( s_i + \nu_i \).

**BoW1:** \( P_2 \) is selected as a top-\( k_2 \) highest scoring elements from the the randomized bag-of-word (BoW) embeddings \( b \) of goal \( g \) and premise \( p_i \). First we compute the weighted bag of word encoding of each sentence. First we assign a different one-hot vector \( w(t) \) associated with each one the 884 tokens \( t \) occurring in our dictionary. Then we reweight each of the embeddings by \( \tilde{w}(t_i) = \nu_i f_i w(t_i) \), where \( f_i \) is the inverse document frequency and \( \nu_i \) is sampled from log normal distribution with the underlying normal distribution having zero mean and unit variance. For each goal \( g \), we rank the premises \( p_i \) by the cosine similarity \( s(\tilde{w}(g), \tilde{w}(p_i)) \) between their embeddings and pick the top-\( k_2 \) highest scoring premises.

**BoW2:** Same as BoW1, but with \( \tilde{w}(t_i) = \frac{|1+nu_i|}{f_i} w(t_i) \), where \( f_i \) is the frequency of \( t_i \) in the whole dataset and \( \nu_i \) is sampled from normal distribution with zero mean and unit variance.

### 2.3 Seed data

In order to initialize our reinforcement learning loop, we start with a longer run of theorem proving on the 10200 instances of the training set. We call this initial set of proofs our seed data. Then we commence on trying to prove 2000 theorems in each iteration of the loop. We use two sets of seed data to initialize the loop.

1. Using a randomly-initialized policy network. The weights of the goal and premise towers are initialized independently as in the baseline architecture.
2. The weights of the goal and premise tower are initialized to be the same and we use cosine similarity between the goal and premise embeddings to rank the premises.
The former is used to create a baseline, the rest of the experiments use the similarity-based seed data.

2.4 Hyperparameters

All models were trained with Adam optimizer (Kingma and Ba [2014]) and exponentially decreasing learning rate starting at 0.0001 with decay rate 0.98 at every 100000 steps. For evaluation, we use moving exponential parameter averaging at a rate of 0.9999 per step (Polyak [1990], Polyak and Juditsky [1992]). Ratio of fresh training examples (those from latest round in reinforcement learning loop) to historical (earlier rounds) was 5:11.

During proof search inside the reinforcement learning loop, we have used the following meta-parameters:

- Maximum number of top tactics explored is sampled uniformly from the interval [6, 16].
- Maximum successful tactic applications is sampled uniformly from the interval [3, 6].
- Total number of selected tactic arguments is sampled uniformly from the interval [1, 32].

In addition, we have used an individual tactic timeout of 5 seconds and overall proof timeout of 300 seconds.

3 Experimental results

We compare the various approaches experimentally. Baseline employs $\epsilon$-greedy startegy and it was performed as desribed by the first method in subsection 2.3, where we just used the randomly initialized network as usual. Seeded uses second set of seed data as described in subsection 2.3 and rest of the setup same as Baseline (in particular, there is no similarity based exploration in the loop).

3.1 Parameter exploration based on similarity

As described in Section 2.2, we ran two experiments by mixing in a new set $P_2$ of examples, one is created by randomly perturbing the order of the ranking based on the similarity of the premise embeddings, while in the other two experiments, we were mixing in randomly selected examples from randomized bag-or-word based embedding vectors. The number of elements $k_2$ selected for this newly selected subset was varied between 6 and 16. The experimental results can be seen in Figure 2. The ratio of successfully proved theorems in every round is displayed in Figure 3. As one can see, the approach of adding new theorem parameters by perturbing the ranking based on the similarity...
between the embeddings of the trained model performed worse than the one in which we selected the new examples based on the randomized bag-of-word based model.

### 3.2 Reseeding

In addition to new exploration approaches, we hypothesized that the slow learning of the models make it harder for them to learn well in the initial phase and they have a hard time to recover from that effect. To combat this, we have tested restarting the RL-loop with a freshly initialized model in order to train from all the training data that was acquired since the beginning of the training. The effect of restarting the loops with the training data from a first run loop as seed data can be seen in Figure 4. The dotted lines represent the number of proofs generated cumulatively by the first
Table 1: Total percentage of proofs on training set of 10200 theorem found by each loop till 70th round, and till when it was aborted. Percentage of theorems closed using various models on the validation set comprising of 3225 theorems at 70th round. We also report the best fraction proven by each loop where this evaluation was performed every 10th round.

| Experiment | Total till 70 (% of training) | Total till @round (% of training) | Proved @70th (on validation) | Proved (@round) (on validation) |
|------------|-------------------------------|----------------------------------|-----------------------------|--------------------------------|
| Baseline   | 20.63%                        | 22.85% @298                     | 16.96%                      | 18.32% @290                    |
| Seeded     | 38.79%                        | 43.65% @335                     | 31.10%                      | 31.13% @60                     |
| PET        | 42.64%                        | 49.76% @390                     | 30.26%                      | 32.18% @170                    |
| BoW1       | 46.32%                        | 46.58% @73                      | 32.00%                      | 32.00% @70                     |
| BoW2       | 51.20%                        | 55.32% @191                     | 33.02%                      | 33.92% @140                    |
| PET (reseed) | 48.91%                     | 51.57% @195                     | 33.73%                      | 34.26% @20                     |
| BoW2 (reseed) | 53.16%                     | 55.39% @140                     | 33.33%                      | 34.10% @90                     |
| BoW2 (extra -ves) | 52.06%                  | 54.59% @123                     | 35.78%                      | 36.55% @100                    |
| Union      | 58.57%                        | 59.79%                           | N/A                         | N/A                            |

reinforcement learning loop, while the solid lines represent the same metric for the loop reseeded from all the training data collected from the first run of the respective loop.

What one can see that the second iteration is not only training faster – which is an expected, but useless effect for practical purposes – but also levels off at a higher number of theorems proved cumulatively.

3.3 Learning from failed tactic applications

The loop partly improves the ranking during the parameter pruning phase, where-in as described in Bansal et al. [2019], parameters which were ranked highly but not needed are added as negative examples while training on subgoal that close. In the loop we are often attempting the same subgoals over the rounds. We added to the negatives of closed subgoals, parameters from other attempts on the same subgoal and tactic but with different theorem parameters where the tactic applications fail (timeout, unchanged subgoal, or any other error). We call this variation in the loop with other settings same as in BoW2 as BoW2 (extra negatives). In the initial rounds, when there aren’t many multiple proof attempts per subgoal, the performance is very similar. In later rounds, the additional data appears to help. It particularly helps the generalization (Section 3.5).

3.4 Overall Results on the Training Set

Since we do not utilize any human provided training data for proving, our training set performance itself is a useful metric of the strength of the overall reinforcement loop. In left half of Table 1, we report the overall ratio of theorems successfully proved after 70 iterations of the loop and till when it was aborted.

Also we have computed the union of all training set theorems proved by the five best of our reinforcement learning loops and compared them with the overall number of theorems proved via the combination of imitation learning and reinforcement learning as presented in Bansal et al. [2019]. Here we can see that using more computational resources, we have managed to train models that outperform the purely imitation learning based baseline and come close to the performance of the model that used a combination of reinforcement learning and imitation learning. Even more encouraging that the union of all of our reinforcement loops together managed to collect more successful proofs for the training set (59.8%) than the union of all proofs given in the original DeepHOL paper (58.0%). Given that our approach does not utilize any human data, this is an encouraging sign, since this data can be used without imitation learning and therefore successfully demonstrated that human proofs do not seem to be essential for getting a very good automated theorem proving performance for higher-order logic. Also, the results support the hypothesis that improved exploration is essential for a high quality solution regardless of relying on imitating human proofs or not.
3.5 Generalization to Unseen Theorems

Here we measure the generalization performance of our models trained by our reinforcement learning loop to theorems that were not encountered before as goals. In order to keep our experiments comparable to published baselines, we have used the published validation split – consisting of 3225 theorems – of the HOList benchmark as the held-out set. We measure the generalization performance of our provers by running them on this subset of theorems with 1000 second timeout. Note however that these theorems have been used as possible premises to be selected from before, so they are not perfectly unseen by the reinforcement learning loop. These results are reported in right half of Table 1 and in Figure 5.

3.6 Reinforcement Learning Based Proving on the Validation Set

Since we do not use any human provided training data, we argue that the whole reinforcement learning loop can be viewed as an automated prover and measure its performance on the validation set while training on the union of training and validation sets. In essence, we just verify that our success rate on the training set in our previous setup is roughly the same as on the validation set. This allows us to compare these results with earlier published baselines. For comparison, in Bansal et al. [2019], the most proven theorems in validation are 38.9% by “Loop tactic dependent” trained on imitation learning and reinforcement learning. We trained a separate $BOW^2$ loop on training and validation and report the performance here. We prove 44.68% of the 3225 validation theorems if using the checkpoint after the loop has trained for 190 rounds; while cumulatively proving 55.19% (across the rounds in RL loop and runs every 10 rounds on all validation theorems).

4 Conclusion

Here we have presented a hybrid approach named DeepHOL-zero that can learn a better automated theorem prover than the imitation learning based DeepHOL theorem prover by Bansal et al. [2019]. We have demonstrated an alternative to the $\epsilon$-greedy approach by using randomized similarity metrics to be mixed with the output of a learned ranking model and demonstrated the effectiveness of this approach on the HOList benchmark. This approach lowers the technical hurdles of integrating proof assistants other than HOL Light as it removes the necessity of the technically most involved task: the generation of human derived proofs. Our approach is generic enough to be integrated in reinforcement learning tasks other than theorem proving: in those which the action space needs to be continuously expanded to account for an indefinitely growing knowledge base.
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