Learning to Find Proofs and Theorems by Learning to Refine Search Strategies

The Case of Loop Invariant Synthesis

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NEURAL INFORMATION PROCESSING SYSTEMS

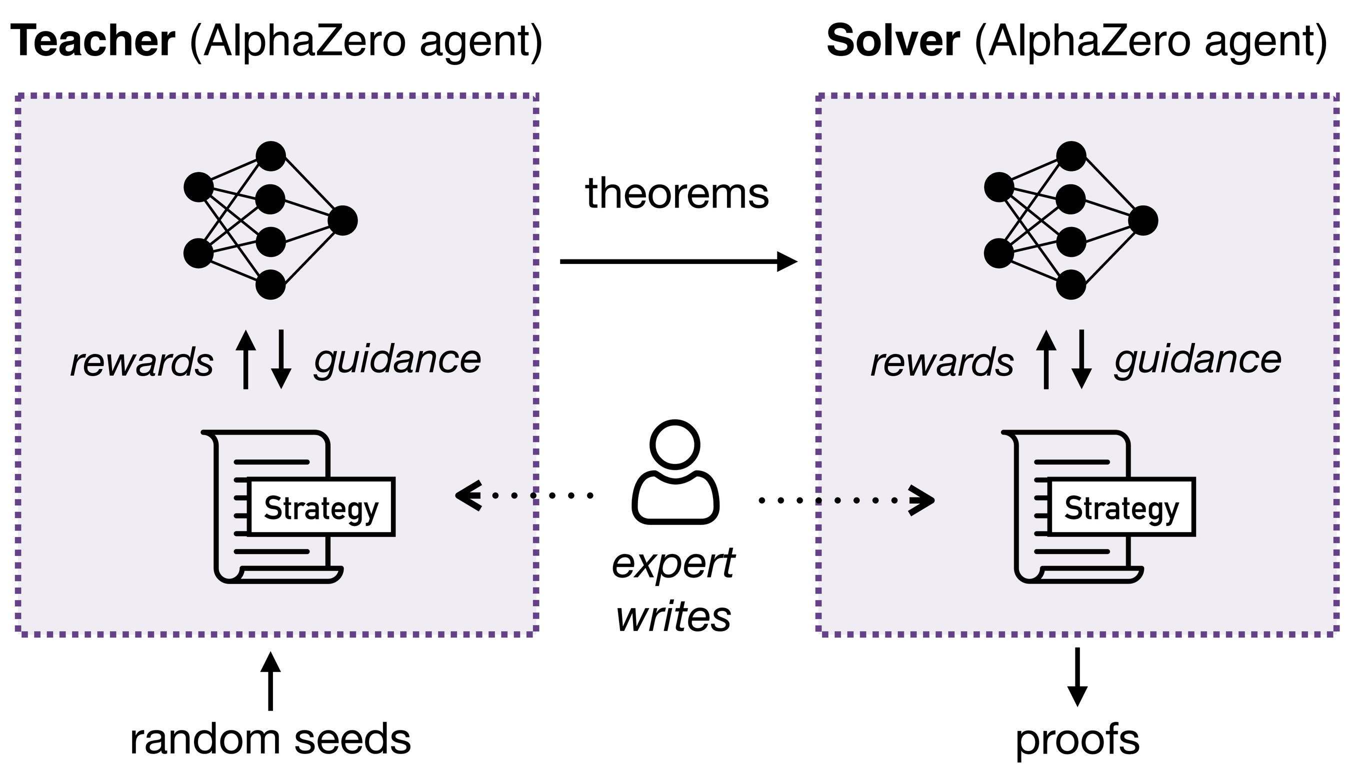
Motivation

Can theorem proving be learned without examples of proofs or theorems?

- **Automated theorem proving** has crucial applications in many fields, including software verification.
- The dominant approach for scaling it up with machine-learning is to use **imitation learning**. However, human proof data is scarce (and nearly nonexistent in many domains).
- **Reinforcement learning** alleviates the need for human proofs but training tasks of suitable relevance and diversity are still needed (equally scarce).

Our approach

A teacher/solver architecture in which both agents use RL to refine generic expert-defined strategies expressed as nondeterministic programs.



Choice points in expert strategies are resolved by neural network oracles that are trained in a purely self-supervised fashion.

Evaluation Setting

Verifying imperative programs by generating loop invariants:

- Training data unavailable and hard to generate!
- No pre-existing deep-learning agent can generalize across instances.

```
assume x ≥ 1
y = 0
while y < 1000 {
    x = x + y
    y = y + 1
}
assert x ≥ y
```

To prove the final assertion, one must find a **loop invariant** that is true before the loop, preserved by the loop body (when the loop guard holds) and implies the final assertion (when the loop guard does not hold).

Invariant: $x \geq y \wedge x \geq 1 \wedge y \geq 0$

A Flexible Strategy Language

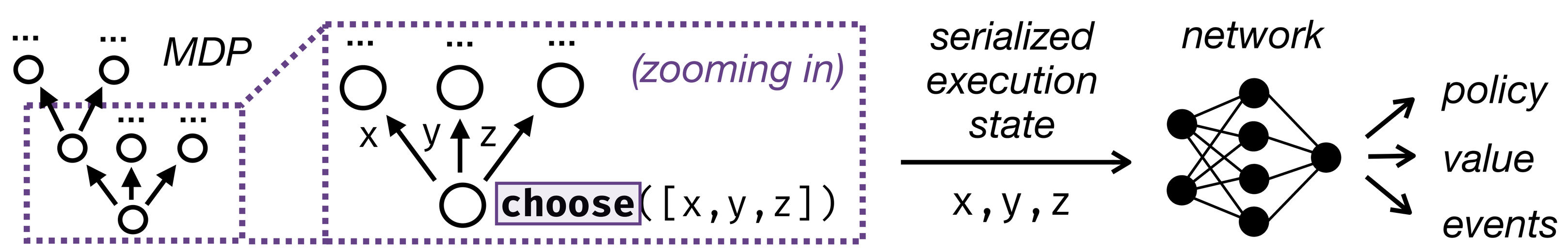
We propose a **flexible language** for experts to define search strategies in the form of nondeterministic programs, using the **choose**, **reward** and **event** operators.

A solver strategy for loop invariant synthesis:

"Start with an invariant candidate that implies the post-condition. If the candidate is not preserved, find a missing assumption that makes it so and prove it invariant recursively."

```
def solver(
    init: Formula, guard: Formula,
    body: Program, post: Formula) → Formula:
    def prove_inv(inv: Formula) → List[Formula]:
        assert valid(Implies(init, inv))
        ind = Implies(And(guard, inv), wlp(body, inv))
        match abduct(ind):
          case Valid:
            return [inv]
          case [*suggestions]:
            aux = choose(suggestions)
            return [inv] + prove_inv(aux)
inv_cand = choose(abduct(Implies(Not(guard), post)))
inv_conjuncts = prove_inv(inv_cand)
reward(max(-1, -0.2 * len(inv_conjuncts))
return And(*inv_conjuncts)
```

Strategies in this language can be **compiled** by our tool **into MDPs** that are amenable to neural-guided search and RL. Non-final states correspond to nondeterministic choice points:



Teacher Strategies

For RL to properly generalize across instances, **diverse** and **relevant theorems** (i.e. initial states in the strategy MDP) must be provided. Generating such theorems is often harder than proving them (for invariant synthesis, naive approaches based on rejection sampling produce low-quality training tasks).

Key insight: teacher agents can be implemented similarly to solver agents, by using RL to refine expert-defined strategies. To do so, we introduce the concept of a **conditional generative strategy**, which generates a problem in two steps:

1. Sample a set of random constraints.
2. Generate a problem nondeterministically and get rewarded for satisfying as many constraints as possible *(amenable to learning)*.

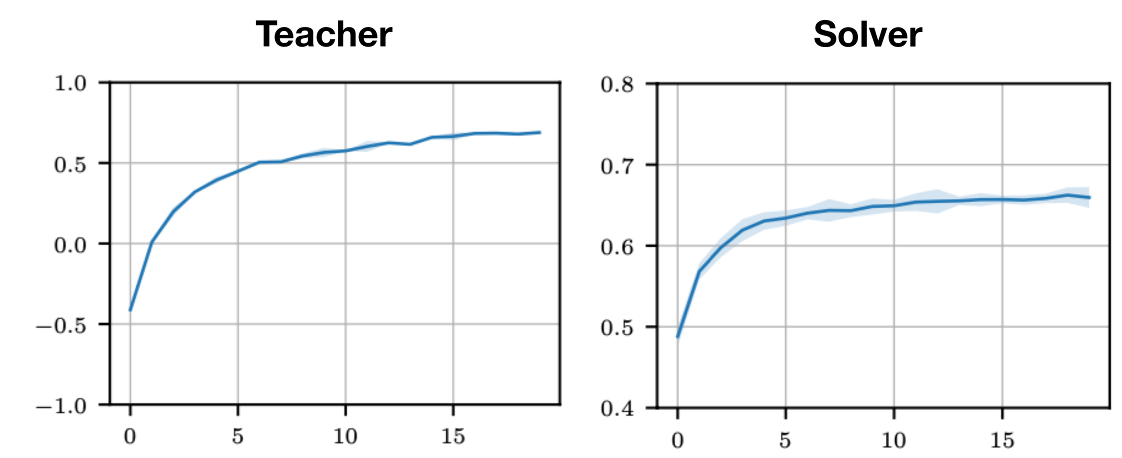
```
def teacher(rng: RandGen) → Prog:
    cs = sample_constraints(rng)
    i = generate_invariant(cs)
    p = generate_program(cs)
    assert valid_invariant(p, i)
    penalize_constr_violations(p, cs)
    return p
```

Outline of a teacher strategy for invariant synthesis. Examples of constraints are:

- *"Use an invariant with 3 conjuncts, only one of which is used to prove the postcondition."*
- *"The loop guard must only be relevant for proving the invariant inductive."*
- *"The postcondition must feature 2 disjuncts and at least one equality."*

Experiments

- We implemented our **strategy language** along with a **toolchain** to write, debug and compile strategies into MDPs.
- We trained a **teacher** and a **solver** agent for **invariant synthesis** based on two strategies written in this language. We used **Dynamic Graph Transformers** with 2M parameters as neural oracles and trained both agents for 160K **AlphaZero** episodes (with 32 MCTS simulations per move).
- Training took 16 hours on a 10-core CPU and 1 Nvidia RTX 3080 GPU.



Average collected reward as a function of the training iteration

- We evaluated the resulting solver on the **Code2Inv benchmark suite** (130 problems involving loops, conditionals and linear integer arithmetic).
- The Code2Inv problems can be solved via pure search so we conducted the evaluation with **no search allowed** (i.e. using the network policy greedily).

Policy	% Problems solved
Random	18.4 ± 0.0
Network (untrained teacher)	39.7 ± 1.6
Network (trained teacher)	**61.5 ± 0.4**

Takeaway: the trained network can solve a majority of problems with *no search* at all despite *never seeing* those during training. Using an untrained teacher leads to an inferior solver with decreased generalization capabilities.

Conclusion and Future Work

We demonstrated the possibility of learning a theorem proving task (invariant synthesis) in the absence of *both* proof and theorem examples.

- **Broader vision:** interactive provers allow users to write teacher and solver strategies for various domains in a distributed way. A large language model is fine-tuned to serve as a shared oracle that generalizes across those.
- **Future work:**
  - Evaluation of our framework in other application domains
  - Intrinsic teacher rewards (curiosity, solver rewarding the teacher directly…)
  - Integration with large pretrained language models