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Towards Reinforcement Learning of Invariants for Model Checking of Interlockings

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Abstract—The application of formal methods, in particular model checking, to verify interlockings operate correctly is well established within academia and is beginning to see real applications in industry. However, the uptake of formal methods research within the UK rail industry has yet to make a substantial impact due to current approaches often producing false positives that require manual analysis during verification. Here, it is accepted that so-called invariants, properties which hold for the entirety or a substantial subregion of the search space, can help reduce the number of such false positives. Invariants are often bespoke, manually designed by engineers making their automatic generation a challenge. In this work we present first steps towards using reinforcement learning to navigate state space representations of ladder logic programs and generate a dataset of state sequences from which invariants could be mined.

Results and what they suggest

1. Introduction

Model checking is a formal verification technique stemming from the need to systematically check whether certain properties hold for different configurations (states) of a given system. Given a transition system T and a formula (or property) F , model checking attempts to verify through refutation that $s \vdash F$ for every system state $s \in T$, such that $T \vdash F$.

The application of model checking in order to verify railway interlockings is well established within academia and is beginning to see real applications in industry. As early as 1995, Groote et al. [1] applied formal methods to verify an interlocking for controlling the Hoorn-Kersenboogse railway station. Newer approaches to interlocking verification have also been proposed in recent years [2], [3], [4]. This includes work by Linh et al. which explores the verification of interlockings written in a similar language to Ladder Logic using SAT-based model checking. In spite of this, such approaches still lack widespread use within the Rail industry.

In particular, one of the limitations of such model checking solutions is that verification can fail due to over approximation, typically when using techniques such as inductive verification []. Inductive verification fails to consider whether system states which violate a given property are

indeed reachable by the system from a defined initial configuration. These false positives often require manual inspection. One solution is to introduce so-called invariants to suppress false positives [5]. Invariants are properties that hold for subregions of the state space. The aim is to introduce invariants that help bound the region of reachable states when model checking. However generating sufficiently strong invariants automatically is complex [].

In this work we take first steps towards using machine learning to generate invariants by providing a first formal mapping of interlocking based state spaces to a reinforcement learning environment. We then explore how such state spaces can be generated in a controlled manner to test the scalability of our approach on environments where the number of reachable states is known. Finally we provide an analysis of how various reinforcement learning algorithms can be used to effectively explore state spaces in terms of their coverage. We see this as a first step towards mining invariants from such state spaces as this approach would indeed require reasonable coverage. Finally we reflect upon future works in directing our approach to improve exploration and learn invariants from a dataset of state sequences generated by our RL agents.

2. Preliminaries

We now briefly discuss model checking of railway interlockings and reinforcement learning. For further details we refer the reader to [6], [7] and [8] respectively.

2.1. Ladder Logic & Interlockings

Interlockings serve as a filter or ‘safety layer’ between inputs from railway operators, such as route setting requests, ensuring proposed changes to the current railway state avoid safety conflicts. As a vital part of any railway signalling system, interlockings are critical systems regarded with the highest safety integrity level (SIL4) according to the CENELEC 50128 standard.

Ladder logic is a graphical language widely used to program Programmable Logic Controllers [?] and in particular the Siemens interlocking systems we consider in this work. From an abstract perspective, ladder logic diagrams can be represented as propositional formulae. Here we follow the definition of James et al— [?]. A ladder logic rung

consists of the following entities. *Coils* represent boolean values that are stored for later use as output variables from the program. A coil is always the right most entity of the rung and its value is computed by executing the rung from left to right. *Contacts* are the boolean inputs of a rung, with *open* and *closed* contacts representing the values of un-negated and negated variables respectively. The value of a coil is calculated when a rung fires, making use of the current set of inputs – input variables, previous output variables, and output variables already computed for this cycle – following the given connections. A horizontal connection between contacts represents logical conjunction and a vertical connection represents logical disjunction.

A interlocking executes such a program from top-to-bottom over and over, indefinitely.

More formally, following [?] a ladder logic program is constructed in terms of disjoint finite sets I and C of input and output/state variables. We define $C' = \{c' \mid c \in C\}$ to be a set of new variables in order to denote the output variables computed by the interlocking in the current cycle.

Defn 1. Ladder Logic Formulae: A ladder logic formula ψ is a propositional formula of the form

$$\psi \equiv ((c'_1 \leftrightarrow \psi_1) \wedge (c'_2 \leftrightarrow \psi_2) \wedge \dots \wedge (c'_n \leftrightarrow \psi_n))$$

Where each conjunct represents a rung of the ladder, such that the following holds for all $i, j \in \{1, \dots, n\}$:

- $c'_i \in C'$ (i.e. c' is a coil)
- $i \neq j \rightarrow c'_i \neq c'_j$ (i.e. coils are unique)
- $vars(\psi_i) \subseteq I \cup \{c'_1, \dots, c'_{i-1}\} \cup \{c_i, \dots, c_n\}$ (i.e. the output variable c'_i of each rung ψ_i , may depend on $\{c_i, \dots, c_n\}$ from the previous cycle, but not on c_j with $j < i$, due to the nature of the ladder logic implementation, those values are overridden.)

2.2. Transition Systems and Model Checking for Ladder Logic

For this work, we have concentrated on trying to produce invariants for the approaches taken by Kanso et al. [6] and James et al. [7]. Here we include their model of ladder logic based railway interlocking programs as we use this as a basis for defining a learning environment.

Building upon the propositional representation of a ladder logic program given in Section ??, we can define, following [?], the semantics of a ladder logic program in terms of labelled transition systems.

Let $\{0, 1\}$ represent the set of boolean values and let

$$Val_I = \{\mu_I \mid \mu_I : I \rightarrow \{0, 1\}\} = \{0, 1\}^I$$

$$Val_C = \{\mu_C \mid \mu_C : C \rightarrow \{0, 1\}\} = \{0, 1\}^C$$

be the sets of valuations for input and output variables.

The semantics of a ladder logic formula ψ is a function that takes the two current valuations and returns a new valuation for output variables.

$$[\psi] : Val_I \times Val_C \rightarrow Val_C$$

$$[\psi](\mu_I, \mu_C) = \mu'_C$$

where μ'_C is computed as follows: the value of each variable c_i is computed using the i th rung of the ladder, ψ_i , using the valuations μ_C and μ_I from the last cycle and the current valuations restricted to those evaluated before the current variable. We refer the reader to [?] for full details.

Defn 2. Ladder Logic Labelled Transition System: We define the labelled transition system $LTS(\psi)$ for a ladder logic formula ψ as the tuple $(Val_C, Val_I, \rightarrow, Val_0)$ where

- $Val_C = \{\mu_C \mid \mu_C : C \rightarrow \{0, 1\}\}$ is a set of states.
- $Val_I = \{\mu_I \mid \mu_I : I \rightarrow \{0, 1\}\}$ is a set of transition labels.
- $\rightarrow \subseteq Val_C \times Val_I \times Val_C$ is a labelled transition relation, where $\mu_C \xrightarrow{\mu_I} \mu'_C$ iff $[\psi](\mu_I, \mu_C) = \mu'_C$.
- $Val_0 \subseteq Val_C$ is the set of initial states.

We write $s \xrightarrow{t} s'$ for $(s, t, s') \in R$. A state s is called *reachable* if $s_0 \xrightarrow{t_0} s_1 \xrightarrow{t_1} \dots \xrightarrow{t_{n-1}} s_n$, for some states $s_0, \dots, s_n \in Val_C$, and labels $t_0, \dots, t_{n-1} \in Val_I$ such that $s_0 \in Val_0$.

add figure example

2.3. Reinforcement Learning and MDPs

Reinforcement Learning (RL) is a machine learning paradigm with demonstrably impressive capacity for modelling sequential decision making problems as the optimal control of some incompletely-known Markov Decision Process (MDP) [9].

Defn 3 Markov Decision Process A finite discounted Markov Decision Process M is a five tuple $\langle S, \mathcal{A}, P_a(s, s'), R_a(s, s'), \gamma \rangle$, where

- S , is a finite set of states, known as the observation space or state space, representing the environment at discrete time steps.
- \mathcal{A} , describes the action space; a set of actions performable at discrete time steps, used to compute new states from the observation space.
- $P_a(s, s') = Pr(s_{t+1} = s' \mid s_t, a_t)$, describe state transition probabilities. The likelihood of observing state s_{t+1} given action a_t is taken from state s_t .
- $R_a(s, s')$ is a reward function feeding a scalar signal back to the agent at each time step t .
- $\gamma \in [0, 1]$ is a discount scalar successively applied at each time step.

In an RL setting we refer to the MDP as our environment, \mathcal{E} where through simulation, software agents sample actions $a \in \mathcal{A}$, observe changes in states, $s \in S$ and learn to optimise learning some objective based on rewards, r issued over discrete time steps t . Simulation can be continuous, where agents indefinitely interact with the environment until some termination criterion is met, such as reaching some reward threshold. Alternatively tasks may be episodic, where training is conducted over a sequence of episodes, defined by a finite number of time steps. An agent's trajectory, $\tau = (s_1, a_1, r_1, s_2, a_2, r_2, \dots, s_h, a_h, r_h)$, summarises experience accumulated over a single episode or continuous training run. Here, h refers to the horizon; a time step

beyond which rewards are no longer considered. Rewards observed from time step t up to some terminal time step T are denoted $G_t = \sum_{i=t}^T \gamma^{i-t} r_i$, and referred to as the return. The discount factor $\gamma \in [0, 1]$ applies to successive rewards at each time step to help enumerate returns over a potentially infinite horizon. Thereafter, learning may conclude having achieved adequate performance or resume from some initial state following an environment reset.

Two principle challenges of RL are those of prediction and control. The first refers to approximating the value function used to estimate state values $v(s)$ or state-action values $q(s, a)$, describing the benefit of being in that state. Values are differentiable and updated based on an empirical average, known as the expectation, taken over observed returns, $\mathbb{E}[G_t | S_t = s, A_t = a]$. Observed returns depend on the action(s) sampled at discrete time steps. The second challenge of control concerns optimising this selection process via the policy $\pi(a|s)$; a probability distribution mapping states to actions most likely to maximise the reward objective. Ultimately an optimal value function will converge to an optimal policy π^* . In practice to scale with complex environments these functions are parametric and approximated with gradient-based methods, such as stochastic gradient ascent.

Determining the reachable state space for LLPs is often intractable, making the complete MDP model unknown to us without computing all transitions. Consequently we trial several gradient-based learning methods. Policy gradient methods [1] utilise parameterised policies which update with respect to their parameter vector and objective function [2]. Actor-critic methods also approximate a parametric value function, separating the learning of action selection from value estimates. In this work we explore the efficacy of basic Deep Q-Networks [11], Proximal Policy Optimisation (PPO) [12], Advantage Actor-Critic (A2C) and its asynchronous counterpart (A3C) [8] in navigating our set of generated LLPs.

3. Mapping Formal Methods to Reinforcement Learning

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 Explain why the LTS in James et al. [17] uses four elements, but we ignore ...

3.1. Ladder Logic Markov Decision Process

We now define the finite Markov Decision Process (MDP), or environment \mathcal{E} used to represent the LLP. A Ladder Logic MDP $M(\psi)$ is a five tuple, where $S = V_I \cup V_C$, observation space to represent the MDP state at discrete time steps. $\mathcal{A} = V_I$, describes the action space; a set of formally defined actions which change the observation space. $P_a(s, s') = Pr(s_{t+1} = s' | s_t, a_t)$, describing the likelihood of observing state s_{t+1} given action a_t taken from state s_t . $R_a(s, s')$ is a reward function fed back to the agent

at each time step γ is a discount scalar applied to the reward estimates for future time steps.

Explain relation between transition probabilities and state transitions

Subsequently the environment unfolds as a set of reachable states for the respective LLP. As workers improve their value estimates according to the reward function, a balance is maintained between stochastic action sampling for exploration and predicted actions from the policy network.

Aiming to maximise state space coverage we implement a reward scheme which positively rewards novel observations and dissuade loops with negative reward and episode termination. Training episodes spawn agents at some initial state, either with all variables set to 0 or from some randomly sampled state from a set of previous observations. Workers are initialised with separate environment instances to accumulate experience independently. A global set of observations is asynchronously updated by workers periodically to compile shared experiences. Early stopping terminates training if a set number of consecutive model updates do not improvement in terms of coverage or reward. Second, training ends in our artificially generated programs if all reachable states have been observed at least once. To aid exploration, on episode resets we randomly initialise workers in some previously visited state, as demonstrated in [23].

4. Related Work

Here we briefly highlight key contributions within related literature, addressing the invariant finding problem for interlocking programs and contemporary RL strategies for environment exploration.

4.1. Invariant Finding

Overview of IC3, other invariant finding techniques for interlockings

From software engineering techniques [24], [25] to hybrid methods incorporating machine learning [26], researchers have proposed various approaches to invariant finding with varying degrees of success.

4.2. Exploration in Reinforcement Learning

Game testing, applied algorithms to 3D environment, postition and player movement used as observations with aim of state coverage for bug finding. FPS paper [27] applies vanilla PPO with no reset logic to identify game exploits. HMI paper [28] apply curiosity function based on an empirical count of state-action pairs to maximise traversal of state transitions over a deterministiv finite state automaton navigation model. Uses vanilla Q-learning with e-greedy exploration. Similar use in web testing [29] simulate user actions to navigate web application, tracking 'uncertain' state transitions for backtracking. Also use vanilla

Q-learning and count-based reward scaling during for Q-function updates. [30] decompose exploration tasks over large, adaptive and partially observable environments into two sub-problems - adaptive exploration policy for region selection and separate policy for exploitation of an area of interest. Others [31] incorporate recurrent networks in policy design, using temporality to recall the performance of past actions and their subsequent consequences according to the reward function. ACER algorithm used to make the A3C algorithm off-policy and constrain updates with TRPO like parameter updates. [32] apply a range of state-of-the-art learning algorithms to help robot navigation in procedurally generated environments. PPO found to have near human-driver level performance, recalling which states are 'expensive' to reach, minimising the frequency of rediscovery.

Existing works have illustrated the efficacy of RL methods in learning such heuristics over large graph structures [33], distributing learning for accelerated performance [34] and prioritising novelty when exploration unfamiliar environments [23], [35], [36].

Reinforcement learning for state exploration

5. Results

We now present a set of results from applying our approach to a series of generated LLPs, modelled as learning environments.

5.1. Environment Generation

Given exhaustive search of large state spaces is often computationally intractable, we have generated a set of LLPs where the number of reachable states and recurrence reachability diameter are known. This has enabled us to analyse the performance of our approach against well understood state spaces. Using existing models of ladder logic structures as a base template [7], we derive progressively larger programs by sequentially introducing additional rungs. This way a constrained yet predictable pattern of growth is devised. If $|S(p_i)|$ represents the number of reachable states for a program p_i , a subsequently generated program p_{i+1} with one additional rung, has $2|S(p_i)| + 1$ reachable states. Through a series of training runs on each environment we record the number of states observed by workers to gauge the overall state space coverage.

Introduce DQN, A2C and PPO

Tried DQN on smaller environments to test the viability of RL in our problem formulation and it solved them (with respect to our reward objective) within an acceptable time frame. DQN doesn't scale well and is too sensitive to hyperparameter tuning, buffer size environment dependent, training delay and gradient step size contingent on complexity of learnable function, which we'd expect to increase with environment size. Algorithm is also off-policy - trains from experiences generated by old (presumably less optimal) policies. Exploration is governed explicitly by the epsilon-greedy strategy and guaranteed to anneal toward a minimum

threshold over a significant number timesteps - this could happen with large regions of an environment unobserved. Methods exist to improve the sample efficiency and learning stability, such as Prioritised experience replay or dueling DQN.

We also try two Actor critic methods, Advantage actor-critic (A2C) and its asynchronous counterpart (A3C) to improve sample efficiency in distributing environment interaction among several workers. Having several workers and an on-policy learning algorithm removes need of replay memory and training delay to accumulate sufficient experience. Actor and critic networks, approximating the behaviour policy and value function, provide better convergence guarantees at the cost of some additional complexity. Paired with randomised reset logic both algorithms accumulate experience faster than Vanilla DQN, achieving good coverage on a range of medium to large state spaces. They are susceptible to parameter updates pushing the model into an unfamiliar region of policy space from which subsequent updates are unable to recover, potentially triggering model collapse.

We then move to trust region methods which constrain the magnitude of gradient updates within some clip range or according to KL-divergence between the current and most recent policy parameters, making the model more resilient to collapse.

5.2. Discussion

Elaborate on the efficacy of approach - is it actually promising?

Add results on some Loch Ness interlocking examples

Preliminary results applying our approach to a number of generated programs are outlined in [ref results]. 'Actions' referenced in column 3 refer to the number of possible assignments over input variables in each LLP. 'K', refers to the greatest number of steps taken before repeating observations in the environment, across all workers.

Coverage metrics are expectedly maximised for environments with a small number of reachable states with acceptable levels of coverage for programs with more than $1e5$ states. Interestingly, we observed longer training durations occasionally increased coverage beyond a certain threshold. It is possible workers learn an optimal search strategy within a subregion of the state space. Additionally, performance in terms of max k and states reached increased by approx. 5% when decreasing the total number of episodes from $3e5$ to $1.5e5$ episodes.

Fix scientific notation

This may be a product of random episode initialisation spawning workers in more desirable states where stochastic action sampling happened to lead to unfamiliar subregions of the environment.

Performance plots illustrating the cumulative reward which failed to maximise coverage often increased linearly before collapsing to some suboptimal reward.

Include performance plots

This may be due to tendencies for large network updates to shift the network gradients into a bad local minima, from which performance does not recover within the allotted training duration. The on-policy nature of actor critic means trajectories generated via an old policy are no longer sampled during minibatch updates for the current policy, thus biasing behaviour to the most recent model updates and introducing sample inefficiency. Adding experience replay [37] may help avoid this in future applications

Given the A3C algorithm requires workers to asynchronously update their shared network every T_{\max} steps or on episode termination, larger values for T_{\max} consolidate more information regarding worker trajectories before applying gradient updates to their local network. We found the most significant improvements to performance in terms of coverage metrics and increasing the k bound when introducing workers to larger environments, was lower update frequencies and random start state initialisation. Prior to these adjustments workers, irrespective of their number, seldom covered 80% of most smaller environments. Similarly, for the largest environment with 2^{50} states, coverage improved from 3.2% to 41.48%

6. Conclusion & Future Work

In this paper we have applied a basic asynchronous deep reinforcement learning method to maximise program state coverage, motivated by a reward scheme

Sentence?

some promising preliminary results but limited in its capacity to scale across large observation spaces.

In light of our findings, we aim to improve several aspects of our approach, predominantly concerning learning stability, sample efficiency and training speed. Experience replay for distributed learning may improve on-policy bias and sample efficiency.

The low dimensionality of our state spaces representation may allow us to introduce count-based exploration models to dampen the reward issued for states repeatedly observed [35]. Intrinsic motivation has also illustrated successes in environment exploration [38].

Applying IMPALA [39] to improve both sample efficiency over A3C and robustness to network architectures and hyperparameter adjustments. The adoption of a Long Short-Term Memory model (LSTM) also improves performance given GPU acceleration is maximised on larger batch updates.

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