Mining Invariants from State Space Observations*

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Abstract. The application of formal methods to verify that railway signalling systems operate correctly is well established within academia and is beginning to see real applications. However, there is yet to be a substantial impact within industry due to current approaches often producing false positive results that require lengthy manual analysis. It is accepted that invariants, properties which hold for all states under which a signalling system operates, can help reduce occurrences of false positives. However automated deduction of these invariant remains a challenge. In this work we report on using reinforcement learning to explore state spaces of signalling systems and generate a dataset of state spaces from which we envisage invariants could be mined. Our results suggest the viability of reinforcement learning in both maximising state space coverage and estimating the longest loop free path for state spaces. Additionally, we use experiences observed by our agents to compute the phi coefficient between sets of variables across unique states. This allows us to both infer invariant properties across states and inform agent exploration by converging coefficients over time.

Keywords: First keyword · Second keyword · Another keyword.

1 Introduction

Review / reframe for invariant approach

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 $s \in T$, resulting in $T \vdash F$.

The application of model checking to verify railway interlockings has a long history within academia and has seen some real applications in industry. As early as 1995, Groote et al. [11] applied formal methods to verify an interlocking for controlling the Hoorn-Kersenbooger railway station. Newer approaches to interlocking verification have also been proposed in recent years [9, ?,?]. This includes work by Linh et al. [25] which explores the verification of interlockings

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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 railway 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 [21]. Inductive verification fails to consider whether system states that violate a given property are indeed reachable by the system from a defined initial configuration. These false positive often require manual inspection, alternatively one solution is to introduce so-called invariants to suppress false positives [2]. Invariants are properties that hold for sub-regions 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 [6].

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 (RL) 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. Second, 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 work in directing our approach to improve exploration and learn invariants from a dataset of state sequences generated by our RL agents.

2   Preliminaries

We briefly discuss model checking of railway interlockings and reinforcement learning. For further details we refer the reader to [15, ?] and [19, 22, 18] 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[24] 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. [12]. 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. An interlocking executes such a program from top-to-bottom over and over, indefinitely.

More formally, following [12] 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

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

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

- $c'_i \in C'$ (i.e. c' is a coil)
- $i \neq j \rightarrow c'_i \neq c'_j$ (i.e. coils are unique)
- $vars(\psi_i) \subseteq I \cup \{c'_1, \ldots, c'_{i-1}\} \cup \{c_i, \ldots, c_n\}$ (i.e. the output variable c'_i of each rung ψ_i, may depend on $\{c_i, \ldots, c_n\}$ 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.)

Figure 1, shows a ladder logic formulae for a simple ladder logic program for controlling a pelican crossing. For full details of the program we refer the read to [12]. However for understanding here, consider line one and three. In line 1, the value of the coil CROSSING' is calculated based upon the inputs REQ and CROSSING. Whereas in line 3, the value of the coil TL_1_G (representing a traffic light being set to green), is calculated based upon the already compared coils CROSSING' and REQ' along with the input PRESSED. This illustrates the imperative nature of ladder logic in referencing variables.

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. [15] and James et al. [12]. 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 2.1, we can define, following [12], the semantics of a ladder logic program in terms of labelled transition systems.

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

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

$((\text{CROSSING}' \leftrightarrow (\text{REQ} \wedge \neg \text{ CROSSING})) \wedge$
$(\text{REQ}' \leftrightarrow (\text{PRESSED} \wedge \neg \text{ REQ})), \wedge$
$(\text{TL\_1\_G}' \leftrightarrow ((\neg \text{ CROSSING}') \wedge (\neg \text{ PRESSED} \vee \text{REQ}'))) \wedge$
$(\text{TL\_2\_G}' \leftrightarrow ((\neg \text{ CROSSING}') \wedge (\neg \text{ PRESSED} \vee \text{REQ}'))) \wedge$
$(\text{TL\_1\_R}' \leftrightarrow \text{CROSSING}') \wedge$
$(\text{TL\_2\_R}' \leftrightarrow \text{CROSSING}') \wedge$
$(\text{PL\_1\_G}' \leftrightarrow \text{CROSSING}') \wedge$
$(\text{PL\_2\_G}' \leftrightarrow \text{CROSSING}') \wedge$
$(\text{PL\_1\_R}' \leftrightarrow \neg \text{ CROSSING}') \wedge$
$(\text{PL\_2\_R}' \leftrightarrow \neg \text{ CROSSING}') \wedge$
$(\text{AUDIO}' \leftrightarrow \text{CROSSING}'))$

Fig. 1: Ladder logic program for pelican crossing.

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.

$$[\psi] : Val_I \times Val_C \to Val_C$$
$$[\psi](\mu_I, \mu_C) = \mu'_C$$

where μ'_C is computed as follows: the value of each variable c_i is computed using the ith 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 be fore the current variable. We refer the reader to [12] for full details.

Definition 1 (Ladder Logic Labelled Transition System). *We define the labelled transition system $LTS(\psi)$ for a ladder logic formula ψ as the tuple $(Val_C, Val_I, \to, Val_0)$ where*

- $Val_C = \{\mu_C | \mu_C : C \to \{0, 1\}\}$ is a set of states.
- $Val_I = \{\mu_I | \mu_I : I \to \{0, 1\}\}$ is a set of transition labels.
- $\to \subseteq Val_C \times Val_I \times Val_c$ 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 $s_0 \in Val_0$.

2.3   Reinforcement Learning and MDPs

Rephrase

Reinforcement Learning (RL) is a machine learning paradigm typically used to solve sequential decision making problems by modelling the optimal control of some incompletely-known Markov Decision Process (MDP) [23].

Definition 2 (Markov Decision Process). *A finite discounted Markov Decision Process M is a five tuple $(S, \mathcal{A}, P_a(s, s'), R_a(s, s'), \gamma)$, where*

- S, is a finite set of states, known as the observation space or state space, representing the model state 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.
- $P_a(s, s') = P(s_{t+1} = s'|s_t, a_t)$, 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, r back to the agent at each time step t.
- $\gamma \in [0, 1)$ is a discount scalar successively applied at each time step.

In reinforcement learning the MDP serves as our *environment* $\mathcal{E}$, where through *episodic* or *continuous* simulation, software agents sample their action space, observe state transitions and learn to optimise some objective based on a differential reward signal issued over discrete time steps. Continuous settings allow agents to interact with their environment for an undefined number of time steps, until some termination criterion is met such as reaching a reward threshold or state deadlock. Alternatively tasks may be episodic, where training occurs over T_{Max} sequences of *episodes*. An agent's trajectory, $\tau = (s_1, a_1, r_1, s_2, a_2, r_2, ..., s_h, a_h, r_h)$, summarises experience accumulated over a finite number of time steps, constituting a single episode or continuous training run. Ensuing algorithmic descriptions or problem formulation in this work refer to the episodic case. Here, h denotes the *horizon*; a time step beyond which rewards are no longer influence an agent's prediction. Rewards observed from some time step t up to a 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 $\gamma \in [0, 1)$ downscales rewards over time steps while future rewards are reduced as the discount exponent $i - t$ increases. This helps prioritise immediate rewards over distant ones and enumerate returns over a potentially infinite horizon.

Prediction and *control* refer to two principle challenges of RL. The first challenge is in approximating a value function which accurately estimates a quantitative benefit of being in that state. State values $v(s)$ or state-action values $q(s, a)$, describe this estimate. Values are differentiable and updated based on an empirical average, known as the *expectation* taken over observed returns, $\mathbb{E}[G_t | S_t = s, A_t = a]$. Thus computing expectation over return G_t depends on being in state $S_t = s$, having taken action $A_t = a$ during the most recent time step. Observed returns depend on the actions sampled at discrete time steps.

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. Optimal value functions and optimal policies are reciprocal in that converging to an optimal value function will converge to an optimal policy [17]. 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 industrial ladder logic programs is often intractable, making the complete MDP model unknown to us without exhaustively computing all state-action pairs. Consequently we trial several gradient-based learning algorithms using deep neural networks to approximate both value function and behaviour policy, subject to our reward objective.

Check if we ever refer to the reward objective before this

Policy gradient methods [14] utilise parametrised policies for control, where $\pi(a|s,\theta) = P(A_t = a|S_t = s, \theta_t = \theta)$ describes action selection, without need of value function estimates. Actor-critic methods also approximate a parametric, typically state-value, function $\hat{v}(s,\omega)$ separating predicting and learning action selection and value estimates independently. In practice however, both actor and critic networks share learnable parameters yet produce different predictions. Gradient updates are performed with respect to parameter vector θ and objective function $J(\theta)$. Definitions of $J(\theta)$ vary depending on the learning algorithm. In this work we explore the efficacy of three principle actor-critic algorithms; Proximal Policy Optimisation (PPO) [22], Advantage Actor-Critic (A2C) and its asynchronous counterpart (A3C) [18] in navigating our set of generated ladder logic programs. We discuss the merits and drawbacks of each approach for our setting in Section **??**.

3   Related Work

We briefly highlight key contributions within related literature, addressing contemporary environment exploration strategies, the invariant finding problem for interlocking programs and existing invariant mining techniques.

3.1   Invariant Finding

Elaborate on these citations

From software engineering techniques [7, **?**], to hybrid methods incorporating machine learning [10], researchers have proposed various approaches to invariant finding with varying degrees of success. IC3 [4] is one of the most successful approaches for model checking with invariants. IC3 makes use of of relatively simple SAT problems to incrementally constrain a state space towards only reachable states. In this scenario, IC3 operates only at the Boolean level of the abstract state space, discovering inductive clauses over the abstraction predicates. It has been applied to verification of software [8] and in the context of hardware model checking [5]. Although, we note that this approach explores invariants for a state-space relative to a given property for verification. In our work, we aim to explore invariants that can be mined independent of the given property.

3.2   Exploration in Reinforcement Learning

Techniques on mining and shorten exploration section / focus on mining

Maintaining the desired balance between explorative traversal, for information maximisation, and exploiting existing knowledge of the environment to further improve performance remains a challenge in RL. Means of improving state exploration has seen particular interest in software or user testing communities. In [3], Bergdahl et al. apply vanilla PPO in an episodic 3D environment, incentivising state space coverage to automatically identify in-game bugs and exploits. Peake et al. [20] 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. Other works [1] incorporate recurrent networks [16] in policy design, using temporality to recall the performance of past actions and their subsequent consequences according to the reward function. We incorporate trends in the literature such as state-of-the-art learning algorithms sporting the best performance in research tasks and using environment reset logic to discourage early convergence. We detail this approach further in Section 5.

4 Mining Invariants

Subsec: setting up data gathering - translation, then interaction and generated trajectories

Before any attempts toward invariant finding can be made, it is essential learned properties in an RL environment can be used meaningfully in model checking ladder logic programs. Similarly, any invariant finding approach will require observations from a sufficient proportion of reachable states. In this section we introduce a mapping that, given a ladder logic LTS, constructs an MDP where reinforcement learning can be applied to maximise state space coverage and mine invariants from such observations.

4.1 Ladder Logic Markov Decision Process

Shorten and introduce concept of mining experiences to generate a dataset

Definition 3 (Ladder Logic Markov Decision Process). *A Ladder Logic MDP $M(\psi) = (S, \mathcal{A}, P_a(s, s'), R_a(s, s'), \gamma)$ is a five tuple, where our observation space is the union of program inputs and ladder variables, and:*

- $S = Val_C \cup Val_I$.
- $\mathcal{A} = Val_I$.
- $P_a(s, s') = P(s_{t+1} = s'|s_t, a_t)$.
- $R_a(s, s')$ 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.

Here we note that any unique valuation of Val_C under the dynamics of a ladder logic program constitutes a distinct state. Our action space, describes the set of ladder logic inputs used to compute new valuations after program execution. $P_a(s, s') = P(s_{t+1} = s'|s_t, a_t)$, describes the state transition function in terms of probabilities of observing s_{t+1} given action a_t is taken from state s_t. As here, more transitions are available than described by the ladder logic program, we use this probability distribution to ensure transitions match those defined by the ladder logic (essentially this will be 1 for transitions dictated by the ladder logic program and 0 for transitions that are not). Subsequently as agents build a policy $\pi(s|a, \theta)$ according to $R_a(s, s')$ and state transitions observed under $P_a(s, s')$, the environment unfolds as a set of reachable states that reflect those of the ladder logic LTS.

Finally, our reward function and γ can be tuned to modify the learning objective. Aiming to maximise state space coverage we implement a reward scheme which positively rewards novel observations over distinct episodes, deterring loop traversal through episode termination and negative rewards. Consider the example trajectory $\tau = (S0, [0, 1, 0, 0], +1, S1, [0, 0, 1, 0], +1, S4, [0, 1, 0, 0], +1, S5, [0, 1, 0, 0], -1, S5)$. Computing the expected return on the next episode, starting from $S0$ and using observed rewards from the latest trajectory, discounting factor $\gamma = 0.99$ applies accordingly; $G_t = 1 + 0.99(1) + 0.99^2(1) = 1 + 0.99 + 0.9801$. In Section 5 we discuss these point further.

Consider figure **??**. During the training process we concatenate sequences of trajectories collected across separate episodes, forming an $N \times M$ matrix A_τ, where N refers to total observations collected during training and M the number of program variables $|Val_I \cup Val_C|$, comprising any given observation. A_τ serves as our dataset from which invariants are to be mined.

4.2   Agent Implementation

Here we introduce the network architecture used to train our RL agents. All algorithms presented in this work share the same architecture, adapting the input and output layers according to the environment. Our network input layer consists of $|Val_C \cup Val_I|$ nodes for given ladder logic formula ψ. Similarly, the output layer, responsible for mapping observations to the action space, comprises $|Val_I|$ nodes. All networks include a single fully connected hidden layer as this was empirically shown to produce the best performance. Learning rates for DQN, A2C, A3C and PPO algorithms were tuned individually according to the environment, falling within the range [0.0001, 0.001]. RMSProp was used to optimise the objective function.

5   Results

5.1   Environment Generation

Given exhaustive search of large state spaces is often computationally intractable, we have generated a set of ladder logic programs where the number of reachable

states and depth are known. This enables us to analyse the performance of our approach on state spaces with known ground truths. Using existing models of ladder logic structures as a base environment template [12], we derive progressively larger programs by sequentially introducing additional rungs. This way a predictable growth pattern is devised. Where $|S(\psi_i)|$, represents the number of reachable states for a program ψ_i, a subsequently generated program ψ_{i+1} with one additional rung, has $2|S(\psi_i)|+1$ reachable states. During interaction with each environment we record the number of states observed by agents to gauge the overall state space coverage.

Add fig: pelican state space highlighting gated condition holding for S0, branching off to an extended space

Highlight intended depth effect in correlation time series w.r.t ACT_max

Results presented in Section 5 are based on a set of generated programs ranging from 2^{14} to 2^{50} states[1], referenced in Table 1.

Add fig: illustration of stacked trajectories

5.2   State Space Coverage

Preliminary results applying the A3C algorithm to a number of generated programs are outlined in Table 1. Training was distributed among 32 CPU worker threads. 'Actions' referenced in the third column refer to the number of possible assignments over input variables in each ladder program, from every state. Depth, the first agent column, 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 a theoretical size up to 2^{40}. Interestingly, we observed longer training durations without early stopping 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 depth and states reached increased by approx. 5% when decreasing the total number of episodes from 3×10^5 to 1.5×10^5 episodes. 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 in terms of cumulative reward which failed to maximise coverage often increased linearly before collapsing to some suboptimal reward. 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

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[1] We note that interlocking programs generate much larger state spaces for model checking. However, work on abstractions by James et al. [13] have shown that the state space can be reduced, in many cases, to an approximate size of 2^{50}

the current policy, thus biasing behaviour to the most recent model updates and introducing sample inefficiency. Adding on policy memory strategies[26] 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%

Table 1: A3C Coverage Metrics

Environment			Agent	
States (Theoretical)	States (Reachable)	Actions	Depth	Coverage
2^{14}	15	2	14	100.0
2^{16}	31	4	28	100.0
2^{18}	63	6	48	100.0
2^{20}	127	8	33	100.0
2^{22}	255	10	76	100.0
2^{24}	511	12	49	100.0
2^{26}	1023	14	306	100.0
2^{28}	2047	16	538	100.0
2^{30}	4095	18	1418	99.731
2^{32}	8191	20	1712	96.532
2^{34}	16383	22	1498	95.550
2^{36}	32767	24	2879	84.694
2^{38}	65535	26	1969	89.071
2^{40}	131071	28	2692	82.884
2^{42}	262143	30	1406	76.033
2^{44}	524287	32	1782	62.137
2^{46}	1048575	34	1593	64.053
2^{48}	2097151	36	1598	57.547
2^{50}	4194303	38	2566	41.483

5.3   Variable Correlation

Introduce phi coeffs

Phi coefficients are computed to show the association between a pair of binary variables. Values range $[-1, 1]$ where 1 is complete correlation and -1 is an inverse relation.
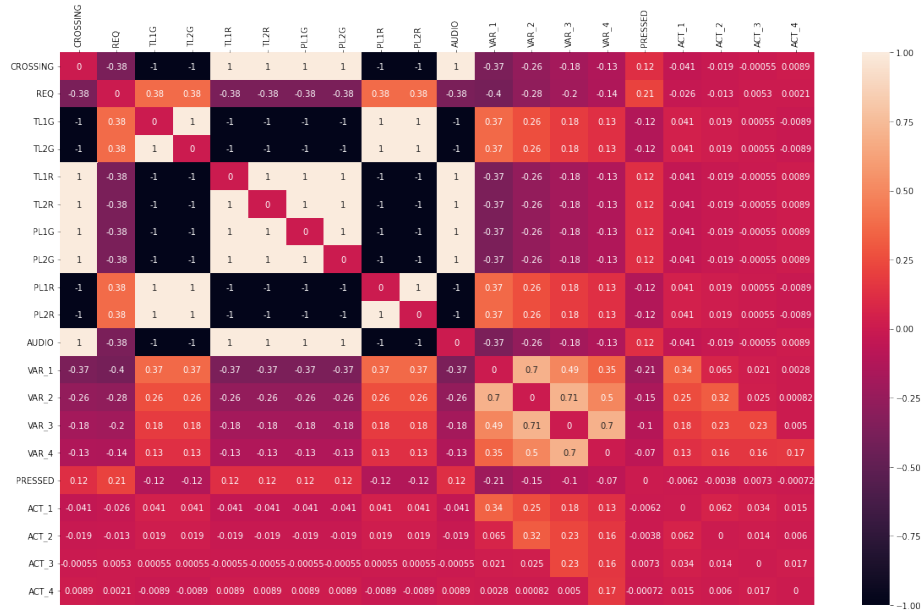
Fig. 2: Correlation matrix for ladder logic program with four additional synthetically generated rungs, 127 reachable states and 2^{20} theoretical states.

Introduce plot - how to read

Consider Figure **??**. Computing the phi coefficients for a set of binary variables produces a symmetric $N \times N$ matrix where element $m_{0,1}$ refers to the phi coefficient between $CROSSING$ and REQ. Entries computing self correlation are read on the diagonal, where they are set to 0.

Highlight program semantics / variable assignment, latch relations)

Highlight generated program / artificially depth

Add fig: correlation time series (w.r.t a variable subset)

Introduce time series plot - how to read

Highlight generated action correlation - suggestion of depth

Discuss optimising phi coeffs to converge over time.

5.4   Use of mining to validate generated data

In generating ladder logic programs to serve as training environments we introduce a condition $VAR\_1 = ACT\_1 \wedge (\neg CROSSING) \wedge \neg REQ \wedge PRESSED)$, which only holds for $S1$ of the original pelican crossing. Subsequent rungs build upon this condition for every additional ACT_N and VAR_N, ensuring every $n^{t}h$

action introduced increases the overall state space depth. We would then expect ACT_1,...,ACT_N to be correlated. Observing the lower right quadrant of Figure **??** we see properties of our program generation in how additional actions and variables become less related to our original program state space.

5.5 Trajectory Clustering

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