Reinforcement Learning in an Adaptable Chess Environment for Detecting Human-understandable Concepts

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Abstract: Self-trained autonomous agents developed using machine learning are showing great promise in a variety of control settings, perhaps most remarkably in applications involving autonomous vehicles. The main challenge associated with self-learned agents in the form of deep neural networks, is their black-box nature: it is impossible for humans to interpret deep neural networks. Therefore, humans cannot directly interpret the actions of deep neural network based agents, or foresee their robustness in different scenarios. In this work, we demonstrate a method for probing which concepts self-learning agents internalise in the course of their training. For demonstration, we use a chess playing agent in a fast and light environment developed specifically to be suitable for research groups without access to enormous computational resources or machine learning models. We provide code for the environment and for self-play learning chess agents, as well as for the state-of-the-art explainable AI (XAI) method of concept detection. We present results for different chess board sizes, discussing the concepts learned by our chess agents in light of human domain knowledge.

Keywords: Reinforcement learning and deep learning in control, Machine learning, Knowledge-based control, Supervision and testing, Discrete event modelling and simulation, Explainable artificial intelligence

1. INTRODUCTION

Autonomous agents are increasingly developed using machine learning (ML), most often with a reinforcement learning (RL) approach. In the RL setting, ML based agents explore their environment freely, with the aim of performing a task or solving a problem. Many control problems greatly benefit from the RL paradigm, since it alleviates many of their inherent challenges. It lets the agent itself be in charge of data collection, meaning that problems with large state spaces can be sufficiently explored without having to hand-tailor a data set to the problem. This can make the agent more robust, despite the fact that most real-life control environments cannot be fully modelled. RL methods also have the benefit of a goal-oriented approach to problems, meaning that we do not need to specify individual decisions in order to reach the end-goal.

While RL for fitting neural network models is an effective approach for creating autonomous agents, it introduces a problem related to human understanding: the resulting models are not interpretable to humans, opening up questions regarding what the agent has learned, and whether it has internalised knowledge human domain experts know to be important. Based on the data processing inequality (see e.g. Beaudry and Renner (2011)), we know that an ML model cannot add to the information contained in its input data. An important goal for explainable AI (XAI) in the context of autonomous agents is therefore to detect what knowledge these agents have conceptualised. We argue that investigating what a model has learned and whether this aligns with human domain knowledge is crucial for human oversight, and ensuring the stability and safety of autonomous agents.

The game of chess is the most thoroughly explored environment in the history of artificial intelligence (AI). We argue that chess is also highly suitable for developing and testing both training and explanation methods for control, for the following reasons. Firstly, the dimensionality of the game is too large for complete exploration of the state space. The RL agent must therefore find an exploration exploitation trade-off in order to succeed in solving its task, as is the case in most real-life control settings. Secondly, the game is extremely complex, meaning that the objective shifts from finding an optimal solution, to producing efficient heuristics for approximating optimal play. Thirdly, the entire game with all its complexity can be completely simulated in a fast and efficient manner, and – with the environment provided in this work – with the desired dimensionality and thus computational cost. This means that it provides a problem that is complex enough for these methods to be relevant, while not being exceedingly computationally expensive, like many other control problems. Finally, the game features a large amount of
available expert knowledge, meaning that explanations of the agent can be readily evaluated.

Today, AlphaZero (Silver et al., 2018) is the state-of-the-art ML based chess playing agent, demonstrating RL agents to be capable of outperforming human experts, and matching the strength of the best chess engines in existence. Recent work, available in the form of a preprint (McGrath et al., 2021), demonstrates that it is possible to probe which human concepts AlphaZero has learned through self-play. This methodology is likely to prove itself highly relevant in control contexts, providing us with the opportunity to investigate what domain knowledge black-box autonomous agents have acquired.

A considerable challenge in this regard is that the re-implementation of the kind of training loop required for such investigation is beyond the computational resources available to most research groups. The classical game of chess is 8x8 dimensional, and requires the evaluation of approximately $10^{123}$ positions in order to determine the value of the initial position (Allis, 1994). It is estimated that AlphaZero performed 44 million self-play games for its peak playing strength. With a large network, this is extremely resource intensive. Additionally, the concept detection method used in McGrath et al. (2021) is based on outputs from the intermediary layer blocks of their network, meaning that the dimensionality of the data set depends on the size of the network. Given their specifications of 256x3x3 dimensions per layer, with a specified maximum sample size of the data set at $5 \cdot 10^5$, this means one needs to find a least-fit regressor on 2304 variables over such a data set for each such layer.

In order to mitigate this challenge and make this promising venue of investigating XAI methods for detecting concepts learned by RL agents in complex environments, we provide

- a fast, open-source chess environment for easy simulation of any chess board size, starting position and piece types¹,
- fully trained RL agents mastering game-play on smaller chess boards,
- code for probing concepts learned by trained agents, together with results showing the detected concepts.

The paper is organised as follows. In Sec. 2, we briefly outline the training of the RL agents, present the environment, and describe the concept detection method. In Sec. 3, we present results for training agents in two different environments, and the evolution of the learned concepts throughout their training processes. In Sec. 4, we analyse the learned concepts, and how they relate to the agents’ learning processes. In Sec. 5, we discuss limitations and possible developments of the concept detection methods, including potential relevance to other areas of application.

2. METHOD

2.1 Training the Agents

The goal is for an agent to master the game of chess via self-play using reinforcement learning. Our agent is

¹ Available piece types are limited to those included in standard 8x8 chess.

![Fig. 1. A block-diagram showing the architecture of the 6x6-ResNet model, as described in the text. The CNN-architecture for the 4x5-model has the same backbone, but without skip-connections and only three initial convolution layers. The 4x5 model has 32 filters per convolutional layer, and the 6x6-model has 64 filters per layer.](https://github.com/patrik-ha/explainable-minichess)
optimal play results in a draw for the Silverman 4x5 variants. Our 4x5-agent reaches this strategy of play, producing draws in almost all simulation games, which we – together with the stagnating validation loss – interpret as having identified and settled on a stable and ideal playing style. In the following section, we provide further details about the training environment.

2.2 Environment

We provide a chess environment for reinforcement learning, with user-defined board-size and starting position, and a simple interface for extracting information about the internal state. The environment also allows customising castling-rules, and creates a representation of each position conforming to the input standard used by AlphaZero. This is highly relevant when used in conjunction with an RL training-loop, and also includes creating a one-to-one mapping for moves between the state-space of the environment, and the state space used for representation in the neural net. The environment is designed for easy extendability. Although it currently only implements standard chess pieces, it can easily be extended with custom move sets and rules. This is particularly relevant for smaller chess variants, where additional artificial rules may be added in order to increase complexity without increasing the dimensionality.

The chess environment is written primarily in Python. We use a standard bitboard representation first proposed by Atkin and Slate (1988), enhanced with “magic-move bitboard generation” introduced in Kannan (2007), providing a significant speedup in move generation. These are both standard techniques for building compact and efficient chess simulators. Python was chosen due to its ease of implementation, and convenience for the wider machine learning community. Although compiled languages, such as C++, are often faster, having access to the backbone of the environment allows direct access to computations done by the main game-play loop, which will be required later, see Sec. 2.3. Almost all operations performed during gameplay are bit-operations, owing mainly to the bitboard representation of the game. These low-level operations are done on NumPy-integers (Harris et al., 2020), since most bit-operations on these have bindings that are pre-compiled in C. This alleviates most of the performance loss from using Python. Some parts of the environment are compiled using Numba (Lam et al., 2015), effectively providing a JIT-compiled version binding of the Python code in C.

The environment is also coupled with a standard variant of Monte Carlo Tree Search (MCTS), first described in Coulom (2007). The implementation utilises simple multi-threading, with minimal communication between the threads. In particular, a tree-parallelized version of MCTS is used, described in Chaslot et al. (2008). Additionally, our implementation exploits the fact that since our neural network is only updated after a given number of self-play iterations, subsequent simulation games between these updates are independent. TensorFlow Lite (Abadi et al., 2015) is utilised to provide fast neural network guidance without having to rely on batching predictions for the GPU. This is doubly important since our implementation requires a separate instance of the predictive model per thread.

This environment is used to train the two agents described in Sec. 2.1.

2.3 Concept Detection

We use the concept detection method used in McGrath et al. (2021), based on the idea introduced in Kim et al. (2018). Briefly described, concepts are detected by learning a set of logistic probes for a data set representing the concept of interest, using the activation outputs for each intermediary layer in the neural network. In the binary case, for a given concept \( C \), an intermediary layer of size \( m \) in the neural network, a given list of inputs \( I_0, I_1,\ldots, I_N \), the corresponding activation outputs \( O_0, O_1,\ldots, O_N \), and binary labels \( P_i \in \{0, 1\} \) for each activation output, the aim is to find the best-fitting logistic regressor with weights \( w \) and bias \( b \) so that

\[
\| \sigma (w \cdot O_i + b) - P_i \|_2^2
\]

is minimized for all \( P_i \) and \( O_i \). Here, \( \sigma \) is the sigmoid function. To ensure that the concepts found are actually compactly represented, an L1-penalty weighted by \( \lambda \) is added to the weights, which in turn gives the final minimization objective:

\[
\| \sigma (w \cdot O_i + b) - P_i \|_2^2 + \lambda \| w \|_1 + \lambda | b | .
\]

The presence of a concept in different layers of the neural network is calculated by splitting the data set representing the concept into a training set and a validation set, learning the logistic regressor on the training set and calculating its binary accuracy on the validation set. In this case, for the logistic probe \( L(\cdot) \), the binary accuracy, corrected for random guessing, is

\[
\frac{2}{N} \left( \sum_{i=1}^{N} H (L(O_i) - 0.5) - P_i \right) - 1,
\]

where \( H \) is the Heaviside step function.

We probe the two agents for four concepts in total, listed in Table 1. The concept probing data sets are created through large amounts of self-play between all of our model checkpoints. Then, a subset containing 10% of the positions is randomly sampled from these games, and the
positions labelled according to the concept they represent. This processed is repeated until enough positions are gathered to form a balanced data set. This differs from the approach in McGrath et al. (2021), where concept data sets are obtained from a database of expert-level games. We choose our approach for two reasons: Primarily, there is no database of recorded games for smaller chess variants. Secondly, we wish to be able to generate balanced data sets of arbitrary sizes, which is not possible when sampling from a fixed-size data set. To avoid any bias in the concept data set in favour of the models being tested, we sample from a large variety of models, in addition to adding noise to the move selection process. This noise also ensures that each model is able to produce a large amount of potential games.

Each of our concept data sets consists of \(2.5 \cdot 10^5\) positive and \(2.5 \cdot 10^5\) negative samples. The validation ratio is 0.2, and the \(L1\) weighting is \(\lambda = 0.01\).

3. RESULTS

The probed concepts for the 4x5 and 6x6 agents are shown in Figs. 3 and 4. Here, we see concepts evolving over the course of training. In Fig. 3a, we see that the 4x5-agent develops a representation for detecting whether it has a material advantage, meaning the ability to count the material value of the opponent’s pieces compared to its own. Soon after in the training process, proceeding approximately 30 iterations, the 4x5-agent learns to represent whether it is the opponent’s queen, see Figs. 3c. Later, after approximately 50 iterations, the 4x5-agent learns to represent whether it has a potential mating attack, see Figs. 3b. Surprisingly, we observe that the agent represents the state of being in check only weakly throughout the entire training process, see Fig. 3d, despite learning to play optimally. Observe that all the probed concepts flatten out after about 100 training iterations, regardless of whether training continues. This indicates that this agent is highly unlikely to allocate more resources to represent these concepts provided more experience.

For the 6x6-agent, we see many of the same trends as for the 4x5 agent, compare Figs. 4a, 4b and 4c. A main difference is that material advantage as well as has_mate_threat are detectable already at the beginning of the training of the opponent, which in turn gives a higher chance of winning. For very weak agents, doing mostly random action selection strategies, it is highly beneficial to have more pieces than the opponent, as it implies controlling more squares than the opponent, which in turn gives a higher chance of winning. This is also reflected in the appearance and development of the ability to detect threats to the opponent’s queen. On average, the queen controls the largest number of squares per piece, and therefore serves as a simple proxy for “the ability to deliver checkmate” when playing in a non-informed way. The same tendency was observed in McGrath et al. (2021).

4. ANALYSIS

In an RL context, most of the early learning takes place because the agent accidentally succeeds, i.e. delivers checkmate. As a consequence, concepts connected to actions that are statistically more likely to win the game for a given agent, appear during the earliest stages of training. For the 4x5-agent, we observe that it quickly creates and bolsters an internal representation of material imbalance, see Fig. 3b. The reason is most likely that this a simple yet highly predictive proxy for which player will win. For very weak agents, doing mostly random action selection strategies, it is highly beneficial to have more pieces than the opponent, as it implies controlling more squares than the opponent, which in turn gives a higher chance of winning. This is also reflected in the appearance and development of the ability to detect threats to the opponent’s queen.

Table 1. Concepts probed in the chess agents.

| Name             | Description                                      |
|------------------|--------------------------------------------------|
| has_mate_threat  | Checkmate is available                           |
| in_check         | Is in check                                      |
| material_advantage| Has more pieces than opponent                    |
| threat_opponent  | Opponent’s queen can be captured                  |
We also observe that there is a difference between the two agents regarding when during training each concept emerges. We also see that the concepts represented in the smaller agent reach a plateau. This is in contrast to the larger agent, which continues developing concepts even after finding a winning playing style. This is as expected, since a larger dimensionality implies that more examples and thus training time are needed to experience a sufficient number of situations in which the different concepts are relevant.

5. DISCUSSION

We have demonstrated that the concept probing method is capable of detecting whether deep neural network models contain a compact, linear representation of a given concept. This allows probing neural network based agents for domain knowledge without having to include it in the training loop. This method is therefore highly relevant for investigating, evaluating and explaining neural network based autonomous agents, as it reveals whether these have internalised domain knowledge as expected. In the following, we discuss challenges and limitations of the method.

While this was not a problem in our case, generating representative concept data sets might prove difficult. Ideally, the concept must be defined programatically, so that concept examples can be distilled from some large sample-repository. This might be challenging, especially for large and complex problems. Also, it requires an efficient simulation-environment. In cases where the environment is a simulation of a real-world application, the simulation must also be able to generate concept samples that are representative of what the agent would encounter in its “true environment”. Otherwise, concept detection might be hindered by subtleties of synthetic data.

Exploration is a fundamental aspect of the RL paradigm, opening up the possibility that the model has observed states that, from a domain expert’s viewpoint, are unlikely to occur. This is important because it makes it more likely that the model is allowed to generalise its concepts, as opposed to if it was trained, e.g., in a supervised fashion. This has also been shown for investigating, evaluating and explaining neural network based autonomous agents, as it reveals whether these have internalised domain knowledge as expected. In the following, we discuss challenges and limitations of the method.

In our implementation, we limit ourselves to probing for linearly represented concepts, although there are no guarantees that the network represents its knowledge in a linearly separable manner. However, as observed in Alain and Bengio (2017), it is expected that most neural networks with sufficient depth will end up representing emergent concepts as simply as possible, i.e. linearly.

Finally, we wish to highlight is the difference between being able to detect concepts, and knowing how the represented concepts are utilised within the given model. In our case, we see that both models develop some representation of material_advantage. For a human, this particular concept is usually used as a heuristic for the result of the game, meaning that the player holding fewer pieces is more likely to lose. However, we cannot guarantee that our model has made the same connection, although this aligns most readily with the relevant domain knowledge.
6. CONCLUSION

In this work, we have demonstrated that concept probing can be used to gain insight into what concepts a neural network model learns. We have also demonstrated the feasibility of using these methods to reason whether the model’s internal representations align with existing domain knowledge. This is highly relevant for all control contexts in which an autonomous agent has learned to navigate in an environment about which humans possess domain knowledge. This implies easy applicability in control contexts, without having to apply constraints on the environment or training loop. While we demonstrate the applicability of the concept detection methods to agents trained in our environment, an important next step will be applying the method to classical control problems, comparing the extracted concepts to domain knowledge.

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