Specifying Goals to Deep Neural Networks with Answer Set Programming

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Abstract

The ability to easily and unambiguously specify a goal to a planner is fundamental to human-AI collaboration and knowledge discovery. Recently, deep reinforcement learning has been used to train deep neural networks (DNNs) as heuristic functions for planning problems. While DNNs can be powerful function approximators that, combined with reinforcement learning, require little to no domain-specific knowledge to learn, there is no formal way to specify goals to DNNs. We introduce a method of training DNN heuristic functions to estimate the distance between a given state and a goal, where a goal is represented as a set of atoms in first-order logic. We then use answer set programming to specify goals, where a set of atoms representing a goal is obtained from the stable model of an answer set program. The DNN heuristic function is then combined with search to reach goals. In our experiments with the Rubik's cube and Sokoban, we show that we can specify and reach a variety of different goals without any need to re-train the DNN. Furthermore, since the specification language is first-order logic, one can specify a goal without having to know what states meet that specification, beforehand. Therefore, our approach can also be used to discover states that meet a given specification.

Introduction

Deep reinforcement learning algorithms (Sutton and Barto 2018), such as DeepCubeA (McAleer et al. 2019; Agostinelli et al. 2019) and Retro* (Chen et al. 2020), have successfully trained DNNs (Schmidhuber 2015) to be informative heuristic functions. Combined with search methods such as A* search (Hart, Nilsson, and Raphael 1968), Q* search (Agostinelli et al. 2021), or Monte Carlo Tree Search (Kocsis and Szepesvári 2006), these learned heuristic functions can solve puzzles, perform retrosynthesis, as well as for compile quantum algorithms (Zhang et al. 2020). However, these DNNs do not generalize across goals where, in this context, a goal is a set of states in the state space that are considered goal states. Instead, these DNNs are either trained for a pre-determined goal or use methods such as hindsight experience replay (Andrychowicz et al. 2017) to generalize across pairs of start and goal states. As a result, specifying a goal to a DNN requires either training a DNN for that specific goal or obtaining the heuristic values for every goal state in the set of goal states and taking the minimum heuristic value. This computationally burdensome process significantly reduces the practicality of DNNs for solving planning problems with dynamic goals.

To address this issue, we present an approach for specifying goals to a DNN using first-order logic. The DNN takes as input a start state and a set of ground atoms that represents what should hold true in a goal state, but does not assume that ground atoms that are not in this set are false. A conversion process then translates these logical atoms to a representation that is convenient for the DNN. To specify a goal, any specification language that can be translated to a set of ground atoms can be used. We choose answer set programming (ASP) (Brewka, Eiter, and Truszczyński 2011), a form of first-order logic programming, as the specification language because one can obtain stable models (Gelfond and Lifschitz 1988), also known as answer sets, for a given specification (answer set program) where each stable model is a set of ground atoms. We also handle the case where the use of negation as failure introduces non-monotonic behavior. That is, conclusions that were previously derived can be retracted by adding new knowledge.

To train the DNN, we generate pairs of states and goals for training by starting from a given start state and taking a random walk to obtain a goal state. Given a process to convert a state to a set of ground atoms that represents what holds true in that state, we then obtain a set of goal states that contains the given goal state by converting the given goal state to a set of ground atoms and simply removing atoms from the set. We then update the estimated cost-to-go with Q-learning. When searching for a path to the goal we employ Q* search (Agostinelli et al. 2021). We evaluate this approach on the Rubik's cube and Sokoban (Dor and Zwick 1999) and results show that one can specify diverse goals to a DNN with simple answer set programs and reach them by combining the DNN with search. Furthermore, the training process is agnostic to the goals that will be specified at test time. An overview of our approach is described in Figure 1. In the Future Work Section, we will discuss handling unreachable goals and representing goals to DNNs using lifted representations.

Preliminaries

Our method builds on the DeepCubeA algorithm (Agostinelli et al. 2019) that was used to train a DNN as a heuristic function using approximate value iteration

(Puterman and Shin 1978; Bertsekas and Tsitsiklis 1996). This heuristic function was then used in a batched version of weighted A* search (Pohl 1970) to solve puzzles such as the Rubik's cube and Sokoban. Recently, research has shown that Deep Q-Networks (DQNs) (Mnih et al. 2015) can be used in a modified version of A* search, called Q* search (Agostinelli et al. 2021), to significantly reduce time and memory requirements of search by calculating the sum of the transition costs and heuristic values of the children of a node with a single forward pass through a DQN. For specifying goals, we use ASP. In this section, we will describe the background of Q-learning and Q* Search, as well as the background of ASP. We also describe the basics of the Rubik's cube.

Q-learning

In the context of deterministic, finite-horizon, shortest path problems, Q-learning is a reinforcement learning (Sutton and Barto 2018) algorithm to learn a function, known as an action-value function, $Q(s, a)$, that maps a state s and action a to the estimated cost-to-go when in state s and taking action a. In this setting, we can write $Q(s, a)$ in terms of the transition cost and the cost-to-go from s', which is the state that results from applying action a to state s, to a closest goal state:

$$Q(s, a) = g^a(s, s') + h(s') \qquad (1)$$

where $g^a(s, s')$ is the cost to transition from state s to state s' using action a and $h(s')$ is the cost-to-go from state s' to a closest goal state and, also, $h(s')$ is equivalent to $\min_{a'} Q(s', a')$. The optimal action-value function, $q^*(s, a)$, represents the cost of a shortest path when in state s and taking action a. The Q-learning algorithm (Watkins and Dayan 1992) takes a given Q and updates it according to Equation 2, where α is the learning rate.

$$Q(s, a) = Q(s, a) + \alpha(g^a(s, s') + \min_{a'} Q(s', a') - Q(s, a)) \qquad (2)$$

In the tabular setting, Q-learning has been shown to converge to q^* as time goes to infinity (Watkins and Dayan 1992). However, for domains with large state spaces, such as the Rubik's cube, we do not have enough memory, or time, to do tabular Q-learning. Therefore, we represent $Q(s, a)$ with a parameterized function $q_\phi(s, a)$ with parameters ϕ. The parameters of the function are trained to minimize the loss function in Equation 3, where ϕ^- are parameters of a target function that remains fixed for a certain number of training iterations and is periodically updated to ϕ. This has been shown to make the training process more stable because the target remains stationary for extended periods of time (Mnih et al. 2015).

$$L(\phi) = (g^a(s, s') + \min_{a'} q_{\phi^-}(s', a') - q_\phi(s, a))^2 \qquad (3)$$

The structure of DQNs is typically one where the input is the state, s, and the output is a vector the size of the action space that represents $q_\phi(s, a)$ for every action a. This allows one to compute the sum of the transition cost and cost-to-go for all possible next states of s with a single forward pass through the DQN, which, in turn, allows for faster heuristic search with the Q* search algorithm.

Q* Search

Q* search (Agostinelli et al. 2021) is a heuristic search algorithm inspired by A* search (Hart, Nilsson, and Raphael 1968) that uses DQNs to do heuristic search. Unlike A* search, Q* search does not need to fully expand nodes by applying every action to it and obtaining the resulting state. Instead, it stores tuples of nodes and actions (node_action tuples) in the priority queue. When removing a node_action tuple from the priority queue, Q* search then applies the action to the corresponding node to obtain the current node. The DQN is then applied to the current node to obtain the estimate of the sum of the transition cost and cost-to-go for all of its children. Then, for all actions, a node_action tuple containing the current node and an action is then pushed to the priority queue with its priority set to its path cost plus the corresponding output of the DQN for that action. The only aspect of this algorithm that directly depends on the size of the action space is pushing node_action tuples to the priority queue. Due to this, results have shown that Q* search can be orders of magnitude faster and more memory efficient than A* search while maintaining similar performance in terms of path cost.

Answer Set Programming

Answer set programming (ASP) (Brewka, Eiter, and Truszczyński 2011) is a form of logic programming that is built on the stable model semantics (Gelfond and Lifschitz 1988) which describes when a set of ground atoms, M, is a stable model, also known as an answer set, of a program, Π. Program Π is restricted to be a set of rules in first-order logic of the form:

$$A \leftarrow B_1, ..., B_m, \neg C_1, ..., \neg C_n \qquad (4)$$

where A, B_i, and C_i are atoms in first-order logic. A is in the "head", or the consequent, and B_i and C_i are in the "body", or the antecedent. In this notation, $\neg$ represents negation, a comma represents conjunction, and $\leftarrow$ represents implication. Since all literals in the body are connected with conjunction, the body is true if and only if all literals in the body are true. Since the head has just has one atom, the head is true if and only if A is true. Since the head and the body are connected by implication, the entire logical sentence is true if and only if one of the two following conditions are met: 1) the body is false; 2) the body is true and the head is true. If there are no literals in the body (also known as "facts"), then semantics dictate that the body is always true; therefore, the head must also always be true. If there are no atoms in the head (also known as "headless" rules), then semantics dictate that the head is always false; therefore, the body must also always be false. In practice, headless rules are used as constraints and are implicitly represented with a literal, A, in the head and a literal, $\neg A$, in the body that is in conjunction with the rest of the body literals. Therefore, headless rules are actually rules with negation in the body.

To determine if M is a stable model of Π, we first must consider the grounded program of Π, which we will denote Π_g. To obtain Π_g, for all rules, R, in Π, every possible grounded version of R, R_g, is obtained and added to Π_g. A ground rule, R_g, is obtained from a rule, R, by substituting all variables in R for a ground term appearing in Π. If there are no rules in Π_g with negation, then there is one unique minimal stable model of Π_g (Van Emden and Kowalski 1976; Gelfond and Lifschitz 1988) which corresponds to all atoms that are derivable from Π_g. An atom is derivable if it is in the head of a rule with a body that is true. If there are rules with negation in Π_g, then we can check if a given set of ground atoms, M, is a stable model of Π_g by first computing the reduct (Marek and Truszczyński 1999) of Π_g with respect to M, which we will denote Π_g^M. Π_g^M is obtained by starting with Π_g and deleting all rules that have a negative literal, $\neg C_i$, in the body if C_i is in M and then deleting all negative literals in the body of the remaining rules. Π_g^M is now a negation free program, which means that it has one unique minimal stable model. If this stable model of Π_g^M is equivalent to M, then M is a stable model of Π. It should be noted that Π can have multiple stable models if it contains negation. Furthermore, some ASP solvers, such as clingo (Gebser et al. 2022, 2014), allow for the use of disjunction, which can result in more than one stable model, even if negation is not present.

In ASP, choice rules may also be employed. Choice rules have a conjunction of literals in the body and a set of ground atoms in the head. If the body is true, then zero or more ground atoms in the head may be added to the stable model. For example for the following choice rule, if the body is true, then no ground atoms in the head may be added, one of the ground atoms in the head may be added, or both of the ground atoms in the head may be added (':-' indicates implication):

```
{a1(c,d); a2(d,c)} :- B_1, B_2, B_3
```

The Rubik's Cube

The Rubik's cube is a three dimensional cube where each face of the cube consists of a 3 x 3 grid of stickers, which 54 stickers in total. Each sticker can be one of six colors: white, yellow, orange, red, blue, or green. These stickers combine where the faces intersect to form cubelets, where center cubelets have 1 sticker, edge cubelets have 2 stickers, and corner cubelets have 3 stickers. There are 6 center cubelets, 12 edge cubelets, and 8 corner cubelets. While the canonical goal state for the Rubik's cube is one where all stickers on each face have the same color, there are many other patterns that interest the Rubik's cube community (Ferenc n.d.).

Methods
Learning Heuristic Functions for Goals

To learn a function that estimates the distance between a state, s, and a goal, $\mathcal{G}$, we must explicitly add the specified goal as an input to the action-value function. Therefore, the action-value function now becomes $Q(s, a, \mathcal{G})$, that represents the cost to go from s to a closest state in $\mathcal{G}$ when taking action a. In our implementation, we use a DQN with

parameters ϕ whose input is s and $\mathcal{G}$ and whose output is a vector representing $q_\phi(s, a, \mathcal{G})$ for all actions, a. We assume a function $G(s)$ that converts states to a set of ground atoms and some process to convert $\mathcal{G}$ to a representation suitable for the DQN. To train the DQN, we must first have the ability to sample state and goal pairs. From these pairs, we can then compute the loss using Q-learning.

To sample state and goal pairs, the agent starts at a randomly generated state, s_0. The agent then takes t actions, where t is drawn from a random uniform distribution between 0 and a given number T. Each action is sampled according to a random uniform distribution[1]. The last observed state, s_t, is then selected to create a goal, $\mathcal{G}$, by first obtaining $G(s_t)$. Since any $G(s_t)$ that is a superset of a goal, $\mathcal{G}$, also represents a goal, we can simply randomly remove atoms from $G(s_t)$ to create $\mathcal{G}$ such that $\mathcal{G} \subseteq G(s_t)$ and; therefore, s_t is a member of the set of goal states.

After obtaining state and goal pairs, we must select an action to update before computing the loss. While we could select the random uniformly selected action that was taken from state s_0 when generating the goal, we would like to prioritize more promising actions over less promising actions during learning to ensure the estimate of the cost-to-go $h(s) = \min_a q_\phi(s, a, \mathcal{G})$ is not biased towards less promising actions. Therefore, we select actions according to a Boltzmann distribution where each action a is selected with probability according to Equation 5, where $|\mathcal{A}|$ is the size of action space and T is the temperature.

$$\frac{e^{(-q_\phi(s,a,\mathcal{G})/T)}}{\sum_{a'=1}^{|\mathcal{A}|} e^{(-q_\phi(s,a',\mathcal{G})/T)}} \quad (5)$$

After action selection, the loss for the DQN is computed according to Equation 6. The parameters of the target network, ϕ^-, are periodically updated to ϕ. This training procedure is outline in Figure 1.

$$L(\phi) = (g^a(s, s') + \min_{a'} q_{\phi^-}(s', a', \mathcal{G}) - q_\phi(s, a, \mathcal{G}))^2 \quad (6)$$

Specifying Goals with Answer Set Programming

A logic program Π used to specify a goal contains background knowledge, B, which is a set of rules that describes relevant domain knowledge, a goal specification, H, which is a set of rules with the atom `goal` in the head, a headless rule, `:- not goal`, that ensures `goal` must be true in all stable models, and a choice rule with an empty body that contains the set of all possible ground atoms, K, that can be used to represent a set of states. Given a stable model M of Π, the subset of M in K, M_K, represents a set of states. With this, we can define goal states and goal models:

Definition 0.1 (Goal state). Given a program Π, a state, s, is a goal state if and only if $G(s)$ is a subset of some stable model of Π.

Definition 0.2 (Goal model). Given a program Π, a set of ground atoms, M, is a goal model if and only if M is a

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[1]Future work could use intrinsic motivation (Barto et al. 2004) to encourage the exploration of diverse states.

Algorithm 1: Reaching a Specified Goal

Input: Program Π, DQN q_ϕ, start state s_0, number of iterations N
for i in $range(0, N)$ **do**
  Sample stable model M of Π
  while M is not None **do**
    s_g = Q*Search(s_0, M, q_ϕ)
    if s_g is not None and $G(s_g)$ is a subset of some stable model of Π **then**
      return s_g
    end if
    Find M' such that M' is a stable model of Π and $M_K \subset M'_K$
    $M = M'$
  end while
end for
return failure

---

stable model of Π and for every state, s, such that $G(s)$ is a superset of M_K, s is a goal state.

If M is indeed a goal model, then M_K represents a set of goal states. However, it is not the case that all stable models of Π are goal models since, in general, logic programs in ASP can exhibit non-monotonic behavior due to the closed world assumption. That is, a logic program is non-monotonic if some atoms that were previously derived can be retracted by adding new knowledge. To handle this, we will combine sampling and iteratively looking for larger models in an attempt to reduce the number of stable models that are not goal models. We will use the clingo (Gebser et al. 2014, 2022) ASP software package to specify goals.

Reaching Goals with Q* Search

Given a DQN trained to estimate the distance between a state and a goal, where a goal is represented as a set of ground atoms, as well as a specification in the form of a logic program, Π, we can now describe how goals are reached. We first start by finding a stable model M of Π. Since M is not guaranteed to be a goal model, it is possible that the terminal state along some path to M is not a goal state. Therefore, we will use the DQN with Q* search to find one or more paths to M. If none of the terminal states along these paths are goal states, we will refine M by searching for a stable model that contains a strict superset of M_K. This corresponds to finding a new stable model, M', where M'_K represents a subset of the states represented by M_K. To accomplish this, M_K are added to Π as facts and a new stable model, M', is found with the constraint that the size of M'_K must be bigger than M_K. This process is outlined in Algorithm 1.

Similar to previous work (Agostinelli et al. 2019, 2021), to take advantage of the parallelism of graphics processing units (GPUs), we do a batched version of Q* search that removes more multiple nodes from the priority queue at each iteration. In addition, we use weighted Q* search that puts a weight between 0 and 1 on the path cost as, in practice, this leads to shorter solve times and less memory usage.

Experiments

Representation and Training

We investigate goal specification for the Rubik's cube. To specify a set of states, we use a predicate, `at_idx`, of arity 2, that holds when a given color is at a given index. For example `at_idx(red,12)` holds if red is at index 12 on the Rubik's cube. `at_idx` is derived from predicate `at_idx_cbl` of arity 3 that holds when the color on a given cubelet is at a given index. This is a conditional literal that can have zero to as many combinations of cubelets, colors, and indices as possible. Below we show how we define colors, cubelets, what color stickers the cubelets have, and `at_idx`:

```
color(w).  color(y). ...  color(g).
white(w). yellow(y). ... green(g).

center_cbl(w_c). center_cbl(y_c). ...
center_cbl(g_c).
edge_cbl(wo_c). edge_cbl(wg_c). ...
edge_cbl(rb_c).
corner_cbl(wog_c). corner_cbl(wob_c).
... corner_cbl(yrg_c).

cubelet(Cbl) :- center_cbl(Cbl).
cubelet(Cbl) :- edge_cbl(Cbl).
cubelet(Cbl) :- corner_cbl(Cbl).

has_col(w_c, w). has_col(y_c, y).
...has_col(g_c, g).
has_col(wo_c, w). has_col(wo_c, o). ...
has_col(rb_c, b).
has_col(wog_c, w). has_col(wog_c, o).
... has_col(yrg_c, g).

index(0..54).
{ at_idx_cbl(Cbl, Col, I) :
cubelet(Cbl), color(Col), index(I) }.
at_idx(Col, I) :- at_idx_cbl(_, Col,
I).
```

In addition, we define directions (clockwise, counter-clockwise, and opposite), faces, their colors (the same as the center cubelet), and their relation to one another (for example, the blue face is a clockwise turn away from the orange face with respect to the white face). We also describe what it means for a cubelet to have a sticker on a face as well as for a cubelet to be "in place" (all colors matching the center cubelet).

We add constraints to the program to prune stable models that represent impossible states. Some constraints used are shown below:

```
% different stickers from the same
cubelet cannot be on the same face
:- onface(Cbl, Col0, F), onface(Cbl,
Col1, F), dif_col(Col0, Col1).

% cannot have a sticker color from same
cubelet be on more than one face
```

Figure 1: The figure outlines our training procedure as well as the goal specification procedure. Steps involving training are solid black lines, steps involving human goal specification are dashed black lines, and steps common to both are grey lines. The DNN is trained with Q-learning and hindsight experience replay. Pairs of start and goal states are obtained by selecting a random start state, taking t steps where t for each training example is randomly distributed between 0 and T, and converting the state at time step t to a set of logical atoms. A subset of the logical atoms is taken to obtain a goal which represents a set of states. After training, a human then describes a start state and a goal, where the goal is then converted to a set of logical atoms and, subsequently, given to the DNN. Note that, given a method to convert the specification to a set of logical atoms, the specification language is independent of the training procedure.

```
:- onface(Cbl, Col, F0), onface(Cbl,
Col, F1), dif_face(F0, F1).

% cannot say a color of a cubelet is on
a face if it does not have that color
:- onface(Cbl, Col, _), not
has_col(Cbl, Col).

% cannot have two stickers from same
cbl on opposite faces
:- onface(Cbl, Col0, F0), onface(Cbl,
Col1, F1), face_rel(_, F0, F1, op).

% cannot have two different colors at
the same index
:- at_idx(Col0, I), at_idx(Col1, I),
dif_col(Col0, Col1).
```

We also make sure the stable model as the fewest number of atoms as possible to obtain the most general stable models possible using the optimization functionality of clingo:

```
count_at_idx(C) :- #count{V0, V1:
at_idx(V0,V1) }=C.
#minimize {C: count_at_idx(C)}.
```

To represent a stable model to the DQN, we use a vector of length 54 to represent each sticker. We then set colors values of 0 through 5 based on the `at_idx` predicate. Unspecified indices in the vector are set to 6. We then use a one-hot representation of this vector as the input to the DQN. The start state is also represented with a one-hot representation, except every sticker is specified, removing the need for the additional value of 6. The architecture of the DQN we use and the optimization procedure is the same as that described in Agostinelli et al. (2021). However, Agostinelli et al. (2021) only trains the DQN for a predetermined goal state. Our training procedure, described in the Methods Section, samples state and goal pairs for training. To randomly generate start states, for each state, we start from the canonical goal state and randomly take between 100 and 200 actions. The temperature, T, for action selection is set to $1/3$. We train and test using two NVIDIA Tesla V100 32 GB GPUs and 48 2.4 GHz Intel Xeon Platinum CPUs.

Specifying and Reaching Goals

Rubik's Cube To test our method, we draw from Ferenc (n.d.) to come up with goals that combine different Rubik's cube patterns shown in Figure 2. We also test our method with the canonical solved state for the Rubik's cube where all faces have a uniform color. All patterns are described using clingo. Given the background knowledge, many patterns only require a few lines of code, as shown below. Note that the training procedure is not told of these patterns and is not aware that these patterns will be used for testing.

```
% cross
cross(F, CrossCol) :- face(F),
color(CrossCol), #count{Cbl:
```

| (a) Cross | (b) X | (c) Cup | (d) Spot |

Figure 2: Examples of patterns that are combined to create goals.

```
edge_cbl(Cbl), onface(Cbl, CrossCol,
F)} = 4.

% X
x(F, XCol) :- face(F), color(XCol),
#count{Cbl: corner_cbl(Cbl),
onface(Cbl, XCol, F)} = 4.

% cup
cup(F1, F2, CCol) :- dif_face(F1, F2),
face_col(F1, F1Col), dif_col(F1Col,
CCol), edge_cbl(ECbl), onface(ECbl,
_, F2), onface(ECbl, F1Col, F1),
#count{Cbl: edge_or_corner(Cbl),
onface(Cbl, CCol, F1)} = 7.

% spot
spot(F, BCol) :- color(BCol), face(F),
face_col(F, FCol), dif_col(FCol, BCol),
#count{Cbl: onface(Cbl, BCol, F),
edge_or_corner(Cbl)} = 8.

% canonical solved state
face_same(F) :- face_col(F, FCol),
#count{Cbl : onface(Cbl, FCol, F)}=9.
canon_solved :- #count{F :
face_same(F)}=6.
```

| (a) Example 1 | (b) Example 2 |

Figure 3: Goal of having a cross on all 6 faces where the center cubelet and cross are the same color.

| (a) Example 1 | (b) Example 2 |

Figure 5: Goal of having a cup adjacent to a spot.

| (a) Example 1 | (b) Example 2 |

Figure 6: Goal of having two checkerboards on opposite faces with all of the other faces the same.

In addition to the canonical goal, we specify four other goals: (1) all faces have a cross where the cross is the same color as the center piece; (2) the red, green, blue, and orange faces have a cup on them (3) there is a spot adjacent to a cup with the opening of the cup facing the spot; (4) there are two checkerboard patterns (a cross combined with an X) on opposite faces and all other faces have uniform color. Given a logic program, we use clingo (Gebser et al. 2014, 2022) to find stable models. To reach goals, we sample up to 10 stable models of the answer set program that represent the goal and find a path to 100 goal states by randomly generating start states and using batch weighted Q* search to find a path from these start states to a goal state. We use a batch size of 10,000 and a weight of 0.6 when doing batch weighted Q* search. Each randomly generated start state is a given a budget of 50 iterations. If a goal is not found in that time, then a new start state is generated. Visualizations of reached goals for the four non-canonical goals are shown in Figures 3, 4, 5, and 6. A table summarizing the time it takes to find stable models, find 100 goals, as well as the average path cost is shown in Table 1.

Table 1: The time it takes to find stable models for each goal, the time it takes to find 100 goal states, and the average path cost from the start states to the goal states.

	Stable Model Time (secs)	Solve Time (secs)	Path Cost
Canon	0.33	625.62	23.82
Cross6	0.35	218.45	11.50
Cup4	11.17	1622.39	24.44
CupSpot	123.04	291.25	14.7
Checkers	0.44	602.03	24.00

Sokoban We also test our method on the Sokoban domain. This domain presents a unique challenge because many stable models can be found for a specification that are not reachable. This is because, unlike the Rubik's cube, Sokoban is not a reversible environment. This is also because the start state determines ground atoms that will be present in a goal

state. In particular, in the Sokoban domain, the walls cannot be modified; therefore, the specification of a goal must also take this into account. To address the fact that many stable models are not reachable, for a given start state, we find 10 goal models and simultaneously find a path from the start state to all goal models. To address the dependence of the goal on the start state, we add the location of the walls to the specification. We discuss more robust potential solutions to these problems in the Future Work Section.

The given background knowledge includes the dimensions of the grid, the relations of coordinates in terms of up, down, left, and right, what it means for a box to be immovable, what it means for a box to be at the edge of the grid, as well as basic constraints that state that two objects cannot share the same location. The predicates `agent(X,Y)`, `box(X,Y)`, and `wall(X,Y)` hold if an agent, box, or wall is at coordinates (X,Y). We investigate the following goals: (1) all boxes are immovable; (2) all boxes form a larger box; (3) the four boxes occupy the four corners next to the agent. Visualizations of reached goals are shown in Figures 7, 8, and 9. Snippets of code used to specify these goals are shown below:

```
box_stuck(X,Y) :- box(X,Y), manhat(D1),
immovable_edge_d(X,Y,D1), adj(D1,D2),
immovable_edge_d(X,Y,D2).
box_stuck_4 :- #count{X,Y:
box_stuck(X,Y)}=4.

box_of_boxes :- box(X,Y), box(X+1,Y),
box(X,Y-1), box(X+1,Y-1).

agent_box_corners :- agent(X,Y),
box(X+1,Y+1), box(X+1,Y-1),
box(X-1,Y+1), box(X-1,Y-1).
```

(a) Example 1   (b) Example 2

Figure 7: Goal where all boxes are immoveable.

(a) Example 1   (b) Example 2

Figure 8: Goal where all boxes form a larger box.

(a) Example 1   (b) Example 2

Figure 9: Goal where four boxes are at the four corners of the agent.

Discussion

To illustrate the power of specifying a set of states as a goal instead of pre-determined states, we note that the Cross6 goal contains the canonical goal state in the set of states that it represents. However, finding the canonical goal state takes about three times as long and has a path cost that is about twice as long when compared to the Cross6 goal. This indicates that this method has the potential to allow us to discover more efficient plans as well as to discover new knowledge by achieving *unanticipated* goal states that even humans have not yet considered. For example, in a domain such as chemical synthesis, this could allow practitioners to discover new synthesis routes as well as learn more about chemistry by examining the properties of the unanticipated molecules that meet their specifications.

When examining solve time and path cost in Table 1, the Cross6 goal takes the least amount of time and has the shortest average path cost. The CupSpot goal is also comparable along these same metrics. This could be because Cross6 and CupSpot need to consider fewer stickers than other goals. However, the Cup4 goal takes the longest to reach out of all the goals even though it also needs to consider fewer stickers than both the canonical goal and the Checkers goal. One indication of the cause of this is that Q* search frequently went over its budget of 50 iterations for the Cup4 goal. This could be because some of the stable models actually represent sets of states that are not reachable. We discuss ways to overcome this in the Future Work Section.

When examining the time it takes to find stable models in Table 1, the CupSpot goal takes the longest out of all the goals. This could be due to having many constraints to consider when finding the stable models. However, dealing with the constraints when solving for the stable models could lead to faster solve times as fewer stable models will represent unreachable goals. It could also be the case that certain constraints could be expressed in a more concise manner.

Related Work

Planning languages such as the Planning Domain Definition Language (PDDL) specify goals using formal logic. Furthermore, a planning problem can be described to a wide variety of planners and heuristics can be computed to guide the planning process. However, when using heuristic functions represented by DNNs, there is no formal way to represent what the goal of the planning problem is. Our approach of

obtaining stable models from logic programs could be extended to descriptions of goals in PDDL. Furthermore, in the Future Work Section, we discuss ways goals can be represented with logic, itself, without having to solve for stable models.

Learning from partial interpretations (Fensel et al. 1995; De Raedt 1997) is a setting in inductive logic programming (Muggleton 1991; De Raedt 2008; Cropper and Dumančić 2022) where the training examples are not fully specified. This setting has also been applied to learning answer set programs from partial stable models (Law, Russo, and Broda 2014). This work has parallels with our work, except, instead of learning an answer set program as in Law, Russo, and Broda (2014), the specification is given in the form of an answer set program. Furthermore, instead of being given partial stable models as examples as in Law, Russo, and Broda (2014), the goal specification produces partial stable models that are then used by the DNN to reach the goal.

Research on training deep neural networks to generalize over both states and goals has mainly focused on goals that are represented by a single state. In reinforcement learning, Universal Value Function Approximators (Schaul et al. 2015) were proposed to learn a value function with an additional input of a goal state. Hindsight Experience Replay (Andrychowicz et al. 2017) built on this approach to learn from failures by using states observed during an episode as goal states, even if they were not the intended goal state. This approach has enabled learning in sparse reward environments, such as those involving object manipulation, and has shown to generalize to goal states not seen during training. After training, one can then specify what the goal state is, provided the practitioner has the ability to fully specify a goal state. However, this approach becomes impractical in cases where there are a diverse set of acceptable goal states that the agent could possibly reach or where only high-level qualities of a goal are known, but the low-level details are not.

Future Work

In this work, we investigated the Rubik's cube, which is a domain in which every state is reachable from every other state. However, in domains such as Sokoban, this is not the case. As a result, not all goals will be reachable from every possible start state. In these cases, the training process could be augmented with mining for "negative" goals (Tian et al. 2021) that cannot be reached. The DQN should then give a very high cost-to-go when a goal is not reachable from a given start state. We can then sample start and goal state pairs that are below some threshold. This sampling procedure could also be imbued with a learned heuristic to guide the ASP solver towards reachable stable models.

In addition to unreachable goals, one could specify goals that only represent impossible states or have some stable models that only represent impossible states. For example, one could specify a Rubik's cube state with two adjacent faces that are entirely white. This is impossible for multiple reasons: 1) There cannot be more than one center cubelet of the same color; 2) Since the faces are adjacent, there would

have to be cubelets with two white stickers, which is impossible because no cubelet has two stickers of the same color; 3) There would be more than nine stickers of the same color. While these constraints could be manually added to the program, we also want to strive for a system that *discovers* new constraints that even humans have not yet discovered. Given a specification, one could use a generality relationship, such as entailment or theta subsumption (Plotkin 1972), to find the most general specification that represents impossible states and add this to the background knowledge as a constraint. Such an approach would build on literature from inductive logic programming.

Our approach of using ground atoms to represent a goal comes with the advantage of being agnostic to the specification language as long as it can produce a set of ground atoms. Therefore, in the case of using ASP as the specification language, changes can be made to the predicates or even the ASP software used without having to re-train the DNN. However, this comes with the computational cost of having to solve for a set of ground atoms given a specification. One could instead train the heuristic function to estimate the distance between a state and a lifted specification that either implicitly or explicitly contains variables. This could be done for any kind of specification, such as first-order logic or even natural language, given the ability to go from a state to a specification representing a set of states of which that state is a member. For example, the specification given to the heuristic function could be a sentence in first-order logic describing the goal. One could obtain training examples by obtaining a goal state and then searching for a first-order logic sentence that represents a set of states of which that goal state is a member. The downside to this approach is that any change in the vocabulary of the specification may require re-training of the DNN.

Conclusion

We have formalized a method for specifying goals to heuristic functions represented by DNNs using a specification language that is accessible to humans. This goal specification is done without any need to re-train the DNN for that particular goal. Furthermore, the language used to specify goals only needs to be able to be translated into a set of ground atoms, which makes the DNN agnostic to the specification language. Using answer set programming, one can easily specify properties that a goal state should have without having to specify any goal state in particular. Therefore, this method has the ability to discover novel goal states and; therefore, facilitate the discovery of new knowledge.

References

Agostinelli, F.; McAleer, S.; Shmakov, A.; and Baldi, P. 2019. Solving the Rubik's cube with deep reinforcement learning and search. *Nature Machine Intelligence*, 1(8): 356–363.

Agostinelli, F.; Shmakov, A.; McAleer, S.; Fox, R.; and Baldi, P. 2021. A* search without expansions: Learning heuristic functions with deep Q-networks. *arXiv preprint arXiv:2102.04518*.

Andrychowicz, M.; Wolski, F.; Ray, A.; Schneider, J.; Fong, R.; Welinder, P.; McGrew, B.; Tobin, J.; Abbeel, O. P.; and Zaremba, W. 2017. Hindsight experience replay. In *Advances in Neural Information Processing Systems*, 5048–5058.

Barto, A. G.; Singh, S.; Chentanez, N.; et al. 2004. Intrinsically motivated learning of hierarchical collections of skills. In *Proceedings of the 3rd International Conference on Development and Learning*, volume 112, 19. Citeseer.

Bertsekas, D. P.; and Tsitsiklis, J. N. 1996. *Neuro-dynamic programming*. Athena Scientific. ISBN 1-886529-10-8.

Brewka, G.; Eiter, T.; and Truszczyński, M. 2011. Answer set programming at a glance. *Communications of the ACM*, 54(12): 92–103.

Chen, B.; Li, C.; Dai, H.; and Song, L. 2020. Retro*: learning retrosynthetic planning with neural guided A* search. In *International Conference on Machine Learning*, 1608–1616. PMLR.

Cropper, A.; and Dumančić, S. 2022. Inductive logic programming at 30: a new introduction. *Journal of Artificial Intelligence Research*, 74: 765–850.

De Raedt, L. 1997. Logical settings for concept-learning. *Artificial Intelligence*, 95(1): 187–201.

De Raedt, L. 2008. *Logical and relational learning*. Springer Science & Business Media.

Dor, D.; and Zwick, U. 1999. SOKOBAN and other motion planning problems. *Computational Geometry*, 13(4): 215–228.

Fensel, D.; Zickwolff, M.; Wiese, M.; et al. 1995. Are substitutions the better examples? Learning complete sets of clauses with Frog. In *Proceedings of the 5th International Workshop on Inductive Logic Programming*, 453–474. Citeseer.

Ferenc, D. n.d. Pretty Rubik´s Cube patterns with algorithms. Accessed March 28, 2023. https://ruwix.com/the-rubiks-cube/rubiks-cube-patterns-algorithms/.

Gebser, M.; Kaminski, R.; Kaufmann, B.; and Schaub, T. 2014. Clingo= ASP+ control: Preliminary report. *arXiv preprint arXiv:1405.3694*.

Gebser, M.; Kaminski, R.; Kaufmann, B.; and Schaub, T. 2022. *Answer set solving in practice*. Springer Nature.

Gelfond, M.; and Lifschitz, V. 1988. The stable model semantics for logic programming. In *ICLP/SLP*, volume 88, 1070–1080. Cambridge, MA.

Hart, P. E.; Nilsson, N. J.; and Raphael, B. 1968. A formal basis for the heuristic determination of minimum cost paths. *IEEE transactions on Systems Science and Cybernetics*, 4(2): 100–107.

Kocsis, L.; and Szepesvári, C. 2006. Bandit based montecarlo planning. In *European conference on machine learning*, 282–293. Springer.

Law, M.; Russo, A.; and Broda, K. 2014. Inductive learning of answer set programs. In *Logics in Artificial Intelligence: 14th European Conference, JELIA 2014, Funchal, Madeira, Portugal, September 24-26, 2014. Proceedings 14*, 311–325. Springer.

Marek, V. W.; and Truszczyński, M. 1999. Stable models and an alternative logic programming paradigm. *The Logic Programming Paradigm: a 25-Year Perspective*, 375–398.

McAleer, S.; Agostinelli, F.; Shmakov, A.; and Baldi, P. 2019. Solving the Rubik's Cube with Approximate Policy Iteration. In *International Conference on Learning Representations*.

Mnih, V.; Kavukcuoglu, K.; Silver, D.; Rusu, A. A.; Veness, J.; Bellemare, M. G.; Graves, A.; Riedmiller, M.; Fidjeland, A. K.; Ostrovski, G.; et al. 2015. Human-level control through deep reinforcement learning. *Nature*, 518(7540): 529–533.

Muggleton, S. 1991. Inductive logic programming. *New generation computing*, 8: 295–318.

Plotkin, G. 1972. Automatic methods of inductive inference.

Pohl, I. 1970. Heuristic search viewed as path finding in a graph. *Artificial intelligence*, 1(3-4): 193–204.

Puterman, M. L.; and Shin, M. C. 1978. Modified policy iteration algorithms for discounted Markov decision problems. *Management Science*, 24(11): 1127–1137.

Schaul, T.; Horgan, D.; Gregor, K.; and Silver, D. 2015. Universal value function approximators. In *International Conference on Machine Learning*, 1312–1320.

Schmidhuber, J. 2015. Deep learning in neural networks: An overview. *Neural networks*, 61: 85–117.

Sutton, R. S.; and Barto, A. G. 2018. *Reinforcement learning: An introduction*. MIT press.

Tian, S.; Nair, S.; Ebert, F.; Dasari, S.; Eysenbach, B.; Finn, C.; and Levine, S. 2021. Model-Based Visual Planning with Self-Supervised Functional Distances. In *International Conference on Learning Representations*.

Van Emden, M. H.; and Kowalski, R. A. 1976. The semantics of predicate logic as a programming language. *Journal of the ACM (JACM)*, 23(4): 733–742.

Watkins, C. J.; and Dayan, P. 1992. Q-learning. *Machine learning*, 8(3-4): 279–292.

Zhang, Y.-H.; Zheng, P.-L.; Zhang, Y.; and Deng, D.-L. 2020. Topological Quantum Compiling with Reinforcement Learning. *Physical Review Letters*, 125(17): 170501.