Deep Learning, Reinforcement Learning, and Heuristic Search

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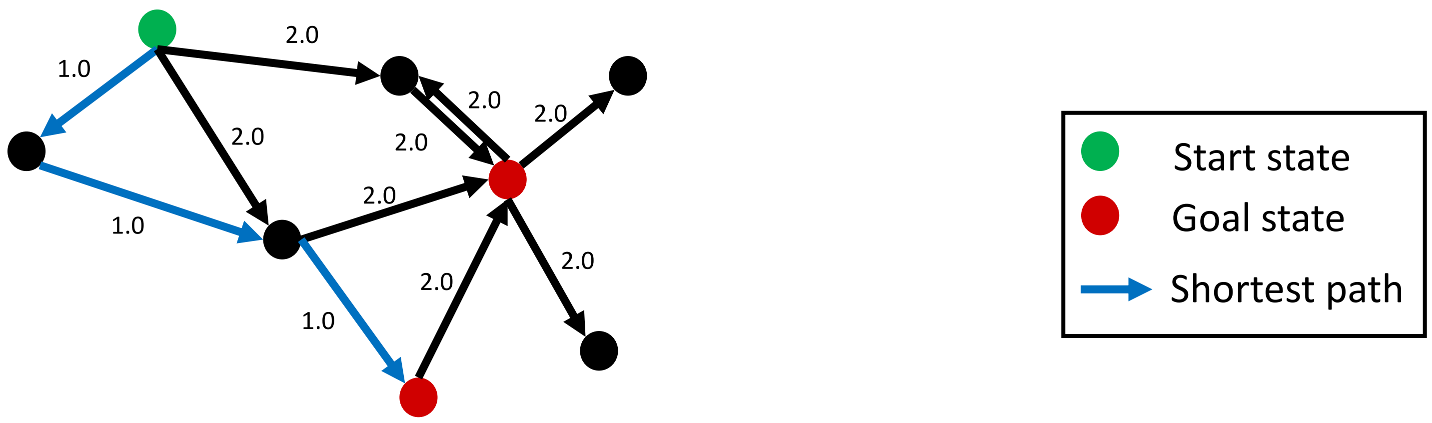
Outline

- Background
- Approximate value iteration and batch weighted A* search
- Approximate Q-learning and batch weighted Q* seaerch
- Generalization
  - Generalizing over goals
  - Generalizing over domains
  - Generalizing to domains with unknown transition functions
- Applications

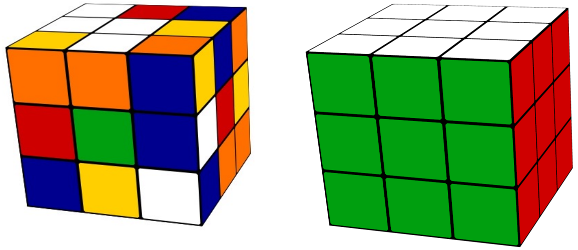
Pathfinding

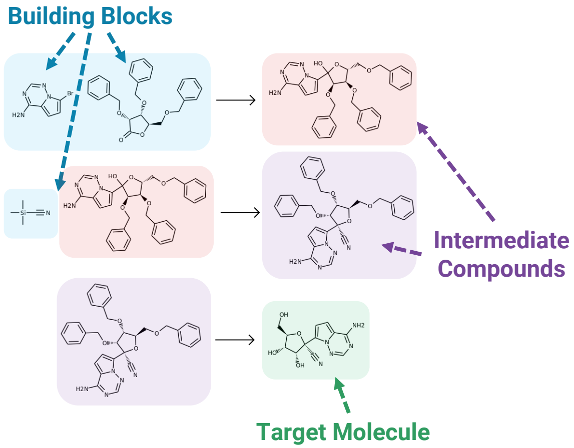
- The objective of pathfinding is to find a sequence of actions that forms a path between a given start state and a given goal
  - A goal is a set of states
  - Preference for minimum cost paths
- A pathfinding problem can be represented as a weighted directed graph where nodes represent states, edges represent actions that transition between states, and edge weights represent transition costs
  - The cost of a path is the sum of transition costs

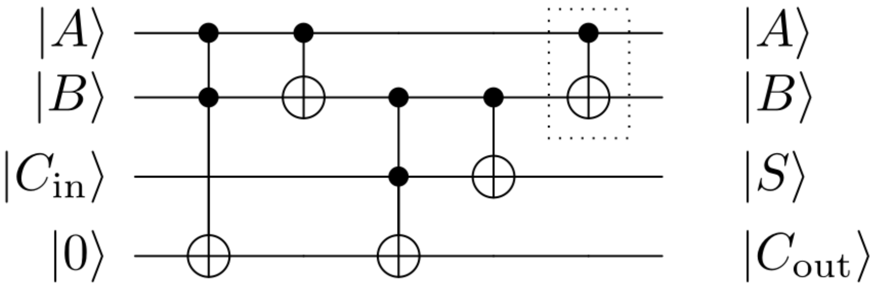


Pathfinding Domains

- Pathfinding problems can be found throughout mathematics, computing, and the natural sciences
  - Puzzle solving, chemical synthesis, quantum circuit synthesis, theorem proving, program synthesis, robotics







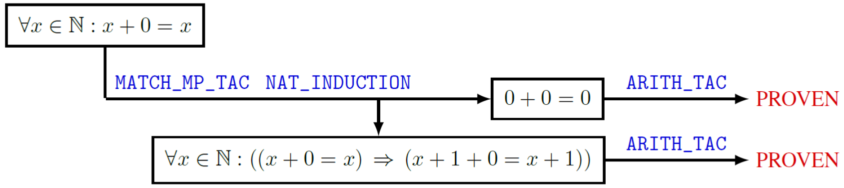
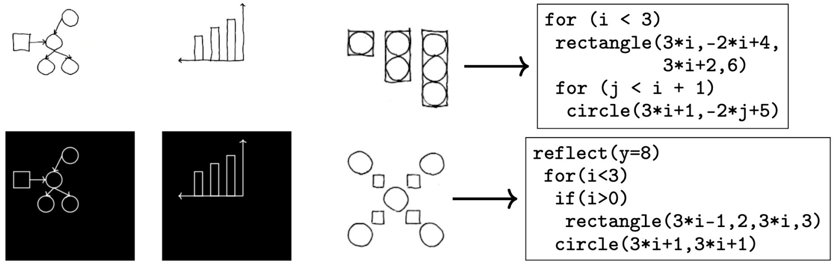


Figure 1: Formally proving $\forall x \in \mathbb{N} : x + 0 = x$.



Pathfinding Domain Definition

- The entire state space graph cannot be given to a pathfinding problem solver because the number of states in a pathfinding problem can be very large.
  - Rubik's cube: $\sim 10^{19}$
  - 48-puzzle: $\sim 10^{62}$
  - Organic chemistry: $\sim 10^{60}$ (exact number unknown)
- Assumptions on what is given
  - Action space
  - State transition function
  - Transition cost function
  - Goal test function
  - Goal specification language
- **Objective: Create a domain-independent algorithm that learns domain-specific heuristics**

Scope of Problems

- What pathfinding problems can be solved with deep reinforcement learning and heuristic search?
  - Sufficient data
  - Sufficient expressivity of deep neural network (DNN)
- Deep learning is data hungry
- Defining models and generating data is easy for many important and difficult problems
  - Theorem proving
  - Program synthesis
  - Quantum algorithm compilation
- Also possible for other environments
  - Chemical synthesis
  - Robotics (sim2real)
- What if we don't have enough data or time?
  - Foundation models
  - Generative model of domains?

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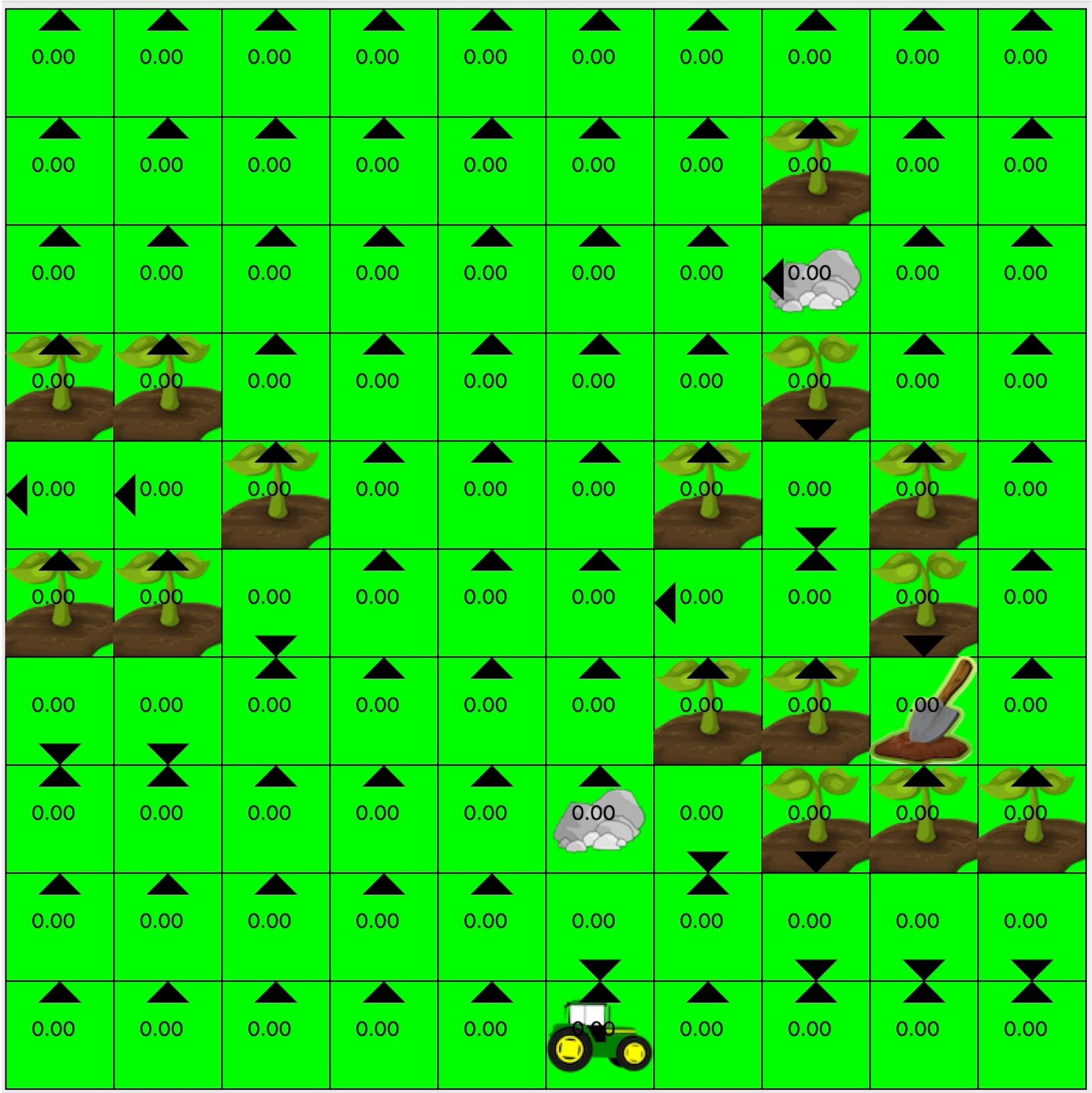
Value Iteration

- Value iteration is a dynamic programming algorithm and is a foundational algorithm in reinforcement learning
- In the context of pathfinding, value iteration is an algorithm for computing the cost-to-go of finding a shortest path for each state in the state space
- Tabular value iteration loops over all states and applies the following update until convergence (h stops changing)
  - $h(s) = \min_a (c^a(s) + h(T(s, a)))$
  - Guaranteed to converge to h^* in the tabular setting
- s: state
- a: action
- T: state transition function
- c^a: transition cost function

Value Iteration: Visualization

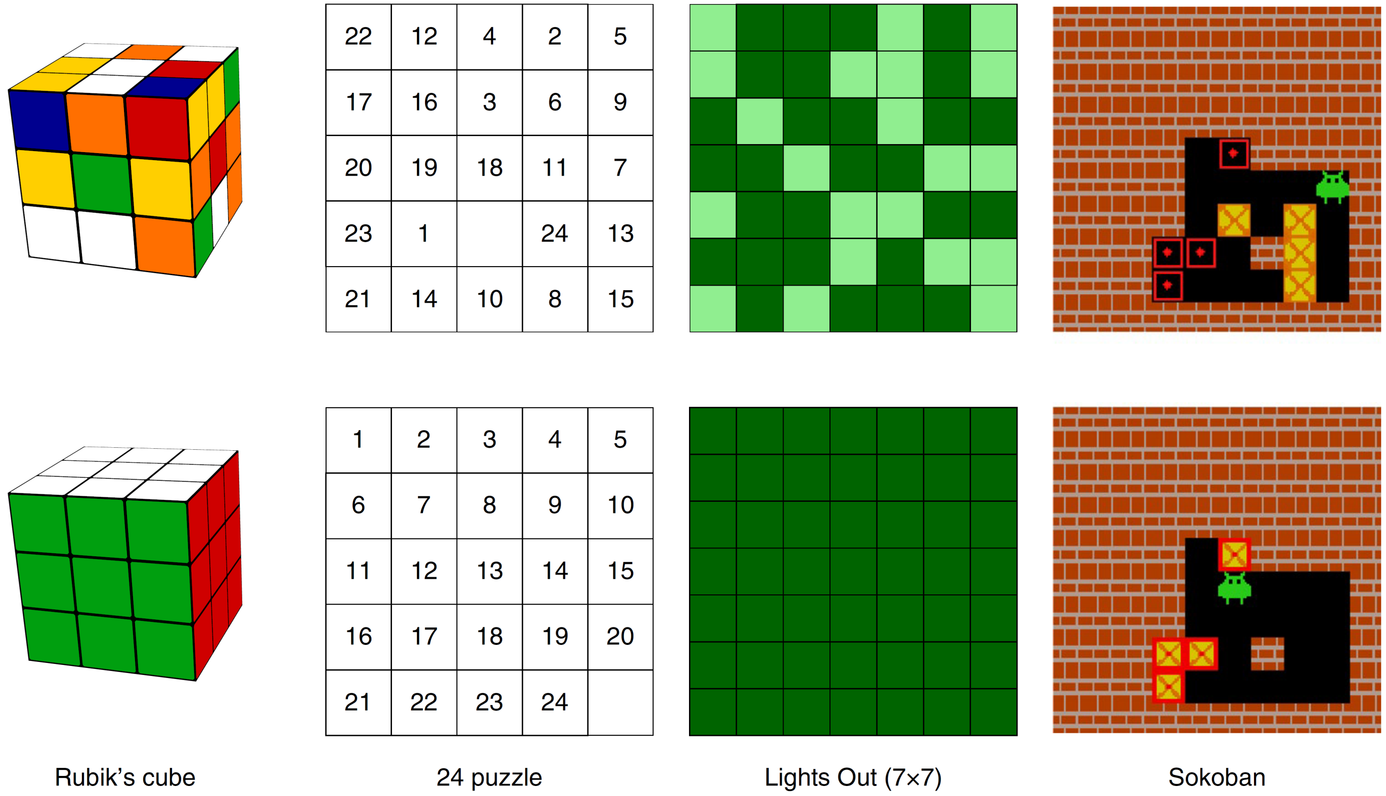
- Actions: up, down, left, right
- Transition costs
  - 1 if square is blank
  - 10 if square has a rock
  - 50 if square has a plant
- Goal: shovel
- Updates propagate outwards from the goal
  - $h(s) = \min_a (c^a(s) + h(T(s,a)))$



Approximate Value Iteration

- As the state space grows, tabular value iteration becomes infeasible
- Approximate value iteration uses an approximation architecture to approximate the value iteration update
- When using a deep neural network as the approximation architecture, we refer to this as deep approximate value iteration (DAVI)
- The update is approximated using the following loss function
  - $L(\theta) = \left(\min_a (c^a(s) + h_{\theta^-}(T(s,a))) - h_\theta(s)\right)^2$
  - Target is set to zero if s is a terminal state
- s: state
- a: action
- T: state transition function
- c^a: transition cost function
- θ: parameters
- θ^-: parameters for target network
  - Is periodically updated to θ throughout training

Application to Puzzle Solving

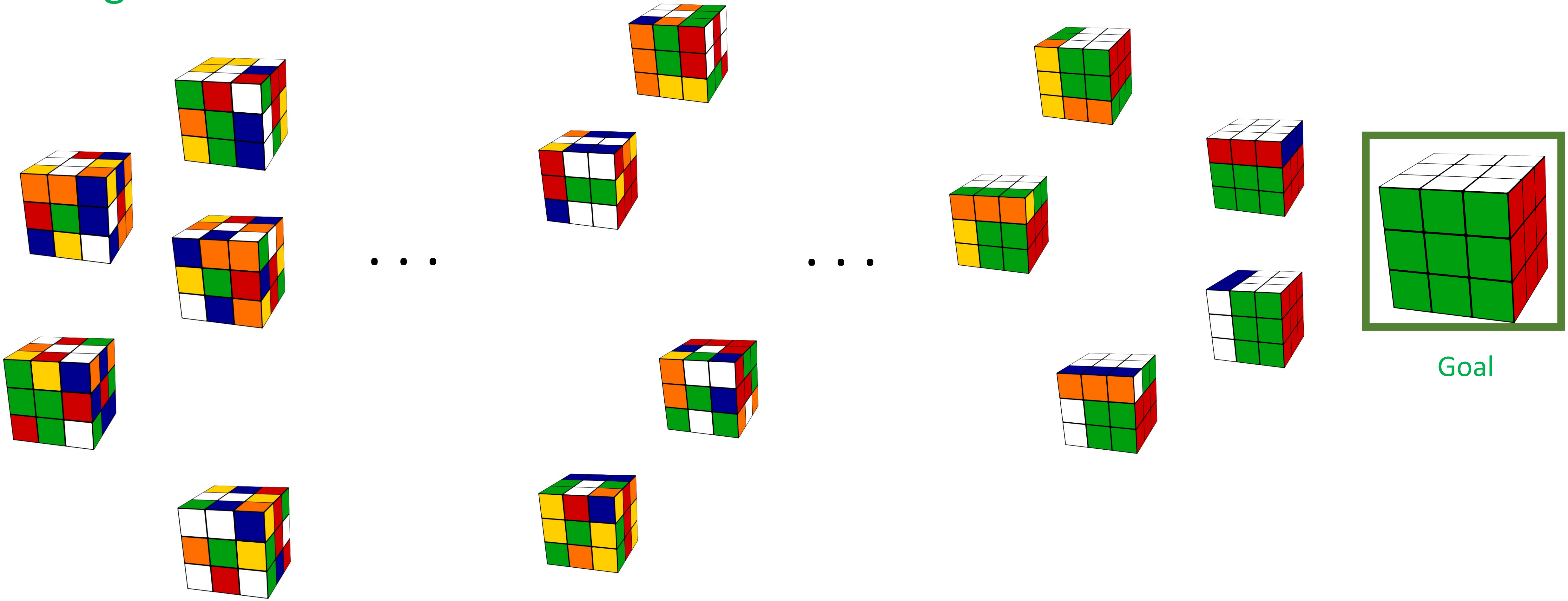


1. Rubik's Cube
2. 15-puzzle
3. 24-puzzle
4. 35-puzzle
5. 48-puzzle
6. Lights Out
7. Sokoban

Largest state space is 3.0×10^{62} (48-puzzle)

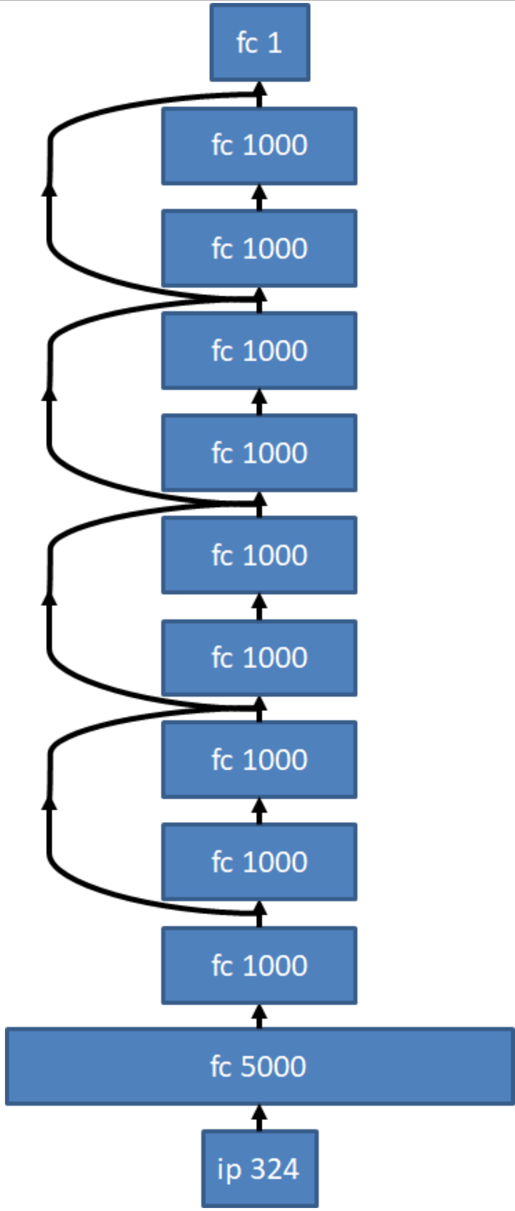
Generating States

- Prioritized sweeping: Generate training data by taking moves in reverse from the goal



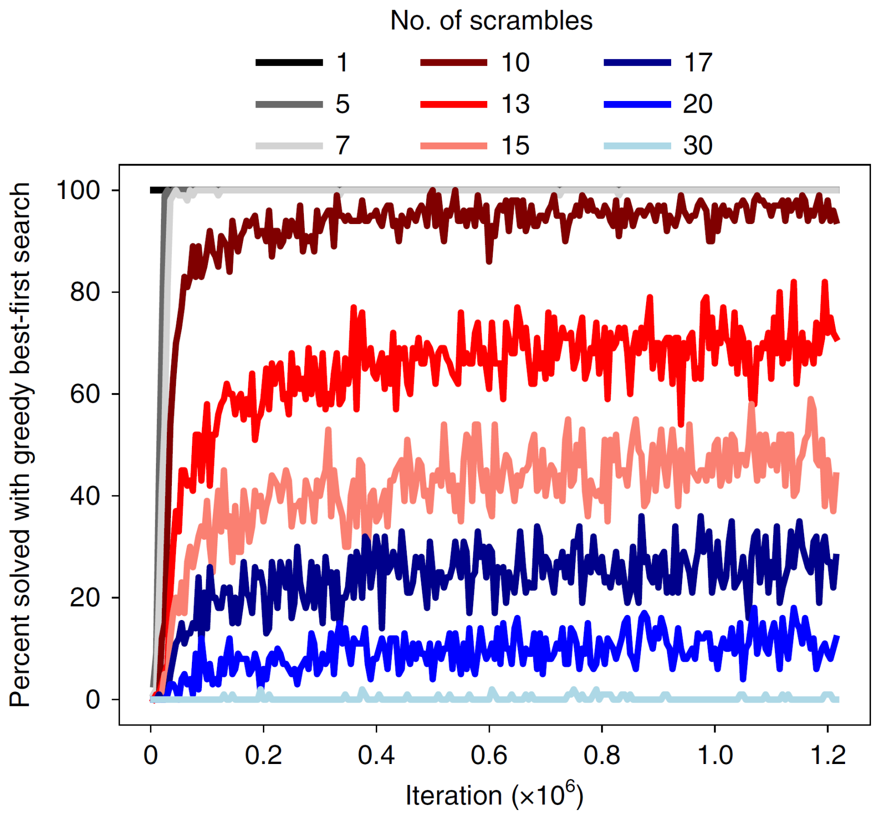
Training

- Deep neural network
  - Input layer -> Two fully connected layers -> Four residual blocks -> Linear output layer
  - Same type of architecture used for all puzzles
    - 24-puzzle has two more residual blocks
- Training
  - Batch size of 5,000
  - ~1,000,000 training iterations
  - Parameters for target network updated when loss goes below some target threshold
    - Future work updates based on greedy policy performance



Greedy Policy Performance

- Behave greedily with respect to the heuristic function
- $\pi(s) = \underset{a}{\operatorname{argmin}}(c^a(s) + h_\theta(T(s,a)))$
- Does not solve all states
- Supervised learning yields similar performance
- We need heuristic search!



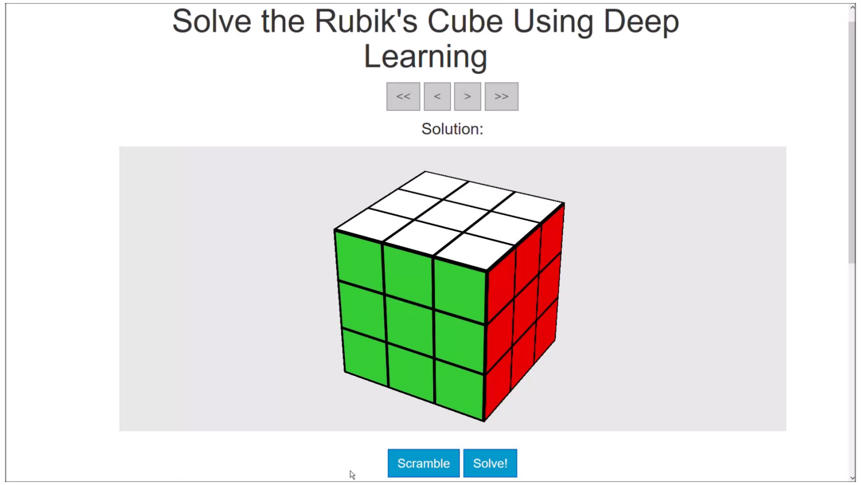
Batch Weighted A* Search

- To take advantage of parallelism provided by GPUs, we can expand multiple nodes at once
- Guaranteed to be bounded suboptimal if
  - The heuristic function is admissible
  - If we terminate when the lower bound >= the upper bound

Agostinelli, Forest, et al. "Obtaining approximately admissible heuristic functions through deep reinforcement learning and A* search." *ICAPS PRL Workshop*. 2021.
Li, Tianhua, et al. "Optimal search with neural networks: Challenges and approaches." *Proceedings of the International Symposium on Combinatorial Search*. Vol. 15. No. 1. 2022.

DeepCubeA: Results

- When applied to seven different puzzles, it was able to solve all test instances and found a shortest path in the majority of verifiable cases
- http://deepcube.igb.uci.edu/



Puzzle	Solution Length	Percent Optimal	Time (seconds)
Rubik's Cube	21.50	60.3%	24.22
15-puzzle	52.03	99.4%	10.28
24-puzzle	89.49	96.98%	19.33
35-puzzle	124.64	N/A	28.45
48-puzzle	253.35	N/A	74.46
Lights Out	24.26	100.0%	3.27
Sokoban	32.88	N/A	2.35

Agostinelli, Forest, et al. "Solving the Rubik's cube with deep reinforcement learning and search." *Nature Machine Intelligence* 1.8 (2019): 356-363.

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Q-learning

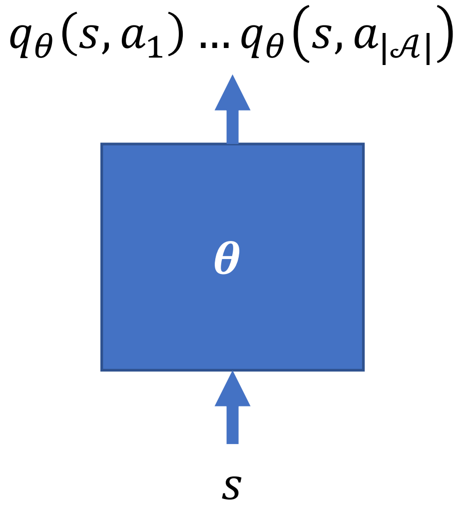
- In the context of pathfinding, Q-learning is used to compute the cost of a path when in a given state, taking a given action, and taking a shortest path from the next state
  - $Q(s,a) = Q(s,a) = c^a(s) + h(T(s,a))$
  - $h(s) = \min_a Q(s,a)$
- Tabular Q-learning applies the following update to each state seen in an episode
  - $Q(s,a) = Q(s,a) + \alpha[c^a(s) + \min_{a'} Q(T(s,a),a') - Q(s,a)]$
  - α is the learning rate
  - Guaranteed to converge to q^* in the tabular setting if certain conditions are met

Approximate Q-learning

- Q-learning loss
  - $L(\theta) = \left(c^a(s) + \min_{a'} q_{\theta^-}(T(s,a),a') - q_\theta(s,a)\right)^2$
- For each training iteration, an action to update is sampled randomly
- Since it is possible most actions are not part of a shortest path, this could bias the estimator to overestimate the cost-to-go
- Therefore, we sample actions according to a Boltzmann distribution
  - $\pi(a|s) = \frac{e^{(-\frac{h_\theta(s,a)}{T})}}{\sum_{a'=1}^{|\mathcal{A}|} e^{(-\frac{h_\theta(s,a')}{T})}}$

From A* Search to Q* Search

- A* search: the number of nodes generated and number of heuristic function applications during each iteration of search grows linearly with the size of the action space
- Deep Q-networks (DQNs) can compute the estimated cost of taking all actions with a single forward pass
- Q* search: the number of nodes generated and number of heuristic function applications is independent of the size of the action space



Batch Weighted Q* Search

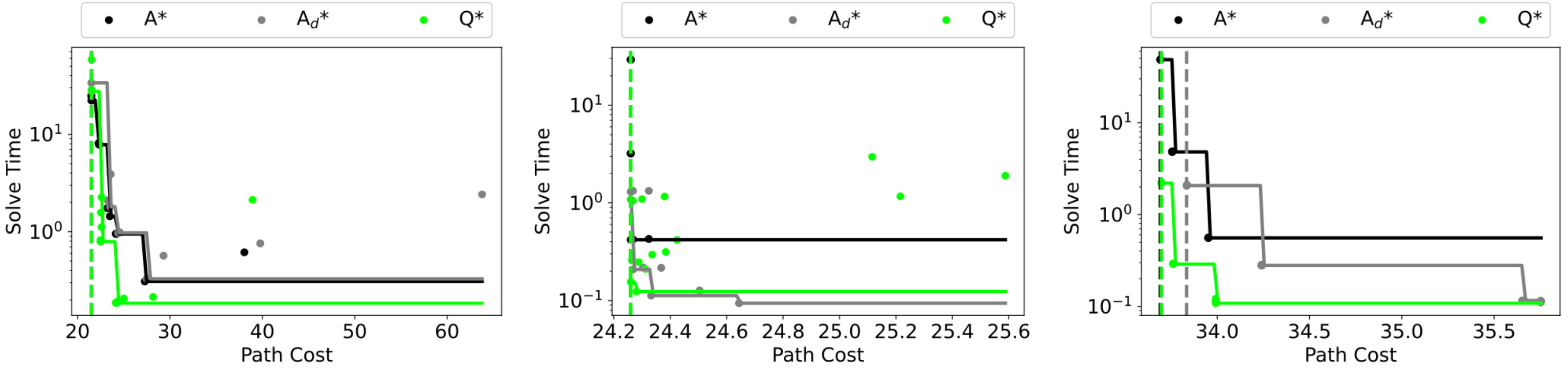
- Given a node, compute the transition cost and heuristic value for all child nodes with a single pass through a DQN
- Store tuples of nodes and actions in OPEN
  - Only part that grows linearly with action space
- Apply popped actions to popped nodes
- Batch weighted version can also be used
- Guaranteed to be bounded suboptimal if
  - The heuristic function never overestimates
    - $c^a(s) + \min_{a'} q^*(T(s,a), a')$
  - If we terminate when the lower bound >= the upper bound

Experiments

- Domains: Rubik's cube, Lights Out, 35-pancake puzzle
- Case study: Adding combinations of actions to the Rubik's cube: 12 actions, 156 actions, 1884 actions
- Comparisons
  - A* search
  - Deferred heuristic evaluation: assign heuristic of parent to children
- Did batch weighted search for all search methods
  - Weight in {0.0, 0.2, 0.4, 0.6, 0.8, 1.0}
  - Batch size in {100, 1000, 10000}

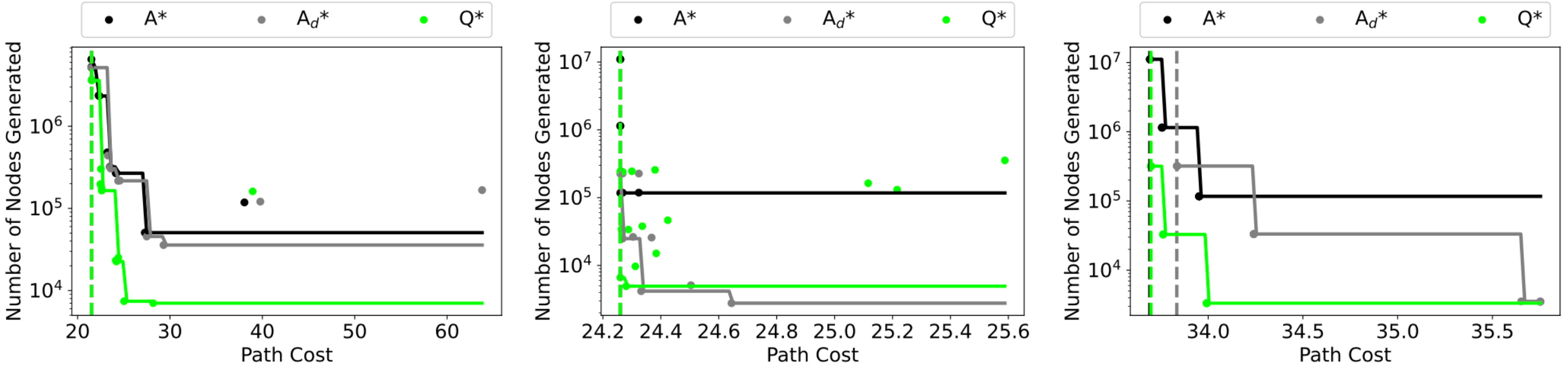
Results

- Each point is a different search parameter setting
- Dashed line: Best path cost
- Solid line: Best of all parameter settings at that path cost
- Q* search often outperforms A* and deferred A* by orders of magnitude
- Best average path cost is either the same or slightly longer



(a) RC (b) Lights Out (c) 35-pancake

Figure 1: Relationship between the average path cost and the average time to find a solution.



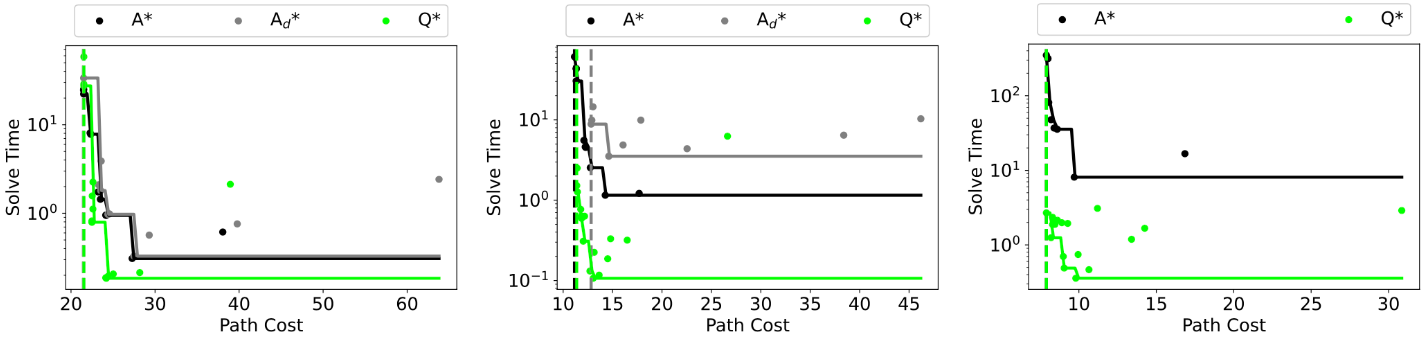
(a) RC(12) (b) Lights Out (c) 35-Pancake

Figure 2: Relationship between the average path cost and the average node generations.

Agostinelli, Forest, et al. "Q* Search: Heuristic Search with Deep Q-Networks." *ICAPS PRL Workshop 2024*

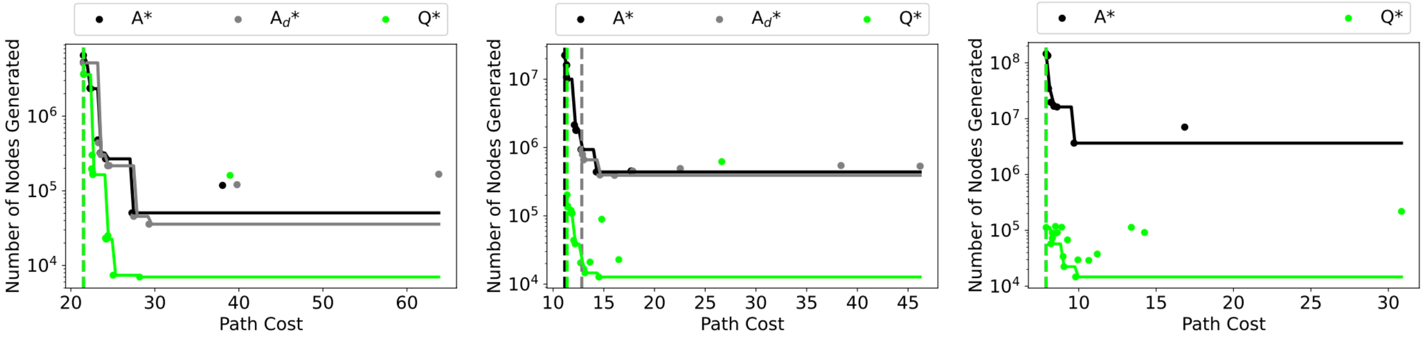
Results

- With 157 times more actions, Q* is only 3.7 times slower and uses 2.3 times more memory



(a) RC(12) (b) RC(156) (c) RC(1884)

Figure 3: Action space size ablation study on Rubik's cube: average path cost vs average time to find a solution.



(a) RC(12) (b) RC(156) (c) RC(1884)

Figure 4: Action space size ablation study on Rubik's cube: average path cost vs average node generations.

Puzzle	Actions	Method	Time	Nodes Gen
RC(156)	x13	A*	3.5(1.6)	8.7(2.2)
		Q*	**0.9(0.7)**	**1.4(1.3)**
RC(1884)	x157	A*	37.0(6.5)	62.7(5.2)
		Q*	**3.7(4.0)**	**2.3(3.6)**

Agostinelli, Forest, et al. "Q* Search: Heuristic Search with Deep Q-Networks." *ICAPS PRL Workshop 2024*

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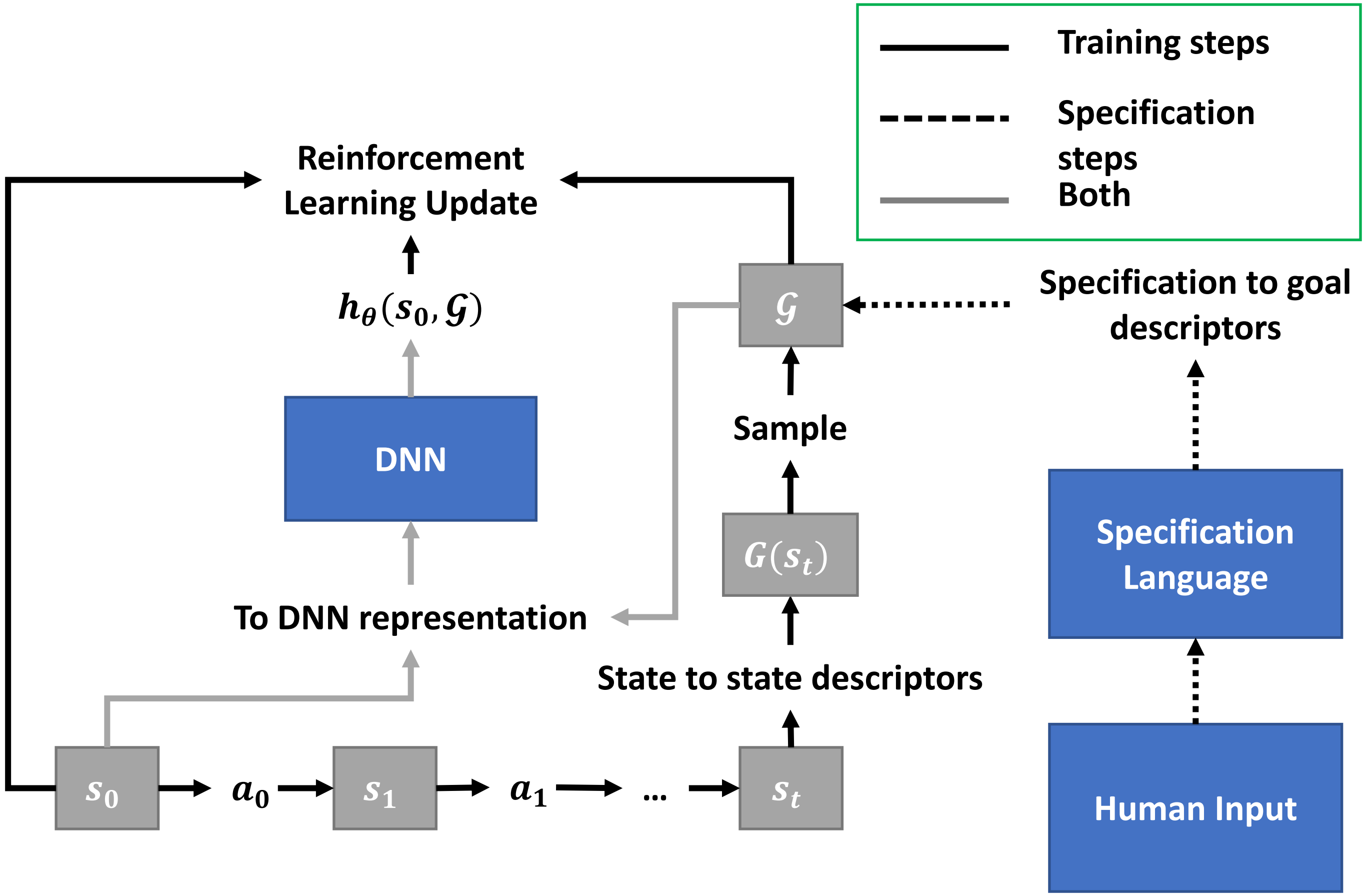
Rojina Panta

Vedant Khandelwal

Generalizing Over Goals: Overview

- In the previous work, the goal is predetermined
- We build on hindsight experience replay to generalize over sets of goal states
- In our work
  - State descriptors: assignments of values to variables
  - Specification language: Answer set programming (ASP)
  - ASP will be used to describe goals at a high-level using formal logic and an answer set solver will be used to find assignments that represent a subset of the goal

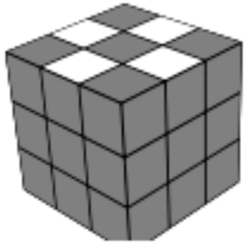


State Representation

- In a given pathfinding domain, there are V variables
  - A variable, x_i, can be assigned a single value from its (variable) domain, $D(x_i)$
- An assignment is an assignment is a set of assignments of values to variables $\{x_i = v_i\}$
  - All $v_i \in D(v_i)$
  - If x_i is not in the assignment then it is unassigned
- An assignment is a complete assignment iff all variables have been assigned values
- A state is a complete assignment
- For example, for the Rubik's cube, variables are stickers and values are their colors

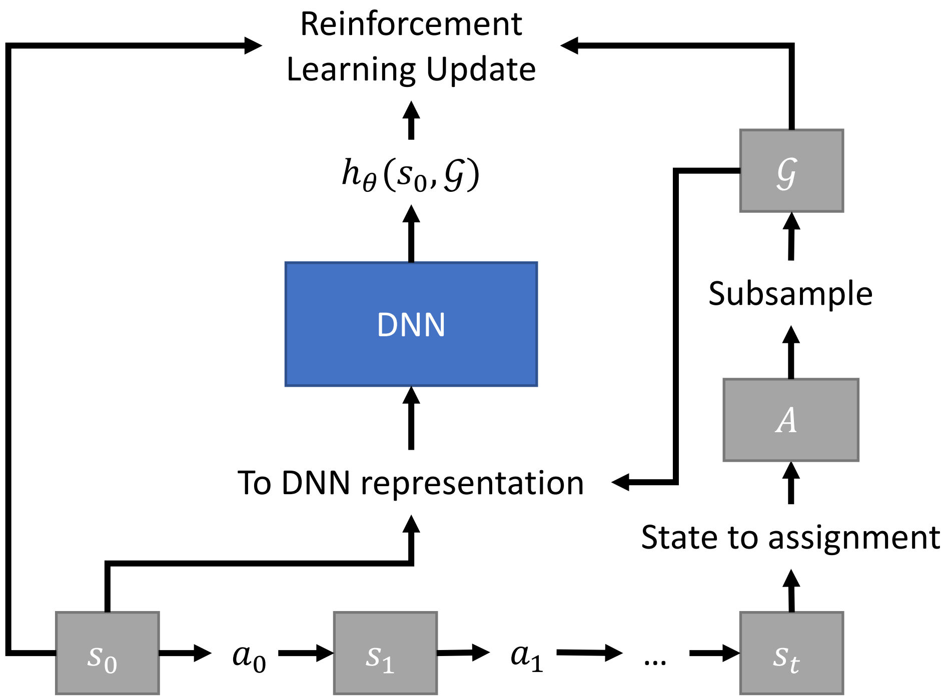
Goal Representation

- An assignment is a partial assignment iff at least one variable has not been assigned a value
- A goal is a complete or partial assignment
- An assignment, A, represents a set of states, $\mathcal{S}_A$
  - A complete assignment always represents a set of states of size 1
- A state, s, is in $\mathcal{S}_A$ iff $A \subseteq s$
  - In other words, all assignments in A are present in s
  - An empty assignment represents the set of all possible states
- For example, a visualization of an assignment for the "white cross" pattern for the Rubik's cube and a state that is in the set of states represented by this assignment



Training

- Generate a start state
- Take a random walk whose length is somewhere between 0 and T
  - Future work could use artificial curiosity
- Convert the end state to its representation as an assignment
- Subsample to obtain a goal
- Convert this representation into one suitable for the DNN
  - One-hot representation
  - Graph
  - Etc.
- RL Update
  - $L(\theta) = \left(\min_{a}(c^{a}(s) + h_{\theta^-}(T(s,a)), \mathcal{G}) - h_{\theta}(s, \mathcal{G})\right)^2$



Experiments

- ASP will be used to find assignments; therefore, we compare our method (DeepCubeA$_g$) to other methods capable of finding paths to goals that can be represented as complete or partial assignments
- 500-1,000 test start and goal pairs
- 200 second time limit to solve test states
- **DeepCubeA**
  - Predefined goal
- **Fast Downward Planner**
  - Can automatically construct heuristics given a formal definition of the domain (including the transition function) in the planning domain definition language (PDDL)
  - Goal count heuristic, fast forward heuristic, causal graph heuristic
  - A* search
- **PDBs**
  - Divides into subproblems and enumerates all possible combinations of the subproblem to create heuristic
  - Predefined goal
  - IDA* search

Performance

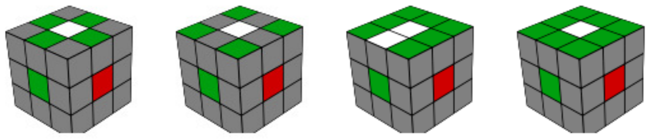
- Canon: Canonical goal states
- Rand: Random assignment selected as goal
  - Can be as small as the empty assignment
  - Methods that require a pre-definied goal cannot be applied to this scenario without considerable overhead
- PDBs+: Also includes group theory knowledge
- DeepCubeA$_g$ consistently outperforms fastdownard in terms of percentage of states solved

Puzzle	Solver	Path Cost	% Solved	% Opt	Nodes	Secs	Nodes/Sec
RC (Canon)	PDBs$^+$	**20.67**	**100.00%**	**100.0%**	**2.05E+06**	**2.20**	**1.79E+06**
	DeepCubeA	21.50	**100.00%**	60.3%	6.62E+06	24.22	2.90E+05
	DeepCubeA$_g$	22.03	**100.00%**	35.00%	2.44E+06	41.99	5.67E+04
	FastDown (GC)	-	0.00%	0.0%	-	-	-
	FastDown (FF)	-	0.00%	0.0%	-	-	-
	FastDown (CG)	-	0.00%	0.0%	-	-	-
RC (Rand)	DeepCubeA$_g$	15.22	**99.40%**	-	1.91E+06	32.24	5.19E+04
	FastDown (GC)	7.18	32.80%	-	2.67E+06	13.79	1.41E+05
	FastDown (FF)	6.49	31.20%	-	4.87E+05	13.83	2.93E+04
	FastDown (CG)	7.85	33.80%	-	1.12E+06	11.62	5.81E+04
15-P (Canon)	PDBs	**52.02**	**100.00%**	**100.0%**	**3.22E+04**	**0.002**	**1.45E+07**
	DeepCubeA	52.03	**100.00%**	99.4%	3.85E+06	10.28	3.93E+05
	DeepCubeA$_g$	**52.02**	**100.00%**	**100.0%**	1.81E+05	2.61	6.94E+04
	FastDown (GC)	36.75	0.80%	0.80%	9.05E+07	102.11	8.66E+05
	FastDown (FF)	52.75	80.80%	24.80%	2.92E+06	42.11	6.93E+04
	FastDown (CG)	41.95	4.40%	1.20%	2.00E+07	80.58	2.47E+05
15-P (Rand)	DeepCubeA$_g$	**33.98**	**100.00%**	-	**1.11E+05**	**1.60**	**6.16E+04**
	FastDown (GC)	14.92	38.00%	-	1.61E+07	18.77	5.46E+05
	FastDown (FF)	32.66	89.20%	-	1.24E+06	17.39	5.65E+04
	FastDown (CG)	20.45	51.20%	-	3.90E+06	21.41	1.20E+05
24-P (Canon)	PDBs	**89.41**	**100.00%**	**100.00%**	8.19E+10	4239.54	**1.91E+07**
	DeepCubeA	89.49	**100.00%**	96.98%	6.44E+06	19.33	3.34E+05
	DeepCubeA$_g$	90.47	**100.00%**	55.24%	**3.38E+05**	**5.22**	6.48E+04
	FastDown (GC)	-	0.00%	0.00%	-	-	-
	FastDown (FF)	81.00	1.01%	0.40%	2.68E+06	89.84	2.91E+04
	FastDown (CG)	-	0.00%	0.00%	-	-	-
24-P (Rand)	DeepCubeA$_g$	66.28	**99.60%**	-	3.10E+05	4.91	6.16E+04
	FastDown (GC)	9.86	10.00%	-	9.54E+06	11.88	4.27E+05
	FastDown (FF)	26.35	26.00%	-	5.99E+05	19.57	2.41E+04
	FastDown (CG)	13.75	12.60%	-	1.42E+06	14.42	6.85E+04
Sokoban	DeepCubeA	32.88	**100.00%**	-	**5.01E+03**	2.71	1.84E+03
	DeepCubeA$_g$	**32.02**	**100.00%**	-	1.80E+04	0.95	1.79E+04
	FastDown (GC)	31.94	99.80%	-	3.17E+06	5.93	5.85E+05
	FastDown (FF)	33.15	**100.00%**	-	2.92E+04	**0.32**	**7.49E+04**
	FastDown (CG)	33.12	**100.00%**	-	4.43E+04	0.51	7.25E+04

Agostinelli, Forest, Rojina Panta, and Vedant Khandelwal. “Specifying Goals to Deep Neural Networks with Answer Set Programming.” *ICAPS 2024*

ASP Specifications

- We build on this using answer set programming to describe goals with first-order logic and use answer set solvers to solve for assignments that make these goals true
- For the Rubik's cube
  - Define basic background knowledge
    - Colors, faces, cubelets
    - Constraints: Cannot have two stickers of the same color on the same cubelet, cannot have two stickers from the same cubelet on opposite faces
  - Given basic background knowledge, specifications often only require a few lines of code
    - `face_same(F) :- face_col(F, FCol), #count{Cbl : onface(Cbl, FCol, F)}=9.`
    - `canon_solved :- #count{F : face_same(F)}=6.`
  - Our specifications contain combinations of common patterns
    - Note: the training procedure is unaware of what the specification will be at test time



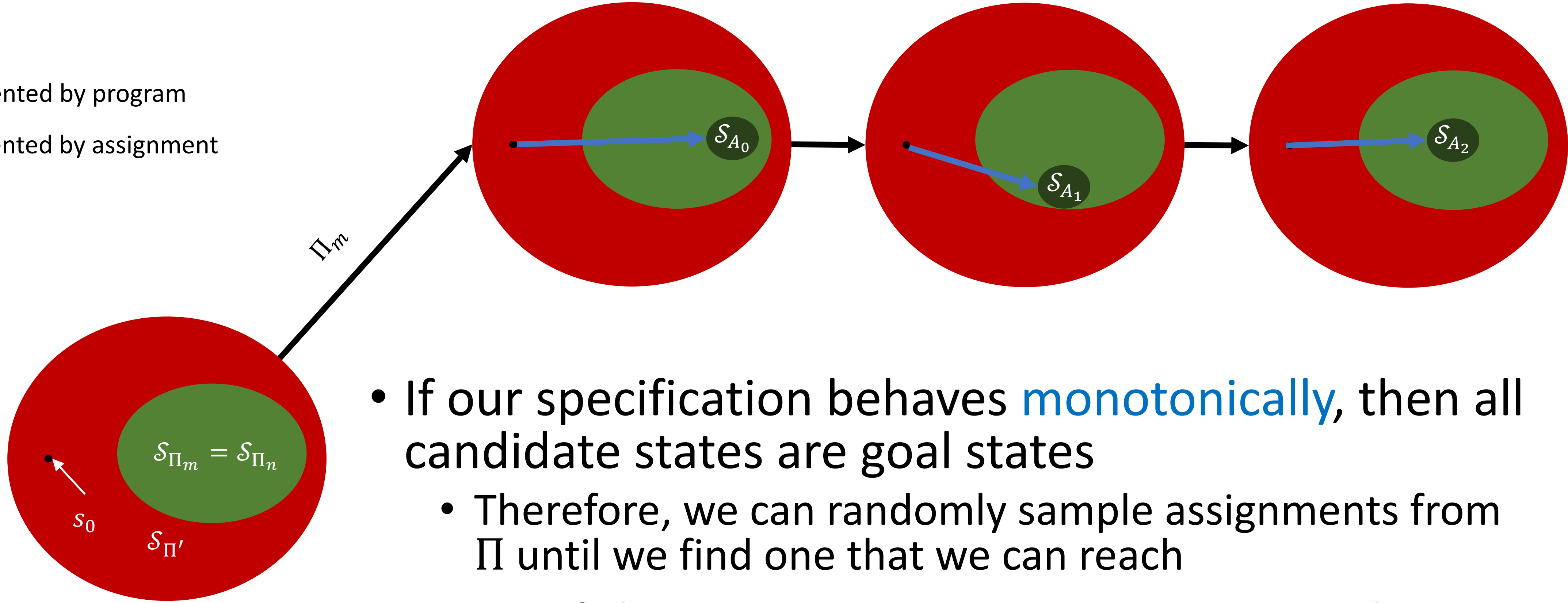
(a) Cross (b) X (c) Cup (d) Spot

Goal Reaching: Monotonic Specification

Π: Answer set program

$\mathcal{S}_\Pi$: set of states represented by program

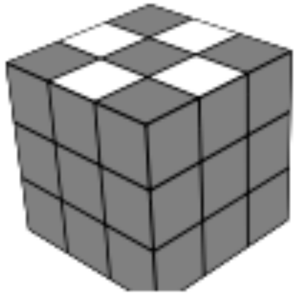
$\mathcal{S}_A$: set of states represented by assignment



- If our specification behaves monotonically, then all candidate states are goal states
  - Therefore, we can randomly sample assignments from Π until we find one that we can reach
- Some of these assignments may represent the empty set
- The answer set solver (we use clingo) used is agnostic to the cost of a shortest path

Handling Non-Monotonicity

- If negation as failure is used in a program, Π, then Π can exhibit non-monotonic behavior
  - A logic program is non-monotonic if some atoms that were previously derived can be retracted by adding new knowledge
  - Therefore, we can have a state that is a candidate state but not a goal state
- For example, a white cross with no yellow stickers on the white face
  - The assignment for this specification is just a white cross
  - However, there can be a state that is a specialization of this assignment, but has yellow on the white face

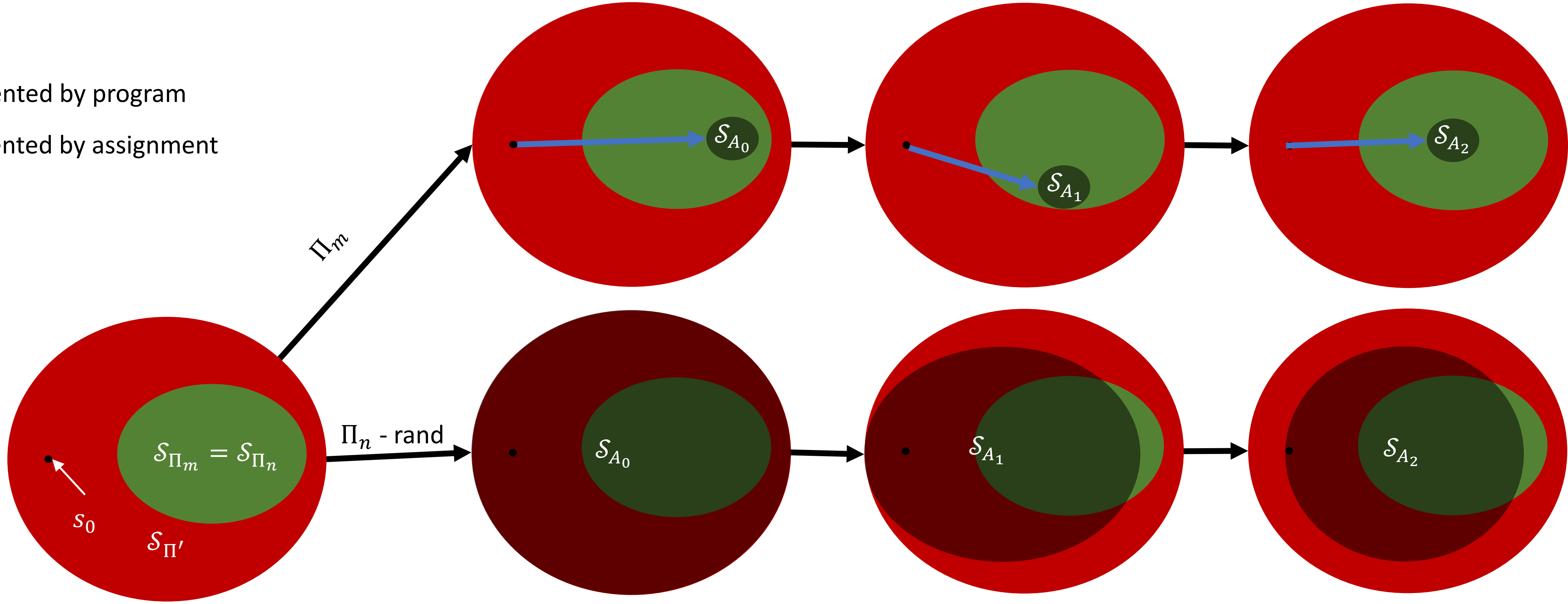


Goal Reaching: Non-monotonic

Π: Answer set program

$\mathcal{S}_\Pi$: set of states represented by program

$\mathcal{S}_A$: set of states represented by assignment

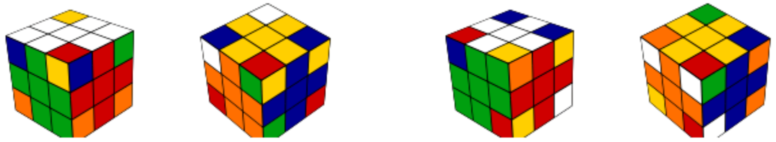


To reduce the size of candidate states while ensuring there is still at least one goal state, find another minimal assignment, A_2, such that

$$A \subset A_2$$
$$A_2 \in \alpha(\Pi)$$

Results

Goal	Path Cost	% Solved	# Models	Model Time	Search Time
Rubik's Cube (Canon)	24.41	100%	1	0.37	4.39
Rubik's Cube (Cross6)	13.11	100%	1	0.41	2.14
Rubik's Cube (Cup4)	24.33	100%	42.5	34.65	374.11
Rubik's Cube (CupSpot)	17.99	100%	27.68	38.66	241.08
Rubik's Cube (Checkers)	23.85	100%	1	0.49	4.2
Sokoban (Immov)	35.15	100%	6.37	6.83	16.16
Sokoban (BoxBox)	33.77	88%	1.89	0.58	6.08
Sokoban (AgentInBox)	34.42	77%	1.26	0.38	4.09



(a) Example 1 (b) Example 2

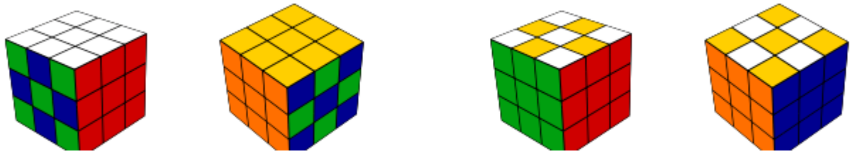
Cross6

(a) Example 1 (b) Example 2

Cup4

(a) Example 1 (b) Example 2

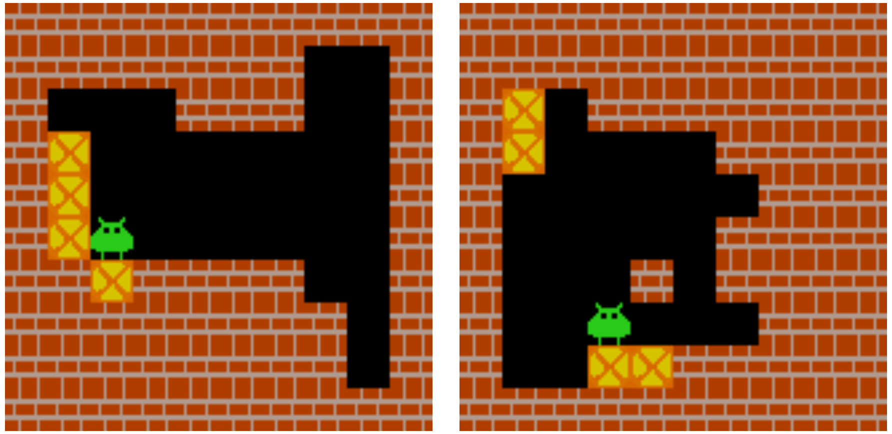
CupSpot



Checkers

Agostinelli, Forest, Rojina Panta, and Vedant Khandelwal. "Specifying Goals to Deep Neural Networks with Answer Set Programming." *ICAPS 2024*

Results



All boxes are immoveable

Goal	Path Cost	% Solved	# Models	Model Time	Search Time
Rubik's Cube (Canon)	24.41	100%	1	0.37	4.39
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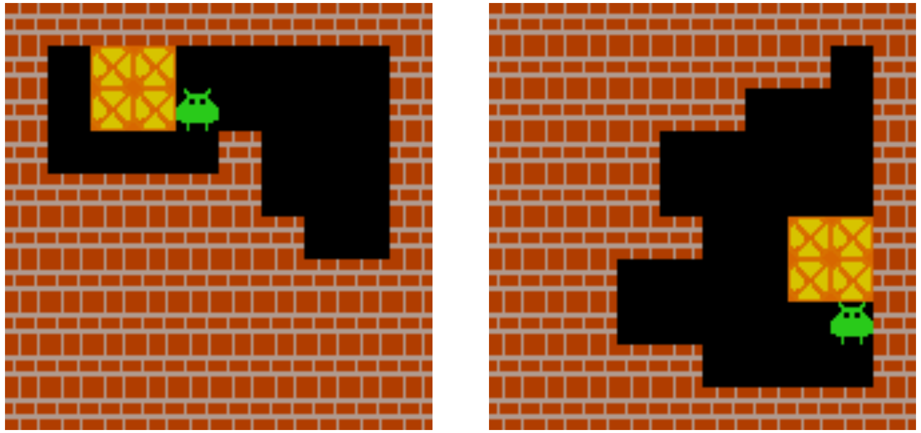
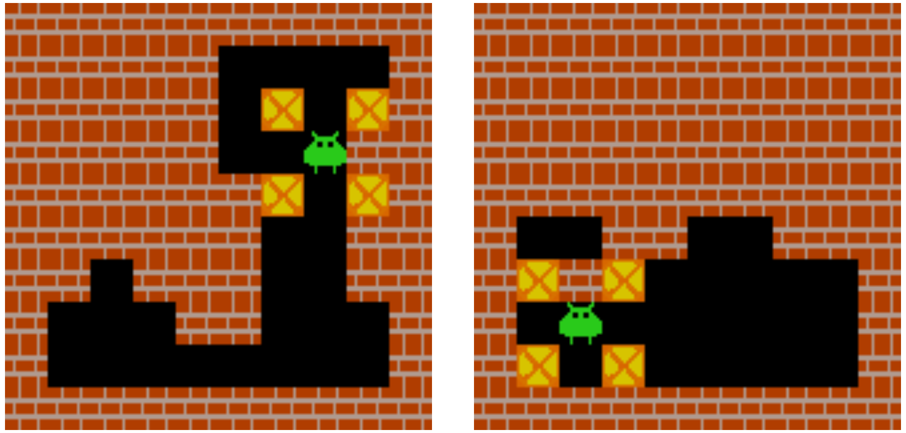


A box of boxes



Boxes at the four corners of the agent

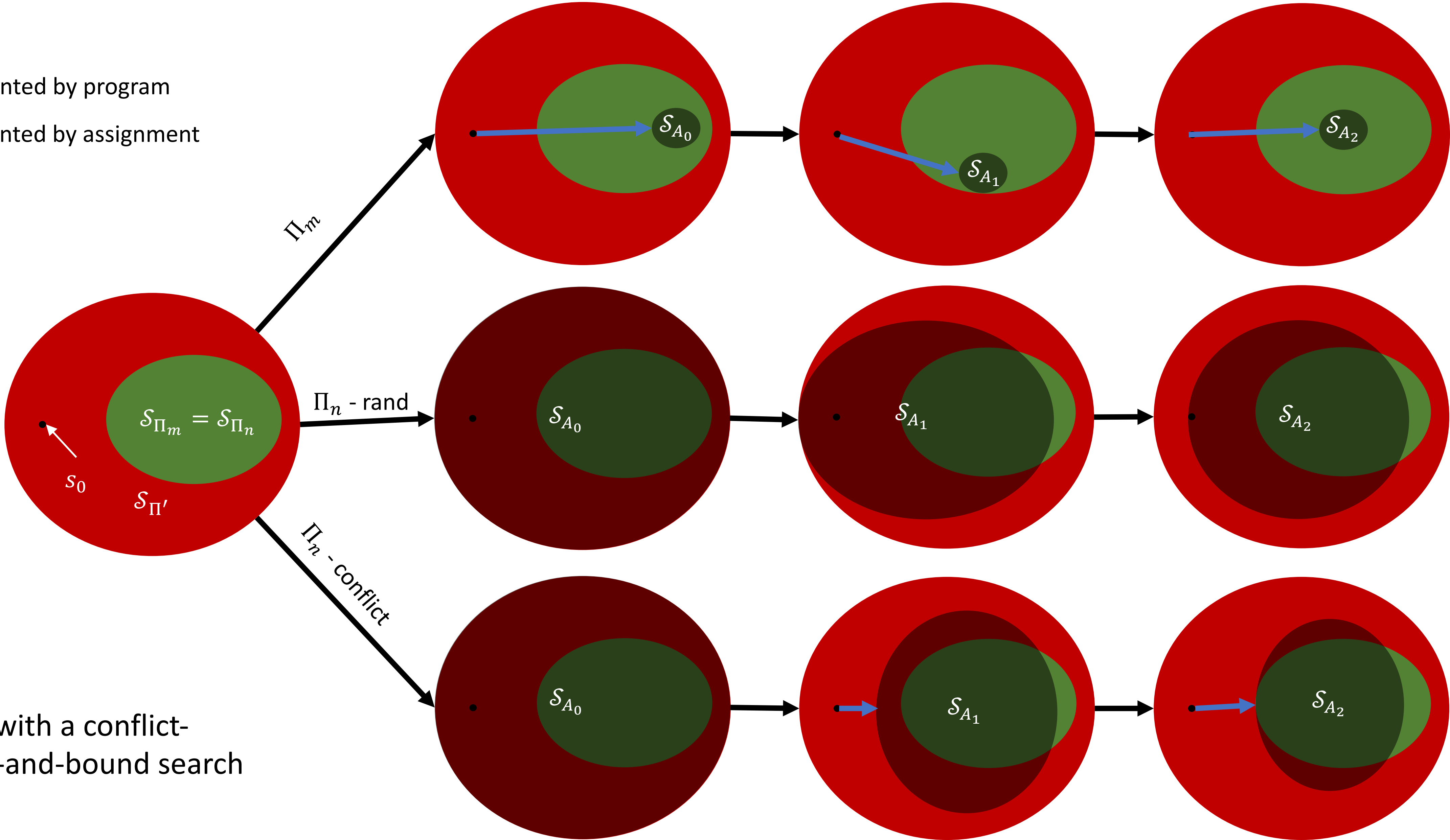
Agostinelli, Forest, Rojina Panta, and Vedant Khandelwal. "Specifying Goals to Deep Neural Networks with Answer Set Programming." *ICAPS 2024*

Goal Reaching: Non-monotonic

Π: Answer set program

$\mathcal{S}_{\Pi}$: set of states represented by program

$\mathcal{S}_{A}$: set of states represented by assignment

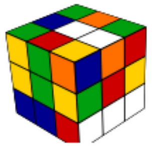


Combine this with a conflict-driven branch-and-bound search

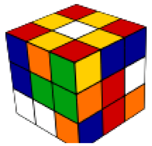
Results

Goal	SpecOp	Cost	%Solve	#Itr	#Assign	%reach	%not goal	Secs/Spec	Secs/Path	Secs
RC:∀diffCtrW	-	11.54	70	**3.34**	**33.43**	7.68	**0**	12.77	7.5	564.94
RC:¬∃sameCtrW	Rand	1.67	99	7.2	63.02	87.84	69.06	**0.06**	1.04	95.46
	Conflict	**1.26**	**100**	5.43	36.31	**99.34**	52.36	**0.06**	**0.07**	**5.98**
24p:r0SumEven	-	24.55	**100**	9.24	92.4	**100**	**0**	**0.2**	0.23	42.52
24p:¬r0SumOdd	Rand	3.16	**100**	4.27	33.6	**100**	38.71	**0.2**	**0.03**	6.64
	Conflict	**2.51**	**100**	**4.06**	**31.6**	**100**	22.13	0.21	0.04	**6.58**
24p:∀rSumEven	-	83.71	**100**	9.19	91.9	50.41	**0**	0.88	1.77	250.18
24p:¬∃rSumOdd	Rand	17.07	**100**	10.23	92.05	99.98	85.51	**0.1**	**0.08**	21.72
	Conflict	**12.87**	**100**	**8.66**	**77.1**	**100**	79.72	0.11	**0.08**	**17.08**

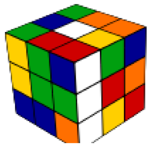
All stickers on the white face are different than the center sticker



Start



Mono: path cost 12



Non-mono: path cost 1

All rows sum to an even number

12	22	6	9	5
7	1	19	2	17
16	13	4	20	21
11	15	10	3	8
	14	18	24	23

Start

17	10	20	5	22
1	6	14	15	16
12	13	23		8
11	3	9	4	7
18	19	2	21	24

Mono: path cost 93

12	22	6	9	5
7	1	19	2	17
16	13	4	20	21
11	15	10		8
14	18	24	3	23

Non-mono: path cost 4

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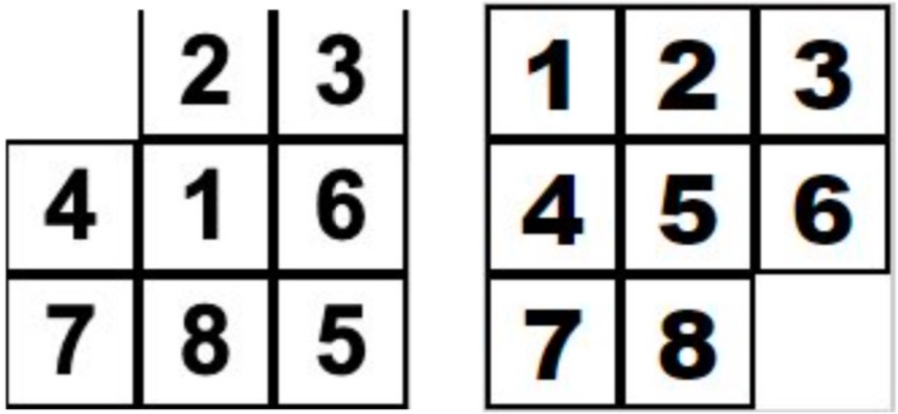
Vedant Khandelwal

Example



Start state

Goal state

- If using only canonical actions, the cost-to-go is 16
- If including diagonal actions, the cost-to-go is 2
- To differentiate between these two scenarios, information about the domain must also be given to the heuristic function

Training

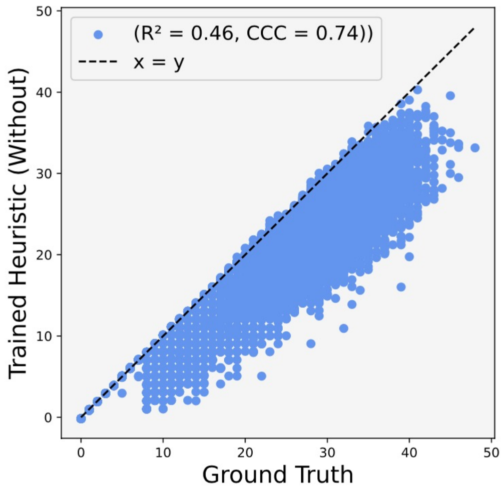
- For each example, randomly sample a domain
- For that domain, randomly sample a state
- RL Update
  - $L(\theta) = \left(\min_a (c^a(s) + h_{\theta^-}(T(s,a), D)) - h_\theta(s, D)\right)^2$
  - D: Domain

Preliminary Experiments

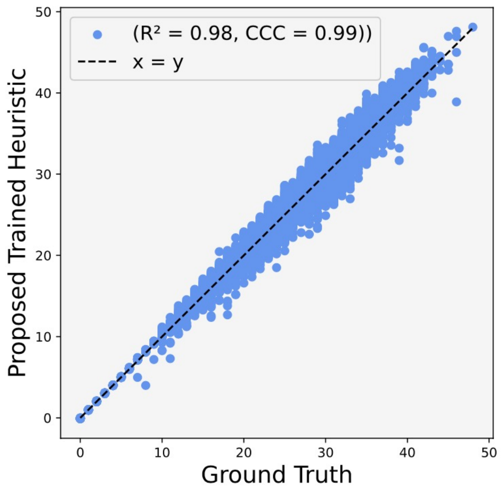
- For the 15-puzzle, generate different domains by sampling a subset of {U, D, L, R, UL, UR, DL, DR} actions for each tile position
  - 8 actions for each of the 16 positions, max $2^{8*16} \approx 3.4\times10^{38}$ domains
  - Ensure all sampled domains are reversible, for simplicity
- Represent the domain as a one-hot vector of which actions are allowed in each position
- Compare heuristic performance with true cost-to-go for random states from domains
  - True cost-to-go computed with merge-and-shrink heuristic
- Compare when training a heuristic function across domains without domain information
- Compare heuristic function with DeepCubeA trained for a fixed domain

Results

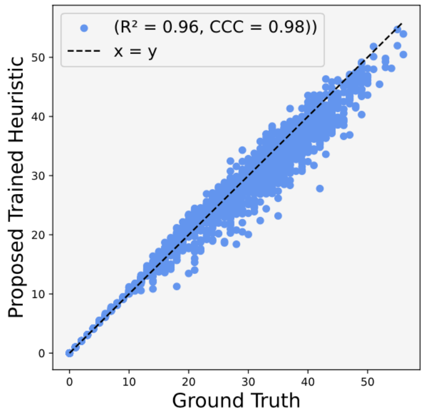
- Adding action information significantly improves performance
- Performs slightly worse when compared to DeepCubeA trained on that specific domain
    - However, unlike DeepCubeA, it does not need to be re-trained for that domain



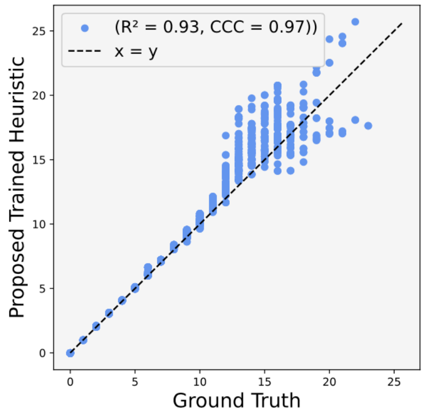
(a) Without Action Info



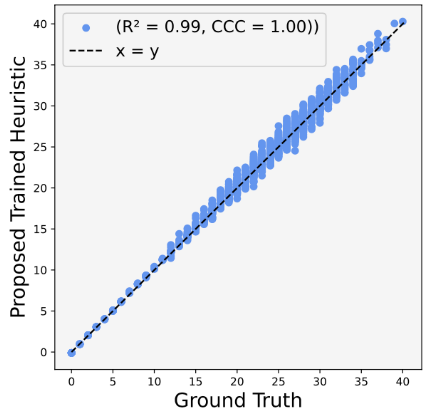
(b) With Action Info



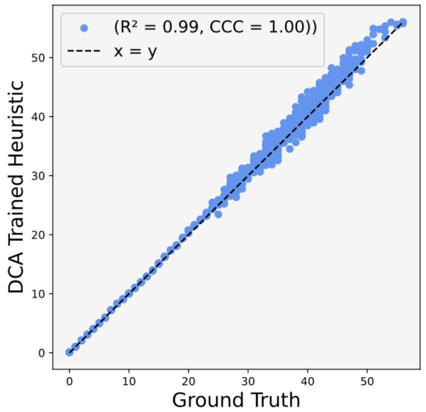
(a) C: P vs GT



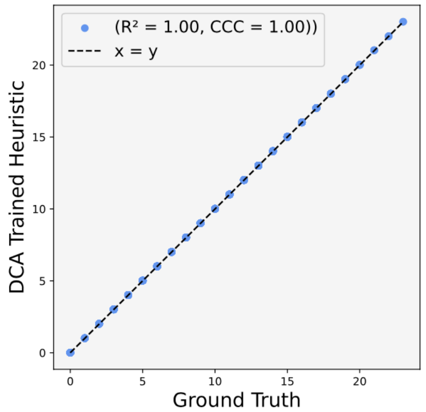
(b) D: P vs GT



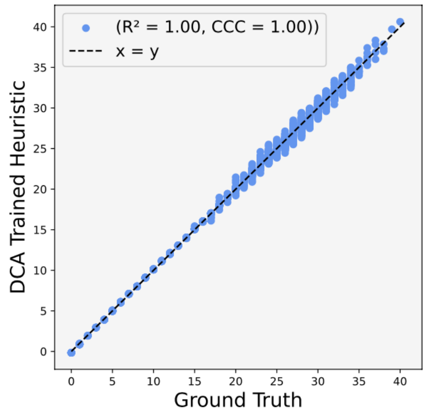
(c) C+D: P vs GT



(d) C: DCA vs GT



(e) D: DCA vs GT



(f) C+D: DCA vs GT

Khandelwal, Vedant, Amit Sheth, Forest Agostinelli. "Towards Learning Foundation Models for Heuristic Functions to Solve Pathfinding Problems." *arxiv, 2024*

Results

- Repeat training for 8-puzzle and 24-puzzle
- Proposed approach compares favorably to the fast downward planner with the fast forward heuristic
- Is slightly worse than DeepCubeA, which must be re-trained for each domain
- Future work could build on work by Felipe Trevizan and Sylvie Thiebaux on using graph neural networks to encode PDDL domains

Domain	Solver	Len	Opt	Nodes	Secs	Nodes/Sec	Solved
8 Puzzle (**C**)	DeepCubeA	**18.38**	**100%**	3.59E+04	0.69	**5.2E+04**	**100%**
8 Puzzle (**C**)	Proposed	**18.38**	**100%**	7.17E+04	1.76	4.07E+04	**100%**
8 Puzzle (**C**)	FD(FF)	18.8	81%	**5.56E+02**	**0.11**	4.7E+03	**100%**
8 Puzzle (**D**)	DeepCubeA	**1.44**	**100%**	1.95E+01	**0.01**	2.92E+03	**100%**
8 Puzzle (**D**)	Proposed	**1.44**	**100%**	4.05E+01	**0.01**	**4.92E+03**	**100%**
8 Puzzle (**D**)	FD(FF)	**1.44**	**100%**	**2.45E+00**	0.2	1.23E+01	**100%**
8 Puzzle (**C+D**)	DeepCubeA	**11.84**	**100%**	6.2E+04	**1.18**	**5.26E+04**	**100%**
8 Puzzle (**C+D**)	Proposed	**11.84**	**100%**	6.23E+04	1.56	3.97E+04	**100%**
8 Puzzle (**C+D**)	FD(FF)	12.9	54.2%	**8.68E+01**	**0.13**	6.59E+02	**100%**
15 Puzzle (**C**)	DeepCubeA	**52.03**	**99.4%**	**1.82E+05**	**4.31**	4.21E+04	**100%**
15 Puzzle (**C**)	Proposed	52.18	93.76%	3.62E+05	10.39	3.49E+04	**100%**
15 Puzzle (**C**)	FD(FF)	52.75	24.80	2.92E+06	42.11	**6.93E+04**	80.80%
15 Puzzle (**D**)	DeepCubeA	**10.8**	**100%**	8.2E+02	**0.03**	2.43E+04	**100%**
15 Puzzle (**D**)	Proposed	10.81	99.8%	1.64E+03	0.05	**3.01E+04**	**100%**
15 Puzzle (**D**)	FD(FF)	10.86	96.8%	**4.18E+01**	0.21	1.96E+02	**100%**
15 Puzzle (**C+D**)	DeepCubeA	**25.66**	**100%**	1.78E+05	3.74	**4.78E+04**	**100%**
15 Puzzle (**C+D**)	Proposed	25.67	99.8%	1.78E+05	4.72	3.78E+04	**100%**
15 Puzzle (**C+D**)	FD(FF)	29.32	13.4%	**8.4E+03**	**1.17**	3.56E+03	**100%**
24 Puzzle (**C**)	DeepCubeA	**89.48**	**96.98%**	**3.34E+05**	**8.05**	**4.15E+04**	**100%**
24 Puzzle (**C**)	Proposed	92.80	22.03%	7.6E+05	24.06	3.16E+04	**100%**
24 Puzzle (**C**)	FD(FF)	81.00	0.40	2.68E+06	89.84	2.91E+04	1.01%
24 Puzzle (**D**)	DeepCubeA	**14.9**	**100%**	2.55E+04	**0.47**	**5.46E+04**	**100%**
24 Puzzle (**D**)	Proposed	14.92	99.8%	5.1E+04	1.35	3.78E+04	**100%**
24 Puzzle (**D**)	FD(FF)	15.16	89.2%	**2.64E+02**	**0.12**	2.05E+03	**100%**
24 Puzzle (**C+D**)	DeepCubeA	**31.33**	**100%**	2.27E+05	**4.83**	**4.69E+04**	**100%**
24 Puzzle (**C+D**)	Proposed	31.34	99.6%	2.27E+05	6.78	3.34E+04	**100%**
24 Puzzle (**C+D**)	FD(FF)	36.81	13.8%	**1.7E+04**	5.35	1.77E+03	99.4%

Khandelwal, Vedant, Amit Sheth, Forest Agostinelli. “Towards Learning Foundation Models for Heuristic Functions to Solve Pathfinding Problems.” *arxiv, 2024*
Chen, Dillon Z., Sylvie Thiébaux, and Felipe Trevizan. "Learning Domain-Independent Heuristics for Grounded and Lifted Planning." *AAAI*. Vol. 38. No. 18. 2024.

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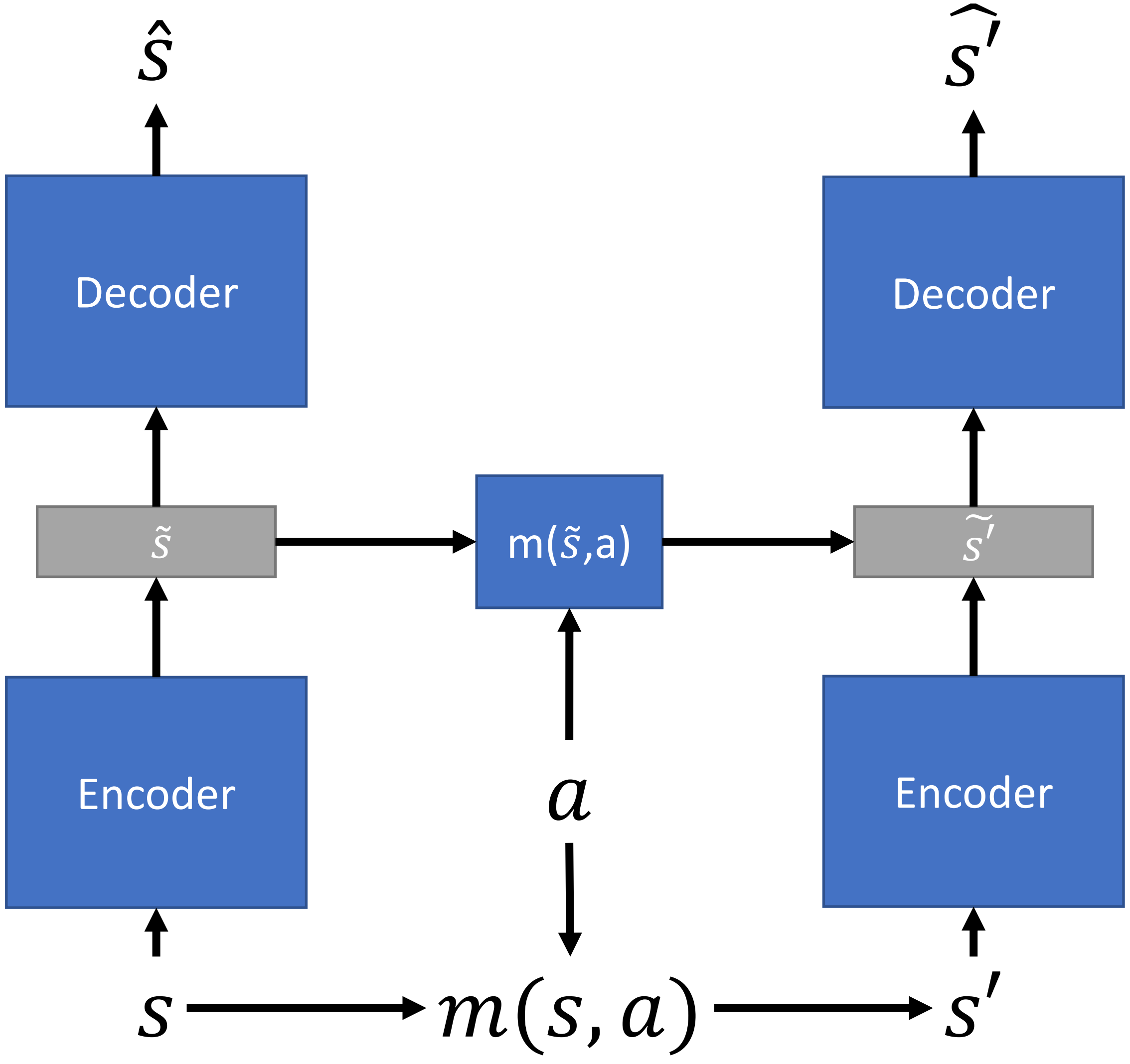
Misagh Soltani

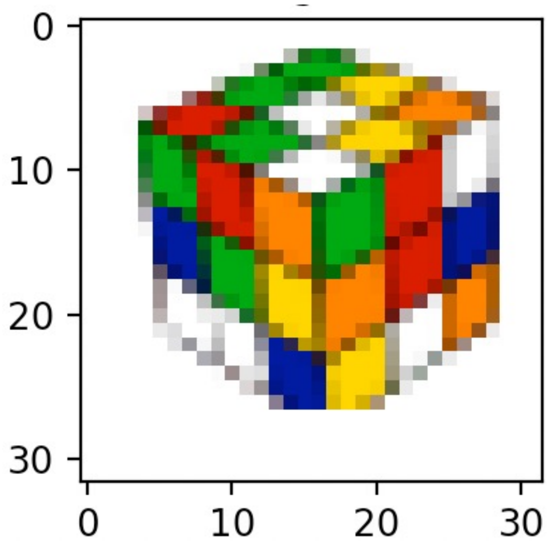
Learning Discrete World Models

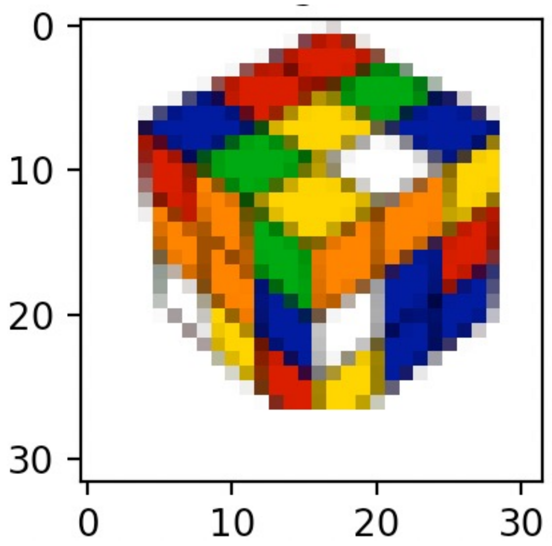
- Addressing previous shortcomings
  - Small errors in prediction can be corrected by simply rounding
  - Can reidentify states by comparing two vectors
- Encoder
  - Maps the state to a discrete representation
  - To allow training with gradient descent, use a straight through estimator
- Decoder
  - Maps the discrete representation to the state
  - Ensures the discrete representation is meaningful
- Environment model
  - Maps discrete states and actions to next discrete state

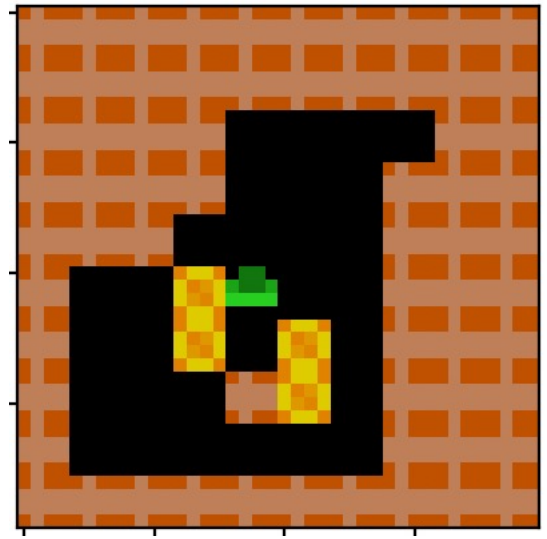


Experiments

- Rubik's cube
  - Two 32x32 RGB images showing both sides of the cube
- Sokoban
  - One 40x40 RGB image
- Generate offline dataset of 10,000 episodes of 30 random steps, each

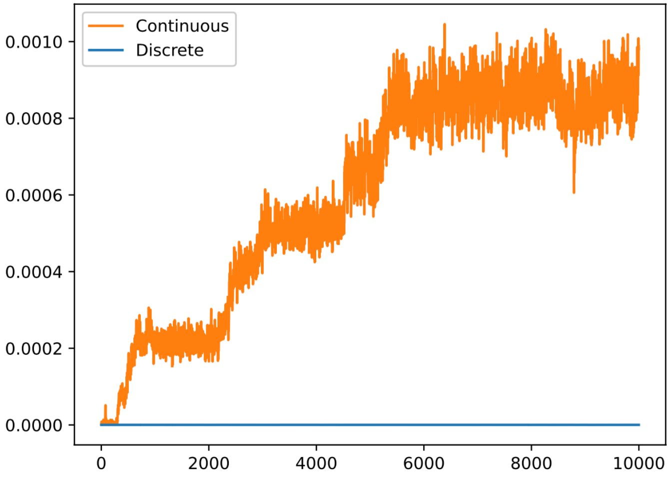




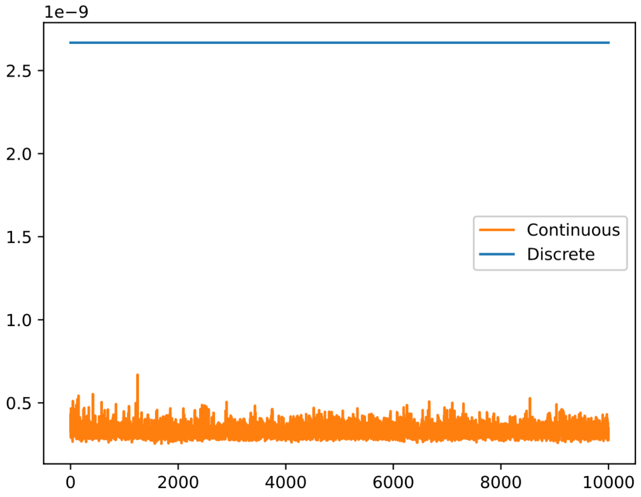


Discrete vs Continuous Model Performance

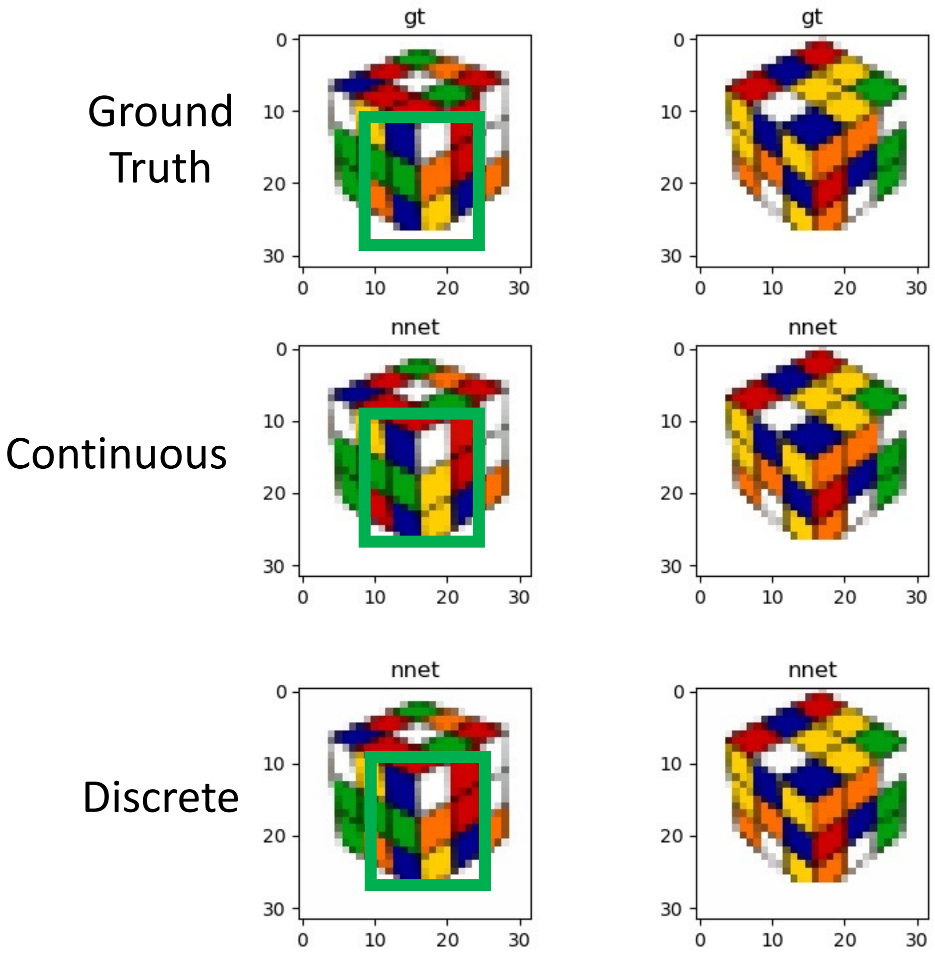
- The continuous model eventually accumulates error for the Rubik's cube



(a) Rubik's Cube



(b) Sokoban



Heuristic Learning and Search with Discrete Model

- DeepCubeAI – DeepCubeA + "Imagination"
  - Learn discrete world model with offline data
  - Use offline data and the learned world model to generate training data
  - Heuristic learning: Q-learning with hindsight experience replay
    - Generalize over goal states
  - Heuristic search: Q* search
    - Helps when model uses computationally expensive DNN

Domain	Solver	Len	Opt	Nodes	Secs	Nodes/Sec	Solved
RC	$PDBs^+$	20.67	100.0%	2.05E+06	2.20	1.79E+06	100%
	DeepCubeA	21.50	60.3%	6.62E+06	24.22	2.90E+05	100%
	Greedy (ours)	-	0%	-	-	-	0%
	DeepCubeAI (ours)	22.85	19.5%	2.00E+05	6.21	3.22E+04	100%
RC_{rev}	Greedy (ours)	-	0%	-	-	-	0%
	DeepCubeAI (ours)	22.81	21.92%	2.00E+05	6.30	3.18+04	99.9%
Sokoban	LevinTS	39.80	-	6.60E+03	-	-	100%
	LevinTS (*)	39.50	-	5.03E+03	-	-	100%
	LAMA	51.60	-	3.15E+03	-	-	100%
	DeepCubeA	32.88	-	1.05E+03	2.35	5.60E+01	100%
	Greedy (ours)	29.55	-	-	1.68	-	41.9%
	DeepCubeAI (ours)	33.12	-	3.30E+03	2.62	1.38E+03	100%

Agostinelli, Forest and Soltani, Misagh "Learning Discrete World Models for Heuristic Search." *Reinforcement Learning Conference 2024*

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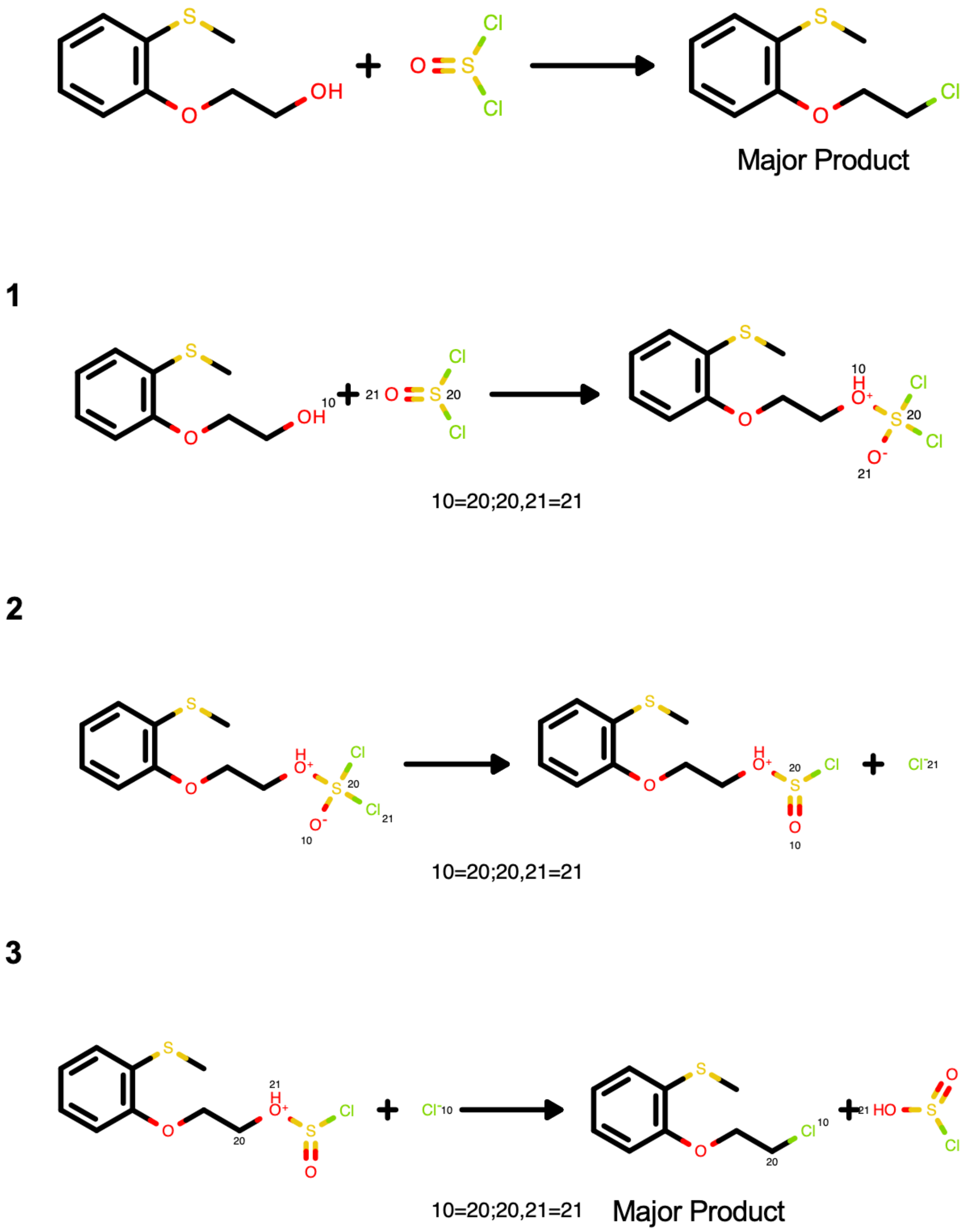
Rojina Panta

Christian Geils

Reaction Mechanisms

- Chemical reactions are composed of smaller steps called reaction mechanisms
- Knowledge of the reaction mechanisms that compose a chemical reaction allows practitioners to
  - Validate reaction feasibility
  - Improve reaction efficiency
  - Predict reaction outcome under different conditions
- Most chemical reaction prediction methods skip reaction mechanisms and predict products directly from reactants



Reaction Mechanism Domain

- We create the state transition function using OrbChain, a model for reaction mechanism steps
  - Can take over a second to expand a state, limiting training data
- For simplicity, we assume all transition costs are 1
  - Future work will use negative log probabilities of reaction mechanism steps as transition costs
- We use extended-connectivity fingerprints to represent a molecule to the heuristic function
  - Future work will use a learned representation using graph neural networks
- We generate data using small molecules from the United States Patent and Trademark Office (USPTO) dataset of chemical reactions
  - Using random walks, we generate new molecules
- The heuristic function also takes a goal state as input
  - $L(\theta) = \left(\min_a \left(c^a(s) + h_{\theta^-}(T(s,a), s_g)\right) - h_\theta(s, s_g)\right)^2$

Results

- Generate test data by performing a random walk between 0 and 6 steps
- The learned heuristic function outperforms uniform cost search and A* search with the Tanimoto similarity metric

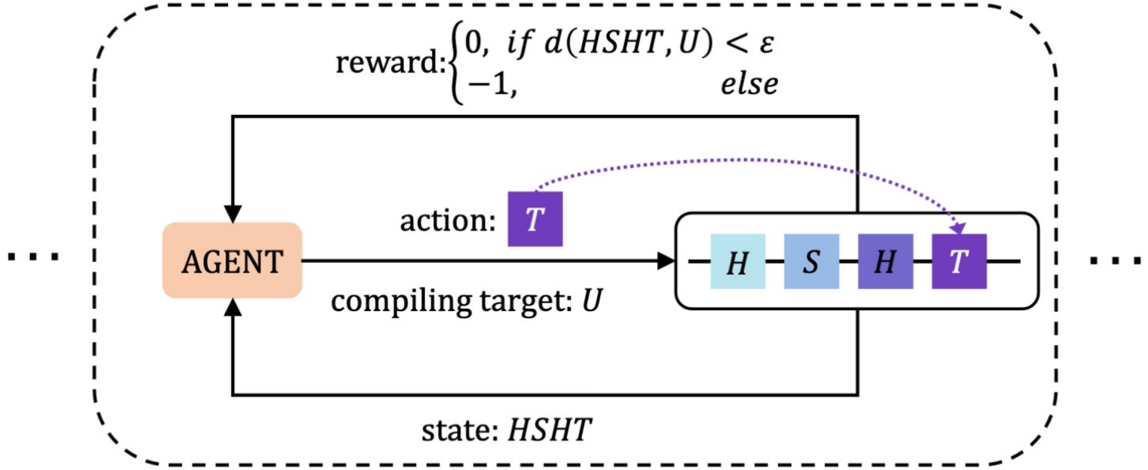
Step/s	Solver	Path Cost	% Solved	Nodes	Secs	Nodes/Sec
Steps=0	DeepCubeA	0.00	**100.00%**	3.09E+2	3.87	79.97
	Uniform Cost Search	0.00	**100.00%**	3.09E+2	4.61	67.13
	Tanimoto Similarity	0.00	**100.00%**	3.09E+2	3.71	83.42
Steps=1	DeepCubeA	1.00	**100.00%**	7.49E+2	9.70	77.26
	Uniform Cost Search	1.00	**100.00%**	4.26E+4	553.33	76.95
	Tanimoto Similarity	1.00	**100.00%**	3.13E+4	429.29	72.97
Steps=2	DeepCubeA	2.07	**100.00%**	1.63E+4	267.16	60.87
	Uniform Cost Search	1.67	20.00%	1.32E+5	1497.77	87.96
	Tanimoto Similarity	1.75	26.67%	1.10E+5	1229.10	89.13
Steps=3	DeepCubeA	2.77	86.67%	4.14E+4	578.88	71.54
	Uniform Cost Search	-	0.00%	-	-	-
	Tanimoto Similarity	-	0.00%	-	-	-
Steps=4	DeepCubeA	3.33	60.00%	6.36E+4	821.64	77.36
	Uniform Cost Search	3.00	6.67%	1.43E+5	1962.28	73.01
	Tanimoto Similarity	3.00	6.67%	2.47E+4	272.15	90.64
Steps=5	DeepCubeA	3.40	33.33%	8.40E+4	968.49	86.69
	Uniform Cost Search	-	0.00%	-	-	-
	Tanimoto Similarity	-	0.00%	-	-	-
Steps=6	DeepCubeA	3.20	33.33%	6.14E+4	933.86	65.73
	Uniform Cost Search	-	0.00%	-	-	-
	Tanimoto Similarity	-	0.00%	-	-	-

Panta, Rojina, et al. "Finding Reaction Mechanism Pathways with Deep Reinforcement Learning and Heuristic Search." *ICAPS PRL Workshop 2024*

Quantum Algorithm Compilation

- Given a quantum algorithm, a compiler must synthesize a quantum circuit for this algorithm from a given set of quantum gates
- If a given circuit is below an error threshold, then the problem is considered solved

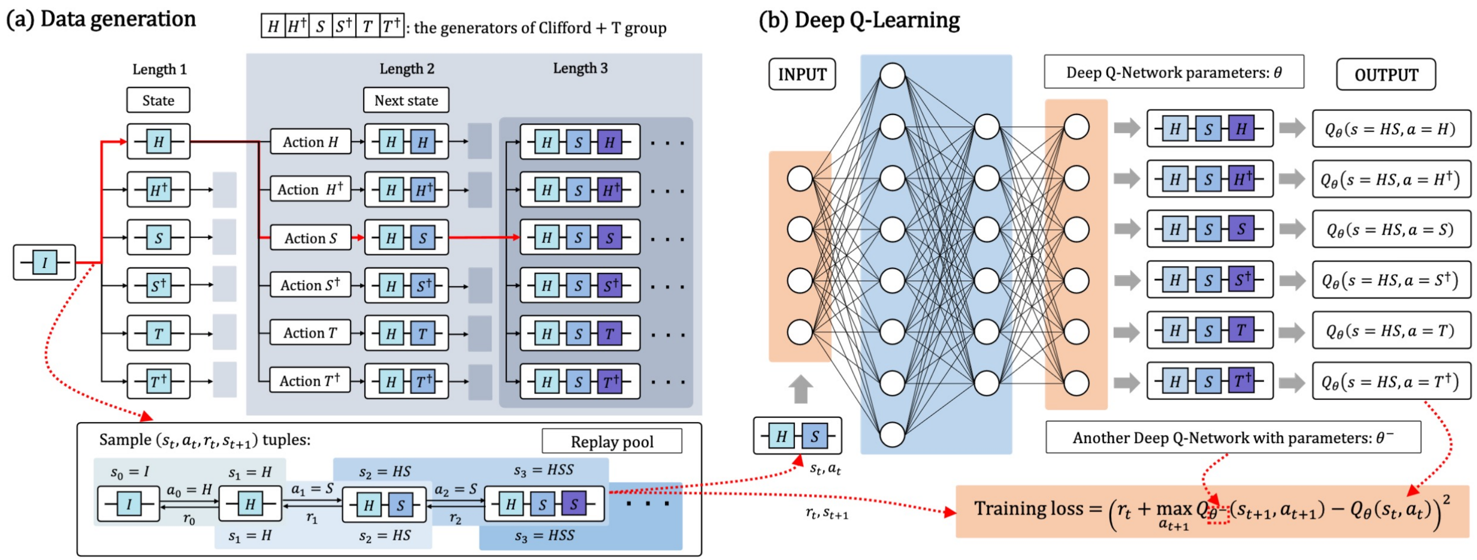
Quantum compiling in the framework of RL

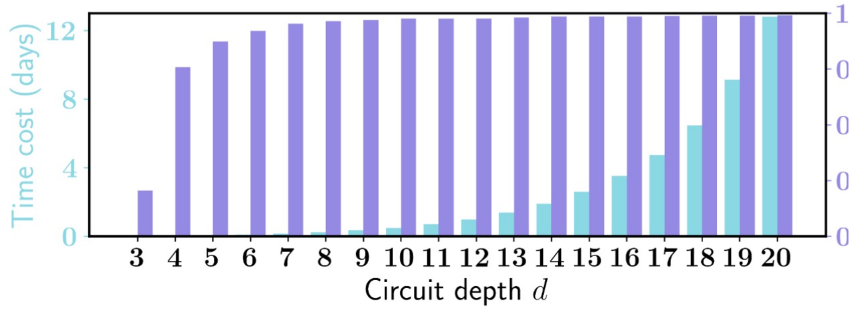


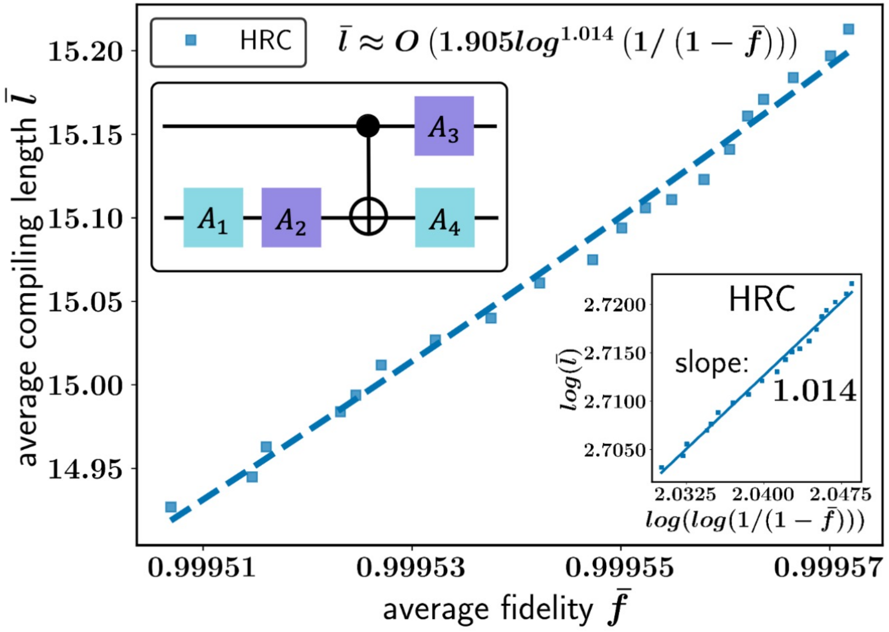
The Markov Decision Process	
action space $\mathcal{A}$	hardware-specific universal basis set
state space $\mathcal{S}$	the circuits composed of $\{A_j; A_j \in \mathcal{A}\}$
reward function r	reward $r = \begin{cases} 0, & if\ d(\prod_{j=0}^{L-1} A_j, U) < \varepsilon \\ -1, & else \end{cases}$
transition probability $\mathcal{P}$	$P(s_{t+1} \mid s_t, a_t) = 1$ (deterministic)

Quantum Algorithm Compilation

- Training data can be generated from a given gate set and a DQN trained to predict the distance of the current quantum circuit to the identity function
- Given a trained DQN, Q* search can be used to search for a circuit for a given algorithm
- Accuracy increases given more time for synthesis





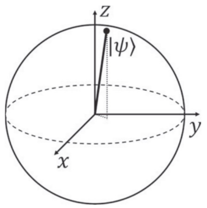
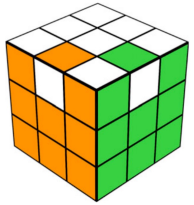


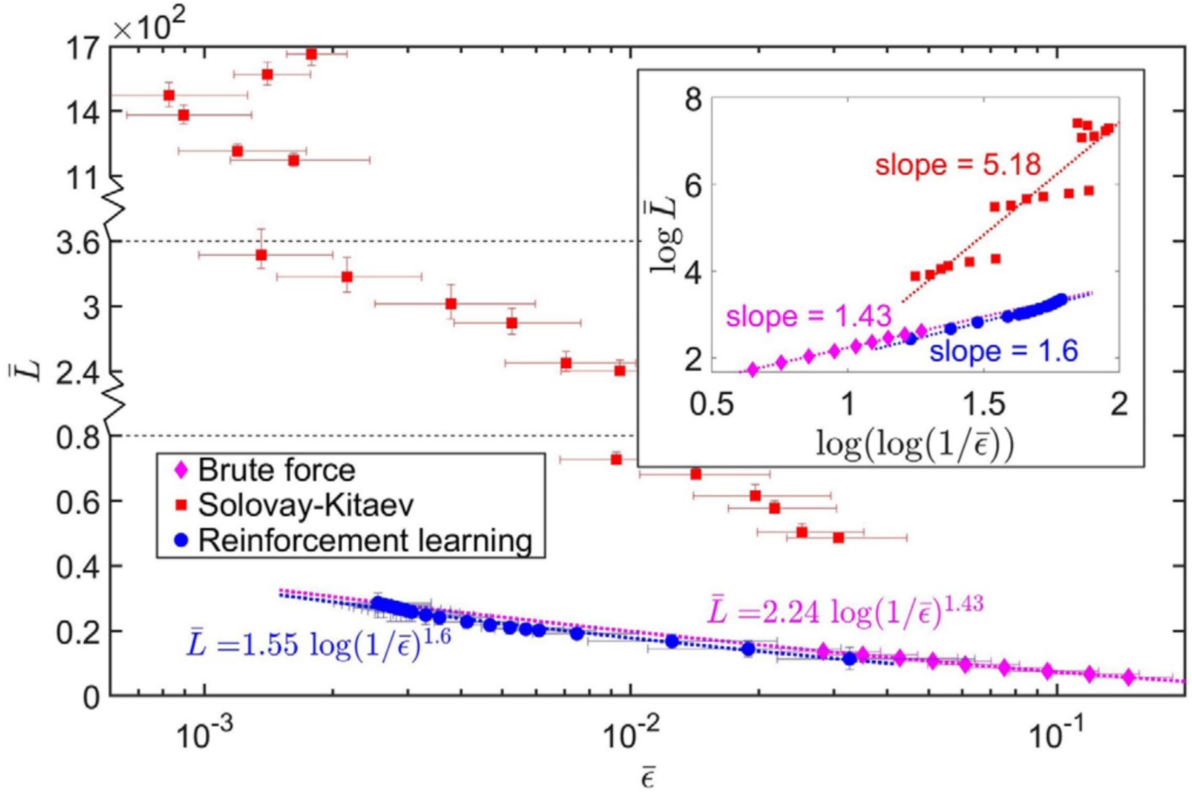
Quantum compilation on two-qubit universal basis set

Qiuhao, Chen, et al. "Efficient and practical quantum compiler towards multi-qubit systems with deep reinforcement learning." Quantum Science and Technology (2024).

Other Applications to Quantum Algorithm Compilation

- Topological quantum compiling
- Clifford synthesis
- Can produce near-optimal solutions

System		
Initial state	The unitary to be approximated	The scrambled cube
Target state	The identity matrix	The solved cube
Basic move	A gate from the universal set	Rotation of one face



Zhang, Yuan-Hang, et al. "Topological Quantum Compiling with Reinforcement Learning." Physical Review Letters 125.17 (2020): 170501.
Bao, Ning, and Gavin S. Hartnett. "Twisty-puzzle-inspired approach to Clifford synthesis." *Physical Review A* 109.3 (2024): 032409.

Questions?

- Papers
  - Agostinelli, Forest, et al. "Solving the Rubik's cube with deep reinforcement learning and search." Nature Machine Intelligence 1.8 (2019): 356-363.
  - Agostinelli, Forest, et al. "Q* Search: Heuristic Search with Deep Q-Networks." *ICAPS PRL Workshop 2024*
  - Agostinelli, Forest, Rojina Panta, and Vedant Khandelwal. "Specifying Goals to Deep Neural Networks with Answer Set Programming." *ICAPS 2024*
  - Agostinelli, Forest. "A Conflict-Driven Approach for Reaching Goals Specified with Negation as Failure." *ICAPS 2024 HAXP Workshop*
  - Khandelwal, Vedant, Amit Sheth, Forest Agostinelli. "Towards Learning Foundation Models for Heuristic Functions to Solve Pathfinding Problems." *arxiv, 2024*
  - Agostinelli, Forest and Soltani, Misagh "Learning Discrete World Models for Heuristic Search." *Reinforcement Learning Conference 2024*
  - Panta, Rojina, et al. "Finding Reaction Mechanism Pathways with Deep Reinforcement Learning and Heuristic Search." *ICAPS PRL Workshop 2024*
- Code
  - Many of these algorithms are publicly available on GitHub
  - https://github.com/forestagostinelli/deepxube

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