Learning More Expressive General Policies for Classical Planning Domains

Simon Ståhlberg[1] Blai Bonet[2] Hector Geffner[1]

[1]RWTH Aachen University, Germany, [2]Universitat Pompeu Fabra, Spain

Introduction

- General policies are strategies for solving many planning instances
  - E.g., general policy for solving **all** Blocksworld problems
- Three main methods for learning such policies (no "synthesis" yet!)
  - **Combinatorial optimization using explicit pool of $\mathcal{C}_2$ features** obtained from domain predicates [B. *et al.*, 2019; Francès *et al.*, 2021]
    - Transparent, can be proved correct, trouble scaling up
  - **Deep learning (DL) using domain predicates but no explicit pool** [Toyer *et al.*, 2020; Garg *et al.*, 2020]
    - Opaque, complex, but scalable
  - **DL exploiting relation between $\mathcal{C}_2$ logic and GNNs** [Barceló *et al.*, 2020; Grohe, 2020; Ståhlberg *et al.*, 2022]
    - **R-GNN architecture** adapted from Max-CSP[Γ] [Toenshoff *et al.*, 2021]
    - More transparent and simple, scalable
    - Supervised and non-supervised training
    - **Problem:** insufficient expressivity for generalized planning

Contributions

- Novel relational architecture R-GNN[t], with parameter $t \geq 0$, that combines the R-GNN architecture with a parameterized encoding $A_t(S)$ of planning states S
- As t increases, the expressive power of R-GNN[t] increases, approaching the full expressivity of $\mathcal{C}_3$ logic
- Significant improvements obtained even with $t = 1$, as shown in experiments
- 2- or 3-GNNs and Edge Transformers unfeasible in practice and limited to binary relations:
  - 2-GNNs: $\Theta(N^2)$ memory, $\Theta(N^3)$ time, $\mathcal{C}_2$ expressivity (yet see below)
  - 3-GNNs: $\Theta(N^3)$ memory, $\Theta(N^4)$ time, $\mathcal{C}_3$ expressivity
  - ETs: $\Theta(N^2)$ memory, $\Theta(N^3)$ time, $\mathcal{C}_3$ expressivity
  - Provably Powerful GNs [Maron *et al.*, 2019]: $\mathcal{C}_3$ expressivity, $\Theta(N^2)$ memory, $\Theta(N^3)$ time

Generalized Planning and First-Order STRIPS

- Generalized planning is about finding **general policies** that solve classes of planning problems
- Task is collection $\{P_1, P_2, \ldots\}$ of instances $P_i = \langle D, I_i \rangle$ over shared **first-order STRIPS** domain
- Each instance $P = \langle D, I \rangle$ consists of:
  - General (reusable) domain D specified with **action schemas** and **predicates**
  - Instance information I details **objects**, **init** and **goal** descriptions

Distinction between **general** domain D and **specific** instance $P = \langle D, I \rangle$ is important for **reusing** action models, and also for **learning** them

Example (Input): 2-Gripper Problem $P = \langle D, I \rangle$ in PDDL

```
(define (domain gripper)
   (:requirements :typing)
   (:types        room ball gripper)
   (:constants    left right - gripper)
   (:predicates   (at-robot ?r - room)
                  (at ?b - ball ?r - room)
                  (free ?g - gripper)
                  (carry ?o - ball ?g - gripper))

   (:action MOVE
       :parameters   (?from ?to - room)
       :precondition (at-robot ?from)
       :effect       (and (at-robot ?to) (not (at-robot ?from)))
   )

   (:action PICK
       :parameters   (?obj - ball ?room - room ?gripper - gripper)
       :precondition (and (at ?obj ?room) (at-robot ?room) (free ?gripper))
       :effect       (and (carry ?obj ?gripper) (not (at ?obj ?room)) (not (free ?gripper)))
   )

   (:action DROP
       :parameters   (?obj - ball ?room - room ?gripper - gripper)
       :precondition (and (carry ?obj ?gripper) (at-robot ?room))
       :effect       (and (at ?obj ?room) (free ?gripper) (not (carry ?obj ?gripper)))
   )
)

(define (problem easy-2balls)
   (:domain  gripper)
   (:objects  roomA roomB - room B1 B2 - ball)
   (:init     (at-robot roomA) (free left) (free right) (at B1 roomA) (at B2 roomA))
   (:goal     (and (at B1 roomB) (at B2 roomB)))
)
```

Relational GNN Architecture [Ståhlberg *et al.*, 2022]

- Planning state S over STRIPS domain D is a **relational structure:**
  - Relational symbols given by predicates in D; **shared** by all such states S
  - Denotation of predicate p given by ground atoms $p(\bar{o})$ true at S
- Adapt architecture of [Toenshoff *et al.*, 2021] for handling relational structures

Relational GNN (R-GNN) Architecture

Input: Set of ground atoms S (state), and objects O
Output: Embeddings $\boldsymbol{f}_L(o)$ for each object $o \in O$

1. Initialize $\boldsymbol{f}_0(o) = 0^k$ for each object $o \in O$
2. **for** $i \in \{0, 1, \ldots, L-1\}$ **do**
3. **for each** atom $q = p(o_1, o_2, \ldots, o_m) \in S$ **do**
4. $m_{q,o_j} := \left[\mathbf{MLP}_p\left(\boldsymbol{f}_i(o_1), \boldsymbol{f}_i(o_2), \ldots, \boldsymbol{f}_i(o_m)\right)\right]_j$
5. **end for**
6. **for each** object $o \in O$ **do**
7. $\boldsymbol{f}_{i+1}(o) := \boldsymbol{f}_i(o) + \mathbf{MLP}_U\left(\boldsymbol{f}_i(o), \mathrm{agg}\left(\{\!\{\boldsymbol{m}_{q,o} \mid o \in q, q \in S\}\!\}\right)\right)$
8. **end for**
9. **end for**

Parameters: embedding dimension k, rounds L, $\{\mathbf{MLP}_p : p \in D\}$, $\mathbf{MLP}_U$, and aggregator

Final Readout, Value Functions, and Greedy Policies

- **Final readout** is **additive readout** that feeds into final MLP:

$$V(S) = \mathbf{MLP}\left(\Sigma_{o \in O} \boldsymbol{f}_L(o)\right)$$

- Training minimize **loss** $L(S) = |V^*(S) - V(S)|$ given by **optimal value function** $V^*(\cdot)$ for small tasks in training set
- **Greedy policy** $\pi_V(S)$ chooses action $a = \mathrm{argmin}_{a \in A(S)} 1 + V(S_a)$:
  - If $V(S) = 0$ for goals, and $V(S) = 1 + \min_a V(S_a)$ for non-goals, π_V is **optimal**
  - If $V(S) = 0$ for goals, and $V(S) \geq 1 + \min_a V(S_a)$ for non-goals, π_V **solves any state** S

  where S_a is state that results of applying action a in state S

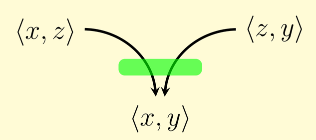
Successful approach for generalized planning, but subject to expressivity of GNNs...

Expressivity of GNNs

- R-GNNs are instances of (1-)GNNs over undirected graphs
- GNNs compute invariant (resp. equivariant) funcs on graphs (resp. vertices)
- Well-understood **expressivity limitations** in terms of **Weisfeiler-Leman** colorings and $\boldsymbol{\mathcal{C}_2}$ **logic** (formulas with counting quantifiers, and at most 2 variables)
- Eg, join $W(x, y) = \exists z.[R(x, z) \wedge T(z, y)]$ of relations R and T **cannot be captured!**
- That is, **no GNN can "track" such implicit relation** $W(x, y)$ on a graph where red and blue edges stand for R and T respectively
- We can augment expressivity by using k-GNNs, $k > 1$, that embed k-tuples of vertices:
  - Expressivity characterized in terms of k-WL colorings
  - Either k-OWL (less poweful) or k-FWL (more powerful) versions
  - Related to, respectively, $\mathcal{C}_{k-1}$ and $\mathcal{C}_k$ logics: counting quant., and k variables
  - **Infeasible by num. objs. in planning problems:** $\Theta(N^k)$ **space,** $\Theta(N^{k+1})$ **time**

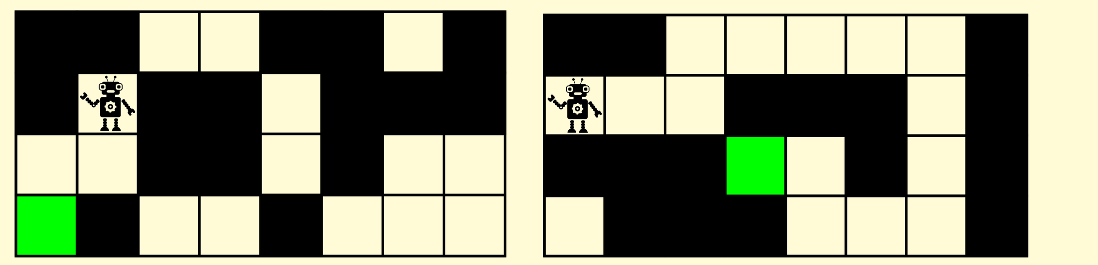
Parametric R-GNN[t] Architecture

- Same R-GNN architecture, different encoding of planning states S
- Embedding of all objects pairs, like in 2-GNNs: $\Theta(N^2)$ space
  - Objects in atoms replaced by pairs: $p(a, b) \to p(\langle a, a \rangle, \langle a, b \rangle, \langle b, a \rangle, \langle b, b \rangle)$
  - Predicate arities expanded from k to k^2
- **New composition predicate** $\Delta(\langle x, z \rangle, \langle z, y \rangle, \langle x, y \rangle)$:



  - Set $A_t(S)$ of added Δ-atoms controlled by integer parameter $t \geq 0$
  - $A_0(S) = \{p(\langle w \rangle^2) \mid p(w) \in S\}$ for $\langle w \rangle^2 = \langle (o_1, o_1), \ldots, (o_i, o_j), \ldots, (o_m, o_m) \rangle$
  - $A_t(S) = A_0(S) \cup \{\Delta(\langle o, o' \rangle, \langle o', o'' \rangle, \langle o, o'' \rangle) \mid \langle o, o' \rangle, \langle o', o'' \rangle \in R_t\}$
  - $\langle o, o' \rangle \in R_t$ iff o and o' in some atom in S (t=1), or $\exists o''[\langle o, o'' \rangle, \langle o'', o' \rangle \in R_{t-1}]$ (t>1)
- R-GNN[t](S, O) = R-GNN$(A_t(S), O^2)$
- **Final readout:** $V(S) = \mathbf{MLP}\left(\Sigma_{o \in O} \boldsymbol{f}_L(o, o)\right)$ aggregates $|O|$ embeddings

Example: Navigation With XY Coordinates



- Navigation in rectangular grid with decoupled coordinates: cells and blocked cells with CELL(x, y) and BLOCKED(x, y), position with AT(x, y), and ADJ$(i, i+1)$
- After 12 hours of training on 105 random $n \times m$ instances, $mn < 30$, greedy policies achieve coverages of **59.72%**, **80.55%**, and **100%** for R-GNN, R-GNN[0], and R-GNN[1] on instances with **different sets of blocked cells and** $nm \leq 32$
- For computing goal distances (ie V^*), cells (x, y) must "communicate" with neighbors (x, y') and (x', y). In the plain R-GNN, there must be atoms involving $\{x, y, y'\}$ (similarly, $\{x, x', y\}$). No such atoms exists in S, except in R-GNN[t] where $A_t(S)$ includes $\Delta(\langle x, x' \rangle, \langle x', y \rangle, \langle x, y \rangle)$ and $\Delta(\langle x, y \rangle, \langle y, y' \rangle, \langle x, y' \rangle)$

Experiments: Setup

- A learned value function V for domain D defines a **general policy** π_V that at state S selects an unvisited successor state S' with lowest $V(S')$ value
- Implemented in PyTorch. Trained on Nvidia A10s with 24Gb of memory over 12 hours, using Adam, lr=0.0002, batches of size 16, and no regularization. Embedding dimension of $k = 64$, and $L = 30$ layers
- For each domain and architecture, 3 models were trained, and best model on validation was selected.
- Standard benchmarks from **International Planning Competition (IPC)**
- **Baselines:** Edge Transformer (ET) [Bergen *et al.*, 2021] designed to do triangulations on graphs, R-GNN$_2$ that adds all Δ atoms, and 2-GNNs that emulates 2-OWL

Expressivity of the R-GNN[t] Architecture

- The architecture R-GNN[t] has the capability to capture compositions of binary relations that can be expressed in $\mathcal{C}_3$

Definition ($\mathcal{C}_3$-Joins)**.** *Let σ be relational language. The class $\mathcal{J}_3 = \mathcal{J}_3[\sigma]$ of relational joins is the* ***smallest class*** *of formulas that satisfies:*

1. *$\{R(x, y), \neg R(x, y)\} \subseteq \mathcal{J}_3$ for relation R in σ,*
2. *$\mathcal{J}_3$ is closed under conjunctions and disjunctions, and*
3. *$\exists y[\phi(x, y) \wedge \phi(y, z)] \in \mathcal{J}_3$ if $\{\phi(x, y), \phi(y, z)\} \subseteq \mathcal{J}_3$.*

Notation *$\phi(x, y)$: ϕ is a formula whose free variables are among $\{x, y\}$*

Theorem. *Let σ be relational language, and let $\mathcal{D} \subseteq \mathcal{J}_3$ be* ***finite collection*** *of $\mathcal{C}_3$-joins. There is parameter $\langle t, k, L \rangle$, where k is embedding dimension and L is number of layers, and network N in* R-GNN$[\sigma, t, k, L]$ *that* ***computes*** *$\mathcal{D}$*

Conclusions

- Novel parametric architecture R-GNN[t] that **provably** increases the expressivity of the relational R-GNN architecture
- R-GNN[t] embeds all pair of objects but does a bounded number of triangulations, determined by the value of parameter $t \geq 0$
- In benchmarks, a small value of $t = 1$ achieves best results
- Other ways to increase expressivity, like k-GNNs for $k \geq 2$, in either the OWL or FWL setting are infeasible in practice due to high number of objects: $\Theta(N^k)$ space, $\Theta(N^{k+1})$ time
- **Future:** consider use of indexicals/markers that can be moved around as an alternative to increase the expressivity in GNN architectures for planning

Experiments: Results

			Plan Length		
Domain	Model	Coverage (%)	Total	Median	Mean
Blocks-s	R-GNN	**17 / 17 (100 %)**	674	38	39
	R-GNN[0]	**17 / 17 (100 %)**	670	36	39
	R-GNN[1]	**17 / 17 (100 %)**	684	36	40
	R-GNN$_2$	14 / 17 (82 %)	922	35	65
	2-GNN	**17 / 17 (100 %)**	678	36	39
	ET	16 / 17 (94 %)	826	38	51
Blocks-m	R-GNN	**22 / 22 (100 %)**	868	40	39
	R-GNN[0]	**22 / 22 (100 %)**	830	39	37
	R-GNN[1]	**22 / 22 (100 %)**	834	39	37
	R-GNN$_2$	**22 / 22 (100 %)**	936	39	42
	2-GNN	20 / 22 (91 %)	750	40	37
	ET	18 / 22 (82 %)	966	39	53
Gripper	R-GNN	**18 / 18 (100 %)**	4,800	231	266
	R-GNN[0]	**18 / 18 (100 %)**	1,764	98	98
	R-GNN[1]	11 / 18 (61 %)	847	77	77
	R-GNN$_2$	**18 / 18 (100 %)**	1,764	98	98
	2-GNN	1 / 18 (6 %)	53	53	53
	ET	4 / 18 (22 %)	246	61	61
Miconic	R-GNN	**20 / 20 (100 %)**	1,342	67	67
	R-GNN[0]	**20 / 20 (100 %)**	1,566	71	78
	R-GNN[1]	**20 / 20 (100 %)**	2,576	71	128
	R-GNN$_2$	**20 / 20 (100 %)**	1,342	67	67
	2-GNN	12 / 20 (60 %)	649	54.5	54
	ET	**20 / 20 (100 %)**	1,368	68	68
Visitall	R-GNN	18 / 22 (82 %)	636	29	35
	R-GNN[0]	21 / 22 (95 %)	1,128	35	53
	R-GNN[1]	**22 / 22 (100 %)**	886	35	40
	R-GNN$_2$	20 / 22 (91 %)	739	33	36
	2-GNN	18 / 22 (82 %)	626	32	34
	ET	18 / 22 (82 %)	670	29	37

			Plan Length		
Domain	Model	Coverage (%)	Total	Median	Mean
Grid	R-GNN	9 / 20 (45 %)	109	11	12
	R-GNN[0]	12 / 20 (60 %)	177	11	14
	R-GNN[1]	**15 / 20 (75 %)**	209	13	13
	R-GNN$_2$	10 / 20 (50 %)	124	11.5	12
	2-GNN	6 / 20 (30 %)	82	11.5	13
	ET	1 / 20 (5 %)	15	15	15
Logistics	R-GNN	10 / 20 (50 %)	510	51	51
	R-GNN[0]	9 / 20 (45 %)	439	48	48
	R-GNN[1]	**20 / 20 (100 %)**	1,057	52	52
	R-GNN$_2$	15 / 20 (75 %)	799	52	53
	2-GNN	0 / 20 (0 %)	–	–	–
	ET	0 / 20 (0 %)	–	–	–
Rovers	R-GNN	9 / 20 (45 %)	2,599	280	288
	R-GNN[0]	**14 / 20 (70 %)**	2,418	153	172
	R-GNN[1]	**14 / 20 (70 %)**	1,654	55	118
	R-GNN$_2$	11 / 20 (55 %)	2,225	239	202
	2-GNN	Unsuitable domain: ternary predicates			
	ET				
Vacuum	R-GNN	**20 / 20 (100 %)**	4,317	141	215
	R-GNN[0]	**20 / 20 (100 %)**	183	9	9
	R-GNN[1]	**20 / 20 (100 %)**	192	9	9
	R-GNN$_2$	**20 / 20 (100 %)**	226	9	11
	2-GNN	Unsuitable domain: ternary predicates			
	ET				
Visitall-xy	R-GNN	5 / 20 (25 %)	893	166	178
	R-GNN[0]	15 / 20 (75 %)	1,461	84	97
	R-GNN[1]	**20 / 20 (100 %)**	1,829	83	91
	R-GNN$_2$	19 / 20 (95 %)	2,428	116	127
	2-GNN	12 / 20 (60 %)	1,435	115	119
	ET	3 / 20 (15 %)	455	138	151

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