Learning More Expressive General Policies for Classical Planning Domains

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Introduction

- General policies represent strategies for solving many planning instances
 - ▷ E.g., general policy for solving **all** Blocksworld problems
- Three main methods for learning such policies (no "synthesis" methods yet!)
 - Combinatorial optimization using explicit pool of C₂ features obtained from domain predicates [B. et al., 2019; Francès et al., 2021]
 - Deep learning (DL) using domain predicates but no explicit pool [Toyer et al., 2020; Garg et al., 2020]
 - DL exploiting relation between C₂ logic and GNNs [Barceló et al., 2020; Grohe, 2020; Ståhlberg et al., 2022]
 - \square **R-GNN architecture** adapted from Max-CSP[Γ] [Toenshoff *et al.*, 2021]
 - $\hfill\square$ More transparent and simple, scalable
 - □ Supervised and non-supervised training
 - □ **Problem:** insufficient expressivity for generalized planning

In this Work

- Novel relational architecture R-GNN[t], with parameter $t \ge 0$, 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 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, C_2 expressivity (yet see below)
 - ▷ 3-GNNs: $\Theta(N^3)$ memory, $\Theta(N^4)$ time, C_3 expressivity
 - ▷ ETs: $\Theta(N^2)$ memory, $\Theta(N^3)$ time, C_3 expressivity [Müller *et al.*, 2024]
 - ▷ Provably Powerful GNs [Maron *et al.*, 2019]: 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 $\{P_1, P_2, P_3, \ldots\}$ of ground instances $P_i = \langle D, I_i \rangle$ over common first-order STRIPS domain D
- 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 $P = \langle D, I \rangle$ 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)
	<pre>(free ?g - gripper) (carry ?o - ball ?g - gripper))</pre>

(:action MOVE

```
:parameters
                   (?from ?to - room)
    :precondition (at-robot ?from)
    :effect
                   (and (at-robot ?to) (not (at-robot ?from))))
(:action PICK
                   (?obj - ball ?room - room ?gripper - gripper)
    :parameters
    :precondition (and (at ?obj ?room) (at-robot ?room) (free ?gripper))
    :effect
                   (and (carry ?obj ?gripper) (not (at ?obj ?room)) (not (free ?gripper))))
(:action DROP
                  (?obj - ball ?room - room ?gripper - gripper)
    :parameters
    :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 for Planning [Stählberg et al., 2022-2024]

• Planning state S over STRIPS domain D is a **relational structure**:

- \triangleright Relational symbols given by predicates in D; shared by all such states S
- \blacktriangleright 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 f_L(o) for each object o \in O
1. Initialize \mathbf{f}_0(o) = 0^k for each object o \in O
2. for i \in \{0, 1, \dots, L-1\} do
       for each atom q = p(o_1, o_2, \ldots, o_m) \in S do
3.
          m_{q,o_{j}} := \left[ \operatorname{MLP}_{p} \left( \boldsymbol{f}_{i}(o_{1}), \boldsymbol{f}_{i}(o_{2}), \dots, \boldsymbol{f}_{i}(o_{m}) \right) \right]_{j}
4.
5.
       end for
      for each object o \in O do
6.
          \boldsymbol{f}_{i+1}(o) := \boldsymbol{f}_i(o) + \mathbf{MLP}_U(\boldsymbol{f}_i(o), \operatorname{agg}(\{\!\!\{\boldsymbol{m}_{q,o} \mid o \in q, q \in S\}\!\!\}))
7.
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:

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

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

where S_a is result of applying action a in state S

Successful approach for GP, but subject to expressivity of GNNs...

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)
- 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 state S

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 C_2 logic (formulas with counting quantifiers, and at most 2 variables)
- Eg, join $W(x,y) = \exists z.[R(x,z) \land T(z,y)]$ 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
- Can augment expressivity with 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
 - \triangleright Related to, respectively, \mathcal{C}_{k-1} and \mathcal{C}_k logics: counting quant., k variables
 - \triangleright Infeasible by num. objs. in planning problems: $\Theta(N^k)/\Theta(N^{k+1})$ space/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: $p(a, b) \rightarrow p(\langle a, a \rangle, \langle a, b \rangle, \langle b, a \rangle, \langle b, b \rangle)$
 - \triangleright 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 $t \ge 0$ ▶ $A_0(S) = \{p(\langle w \rangle^2) \mid p(w) \in S\}$ for $\langle w \rangle^2 = \langle (o_1, o_1), \dots, (o_i, o_j), \dots, (o_m, o_m) \rangle$ ▶ $A_t(S) = A_0(S) \cup \{\Delta(\langle o, o' \rangle, \langle o', o'' \rangle, \langle o, o'' \rangle) \mid \langle o, o' \rangle, \langle o', o'' \rangle \in R_t\}$ ▶ $\langle o, o' \rangle \in R_t$ 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)
- $\mathsf{R}\text{-}\mathsf{GNN}[t](S,O) = \mathsf{R}\text{-}\mathsf{GNN}(A_t(S),O^2)$
- Final readout: $V(S) = \mathsf{MLP}(\sum_{o \in O} f_L(o, o))$ 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** $nm \le 32$
- 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
- We implemented in PyTorch, and trained on Nvidia A10s with 24Gb of memory over 12 hours, using Adam, Ir=0.0002, batches of size 16, and no regularization. Embedding dimension of k = 64, and L = 30 layers were used.
- Standard benchmarks from International Planning Competition (IPC)
- For each domain and architecture, 3 models were trained, and best model on validation was selected.

• Baselines:

- ▶ Edge Transformer (ET) [Bergen *et al.*, 2021] designed to do triangulations on graphs
- \triangleright R-GNN₂ that adds all Δ atoms
- \triangleright 2-GNNs that emulates 2-OWL which captures C_3

Experiments: Results

			Plan Length						Plan Leng		n
Domain	Model	Coverage (%)	Total	Median	Mean	Domain	Model	Coverage (%)	Total	Median	Mean
Blocks-s	R-GNN R-GNN[0] R-GNN[1] R-GNN2 2-GNN ET R-GNN R-GNN[0] R-GNN[1] R-GNN2 2-GNN ET	17 / 17 (100 %) 17 / 17 (100 %) 17 / 17 (100 %) 14 / 17 (82 %) 17 / 17 (100 %) 16 / 17 (94 %) 22 / 22 (100 %) 22 / 22 (100 %) 22 / 22 (100 %) 22 / 22 (100 %) 22 / 22 (91 %) 18 / 22 (92 %)	674 670 684 922 678 826 868 830 834 936 750 966	38 36 36 35 36 38 40 39 39 39 40 30	39 39 40 65 39 51 39 37 37 42 37	Grid	R-GNN R-GNN[0] R-GNN[1] R-GNN2 2-GNN ET R-GNN R-GNN[0] R-GNN[1] R-GNN2 2-GNN ET	9 / 20 (45 %) 12 / 20 (60 %) 15 / 20 (75 %) 10 / 20 (50 %) 6 / 20 (30 %) 1 / 20 (5 %) 10 / 20 (50 %) 9 / 20 (45 %) 20 / 20 (100 %) 15 / 20 (75 %) 0 / 20 (0 %) 0 / 20 (0 %)	109 177 209 124 82 15 510 439 1,057 799 -	$ \begin{array}{c} 11\\ 11\\ 13\\ 11.5\\ 15\\ 15\\ 51\\ 48\\ 52\\ 52\\ -\\ -\\ -\\ -\\ -\\ -\\ -\\ -\\ -\\ -\\ -\\ -\\ -\\$	12 14 13 12 13 15 51 48 52 53 -
Gripper	R-GNN R-GNN[0] R-GNN[1] R-GNN ₂ 2-GNN ET	18 / 18 (100 %) 18 / 18 (100 %) 11 / 18 (61 %) 18 / 18 (100 %) 1 / 18 (6 %) 4 / 18 (22 %)	4,800 1,764 847 1,764 53 246	231 98 77 98 53 61	266 98 77 98 53 61	Rovers	R-GNN R-GNN[0] R-GNN[1] R-GNN ₂ 2-GNN ET	9 / 20 (45 %) 14 / 20 (70 %) 14 / 20 (70 %) 11 / 20 (55 %) Unsuitable dom	2,599 2,418 1,654 2,225 ain: terr	280 153 55 239 nary predic	288 172 118 202 cates
Miconic	R-GNN R-GNN[0] R-GNN[1] R-GNN ₂ 2-GNN ET	20 / 20 (100 %) 20 / 20 (100 %) 20 / 20 (100 %) 20 / 20 (100 %) 12 / 20 (60 %) 20 / 20 (100 %)	1,342 1,566 2,576 1,342 649 1,368	67 71 71 67 54.5 68	67 78 128 67 54 68	Vacuum	R-GNN R-GNN[0] R-GNN[1] R-GNN ₂ 2-GNN ET	20 / 20 (100 %) 20 / 20 (100 %) 20 / 20 (100 %) 20 / 20 (100 %) Unsuitable dom	4,317 183 192 226 ain: terr	141 9 9 9 nary predic	215 9 9 11 cates
Visitall	R-GNN R-GNN[0] R-GNN[1] R-GNN ₂ 2-GNN ET	18 / 22 (82 %) 21 / 22 (95 %) 22 / 22 (100 %) 20 / 22 (91 %) 18 / 22 (82 %) 18 / 22 (82 %)	636 1,128 886 739 626 670	29 35 35 33 32 29	35 53 40 36 34 37	Visitall-xy	R-GNN R-GNN[0] R-GNN[1] R-GNN ₂ 2-GNN ET	5 / 20 (25 %) 15 / 20 (75 %) 20 / 20 (100 %) 19 / 20 (95 %) 12 / 20 (60 %) 3 / 20 (15 %)	893 1,461 1,829 2,428 1,435 455	166 84 83 116 115 138	178 97 91 127 119 151

Experiments: #Objects in Training / Validation, and Test Sets

Domain	Training / Validation	Test
Blocks	4–9	10–20
Gripper	2–14	16–50
Logistics	2–5 / 3–5	15–19 / 8–11
Miconic	2–20 / 1–10	11–30 / 22–60
Rovers	2–3 / 3–8	3 / 21–39
Vaccum	8–38 / 11–6	40–93 / 6–10
Visitall	1–21	100

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 C_3

Definition (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. $\{R(x,y), \neg R(x,y)\} \subseteq \mathcal{J}_3 \text{ for relation } R \text{ in } \sigma$,
- 2. \mathcal{J}_3 is closed under conjunctions and disjunctions, and
- 3. $\exists y[\phi(x,y) \land \phi(y,z)] \in \mathcal{J}_3 \text{ if } \{\phi(x,y),\phi(y,z)\} \subseteq \mathcal{J}_3.$

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[σ, 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 ≥ 0
- In benchmarks, a small value of t = 1 achieves best results
- Other ways to increase expressivity, like k-GNNs for $k \ge 2$, 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 work: consider use of indexicals/markers that can be moved around as an alternative to increase the expressivity in GNN architectures for planning

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