One Model, Any CSP: Graph Neural Networks as Fast Global Search Heuristics for Constraint Satisfaction

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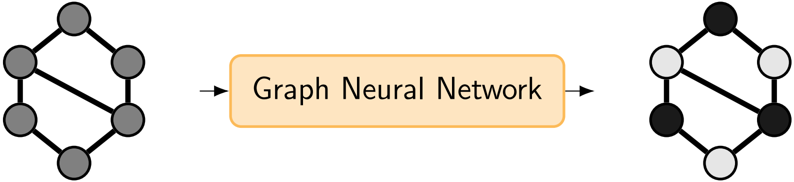
Neural Combinatorial Optimization

Learn heuristics for combinatorial optimization with Graph Neural Networks:



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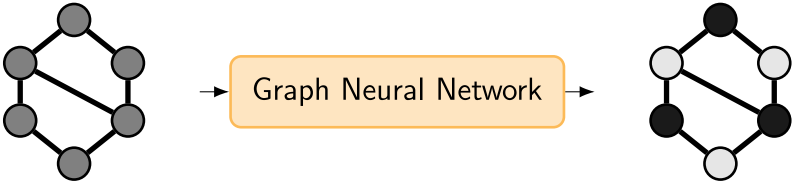

Pros

- Learn novel algorithms from scratch
- Data-driven fine-tuning

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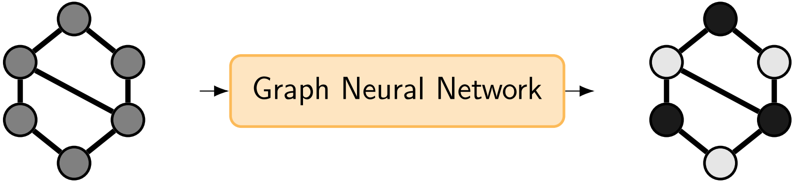

Pros

- Learn novel algorithms from scratch
- Data-driven fine-tuning

Cons

- Computationally expensive
- Problem specific approaches

Constraint Satisfaction Problems

Constraint Satisfaction Problems

$\mathcal{I} = (\mathcal{X}, \mathcal{D}, \mathcal{C})$

- Variables $\mathcal{X} = \{X_1, \ldots, X_n\}$
- Domains $\mathcal{D} = \{\mathcal{D}(X_1), \ldots, \mathcal{D}(X_n)\}$
- Constraints $\mathcal{C} = \{C_1, \ldots, C_m\}$

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Variable assignment α: $\alpha(X) \in \mathcal{D}(X)$

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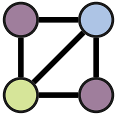
Boolean SAT:

$$f = (X_1 \vee \neg X_2) \wedge X_3$$

Graph Coloring:



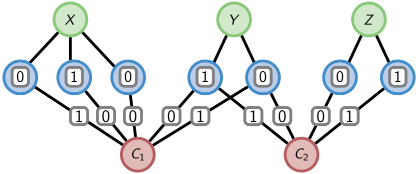
ANYCSP

Are **N**eural Networks great heuristics? **Y**es, for **CSP**s!

- Design unified graph representation and GNN architecture for all CSPs
- Optimize global search heuristic with reinforcement learning

Graph Representation

$$G(\mathcal{I}, \alpha)$$



Learnable Heuristics

$$\pi_\theta$$

$$G(\mathcal{I}, \alpha^{(t)}) \longrightarrow \boxed{\text{GNN } \pi_\theta} \longrightarrow \alpha^{(t+1)}$$

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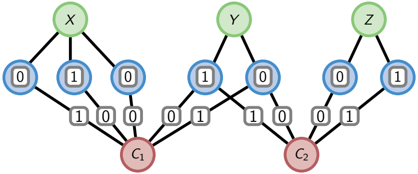

Learnable Heuristics

π_θ

$$(X_1 \lor \neg X_2) \land X_3 \rightarrow \boxed{\text{GNN } \pi_\theta} \rightarrow \begin{array}{l} X_1 = 1 \\ X_2 = 0 \\ X_3 = 1 \end{array}$$

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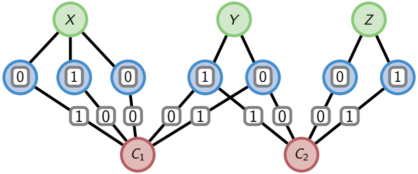

Learnable Heuristics

π_θ

Constraint Value Graph

CSP Instance $\mathcal{I}$:

$\mathcal{X} = \{X, Y, Z\}$

$D_X = \{1, 2, 3\}$
$D_Y = \{1, 2\}$
$D_Z = \{1, 2\}$

$C_1 : X \leq Y$
$C_2 : Y \neq Z$

Assignment $\alpha = (2, 1, 2)$

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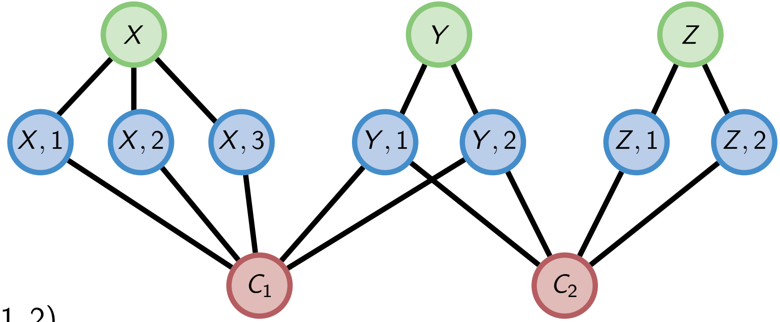
$G(\mathcal{I}, \alpha) = (V, E, L_{\mathcal{D}}, L_{\mathcal{C}})$



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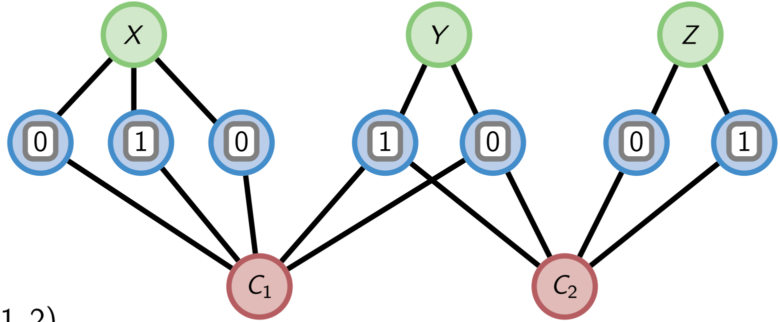

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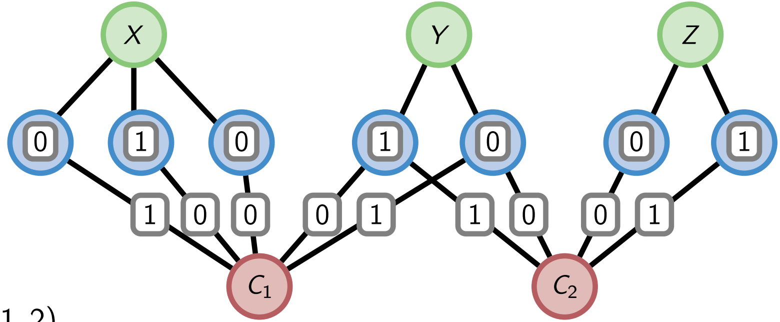
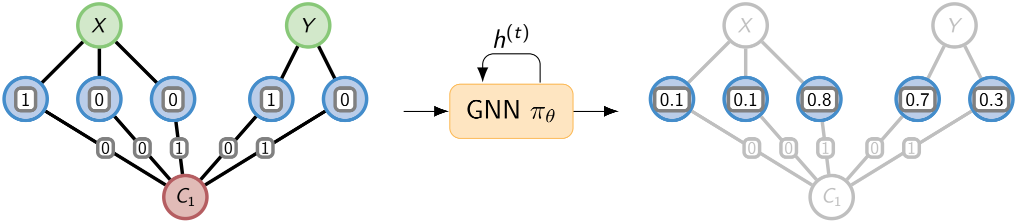


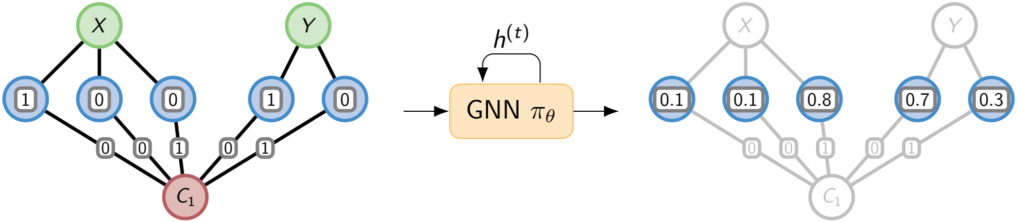
Policy GNN



Our GNN π_θ is a trainable stochastic global search policy:

- Input: $G(\mathcal{I}, \alpha^{(t)})$, recurrent states $h^{(t)}$
- Output: Soft assignment $\varphi^{(t+1)}$

Policy GNN



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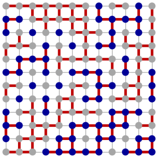
- Input: $G(\mathcal{I}, \alpha^{(t)})$, recurrent states $h^{(t)}$
- Output: Soft assignment $\varphi^{(t+1)}$
- Next assignment: $\alpha^{(t+1)} \sim \varphi^{(t+1)}$

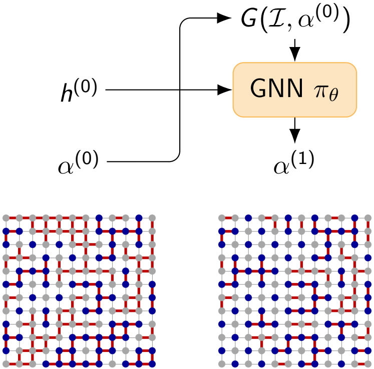
Stochastic Global Search

$h^{(0)}$

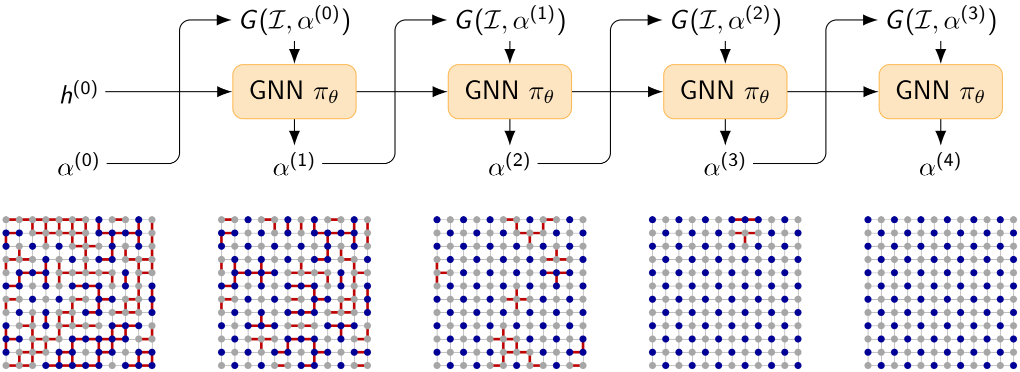
$\alpha^{(0)}$



Stochastic Global Search



Stochastic Global Search



Training

Given a training distribution Ω we optimize π_θ with respect to the reinforcement learning objective

$$\theta^* = \arg\max_{\theta} \mathop{\mathbf{E}}_{\substack{\mathcal{I}\sim\Omega \\ \boldsymbol{\alpha}\sim\pi_\theta(\mathcal{I})}} \left[\sum_{t=1}^{T} \gamma^{t-1} r^{(t)} \right]$$

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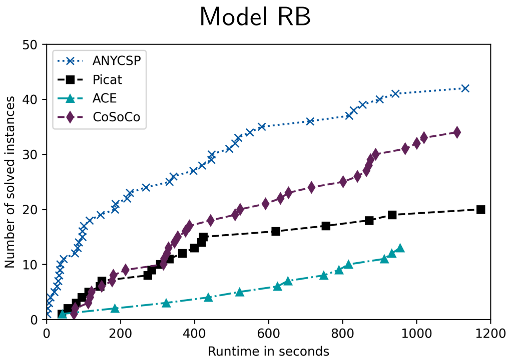
Quality in iteration t:

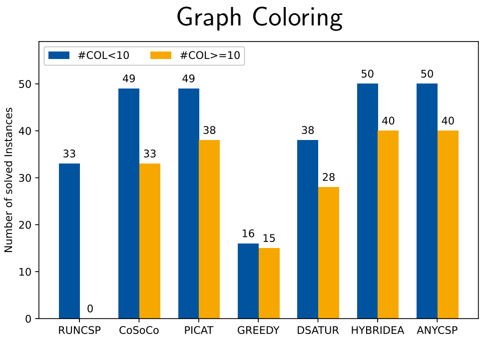
$$Q_{\mathcal{I}}(\alpha) := \frac{|\{C \in \mathcal{C} \ : \ \alpha \models C\}|}{|\mathcal{C}|}$$

Reward in iteration t:

$$r^{(t)} := \max\left\{0,\ Q_{\mathcal{I}}(\alpha^{(t)}) - \max_{0 \leq t' < t} Q_{\mathcal{I}}(\alpha^{(t')})\right\},$$

Experiments





SAT

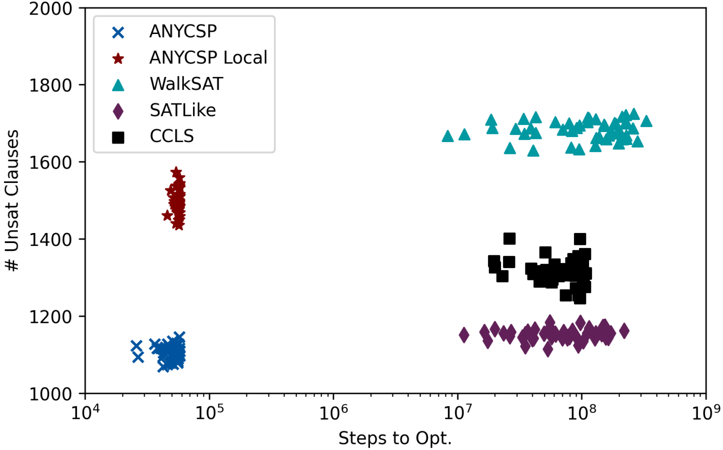
Instances: Random 3SAT Instances from SATLIB.

Metric: Number of satisfied instances.

Method	SL50	SL100	SL150	SL200	SL250
RLSAT	**100**	87	67	27	12
PDP	93	79	72	57	61
WalkSAT	**100**	**100**	97	93	87
ProbSAT	**100**	**100**	97	87	92
ANYCSP	**100**	**100**	**100**	**97**	**99**

MAX-SAT

Instances: 50 5-CNF formulas with 10K variables and 300K clauses.



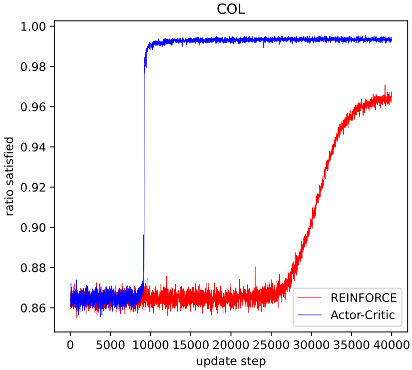
Further Modifications

Changes

- Actor-Critic architecture
- Geometric reward
- Entropy regularization

Results

- earlier, faster, and more robust learning
- better in distribution and on decision problems
- less stable



Conclusion

ANYCSP:

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- Reinforcement learning applied to exponential action spaces

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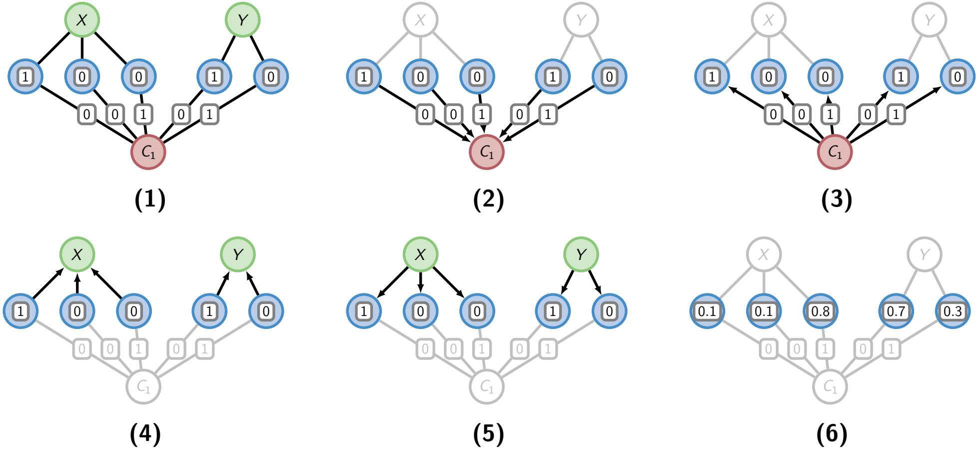
Empirical Observations:

- CSP heuristics can be obtained purely through data-driven training
- GNNs parameterize a powerful and versatile class of global search heuristics

π_θ: Message Passing Scheme



MaxCut

Instances: (Unweighted) GSet graphs

Metric: Mean absolute deviation from best known cut value.

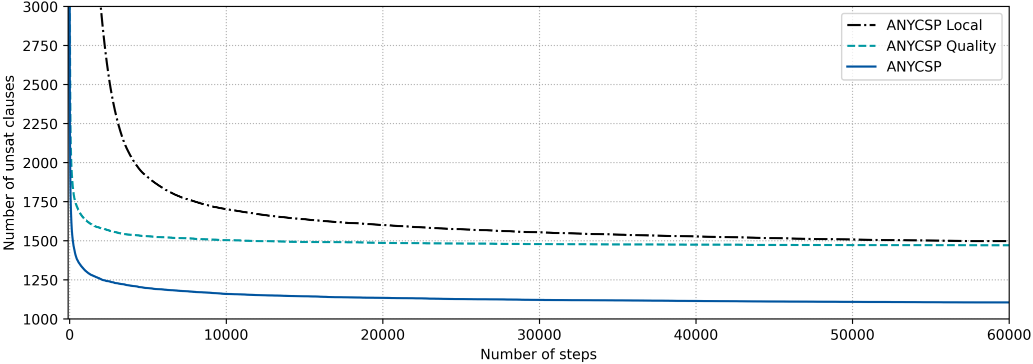
Method	$\|V\|$=800	$\|V\|$=1K	$\|V\|$=2K	$|V|\geq$3K
Greedy	411.44	359.11	737.00	774.25
SDP	245.44	229.22	-	-
RUNCSP	185.89	156.56	357.33	401.00
ECO-DQN	65.11	54.67	157.00	428.25
ECORD	8.67	8.78	39.22	187.75
ANYCSP	**1.22**	**2.44**	**13.11**	**51.63**

Cross-Comparison

Training Distribution Ω vs Test CSPs:

Ω	RB50	$\text{COL}_{<10}$	Gset800	SL250	MAX-5-CNF
$\Omega_{\textbf{RB}}$	**42**	**50**	655.56	98	6192.18
$\Omega_{\textbf{COL}}$	15	**50**	868.22	96	5076.16
$\Omega_{\textbf{MCUT}}$	0	0	**1.22**	0	9048.64
$\Omega_{\textbf{3SAT}}$	0	19	1213.11	**99**	5001.72
$\Omega_{\textbf{MSAT}}$	0	15	1217.67	66	**1103.14**

Ablation


3000
2750
2500
2250
2000
1750
1500
1250
1000
Number of unsat clauses
0
10000
20000
30000
40000
50000
60000
Number of steps
ANYCSP Local
ANYCSP Quality
ANYCSP

REINFORCE

Given a training distribution Ω we optimize π_θ with respect to the reinforcement learning objective

$$\theta^* = \arg\max_{\theta} \mathop{\mathbf{E}}_{\substack{\mathcal{I}\sim\Omega \\ \boldsymbol{\alpha}\sim\pi_\theta(\mathcal{I})}} \left[\sum_{t=1}^{T} \gamma^{t-1} r^{(t)} \right]$$

using the gradient estimation given by REINFORCE (Williams, 1992)

$$-\frac{1}{T} \sum_{t=1}^{T} G_t \frac{\nabla \pi_\theta(\alpha^{(t)} \mid \alpha^{(t-1)}, h^{(t-1)}, \mathcal{I})}{\pi_\theta(\alpha^{(t)} \mid \alpha^{(t-1)}, h^{(t-1)}, \mathcal{I})}$$

where G_t is the empirical gain

$$G_t = \sum_{k=t}^{T} \gamma^{k-t} r^{(k)}$$

Critic

A **critic** $\mathfrak{c}$ learns to estimate gain G_t from recurrent state $h^{(t)}$, which speeds up learning through a baseline (replacing G_t in policy gradient):

$$A_t = G_t - \mathfrak{c}(h^{(t)})$$

and temporal difference learning (replacing G_t everywhere):

$$G_t^{(n)} = \gamma^{n+1}\mathfrak{c}(h^{(t+n+1)}) + \sum_{k=t}^{t+n} \gamma^{k-t} r^{(k)},$$

$$G_t(\lambda) = \lambda^{T+1} G_t + (1-\lambda) \sum_{n=0}^{T} \lambda^n G_t^{(\min(n,T-t))}$$

Modified Reward

Geometric reward including quality and improvement:

$$r_g^{(t)} = \sqrt{(Q_{\mathcal{I}}(\alpha^{(t)}) - Q_{\mathcal{I}}(\alpha^{(0)})) \cdot r^{(t)}}$$

Entropy regularization incentivizes exploration:

$$r_e^{(t)} = r_g^{(t)} - \sigma \log \mathbf{P}(\alpha^{(t)} \mid \varphi_\theta^{(t)})$$

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