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

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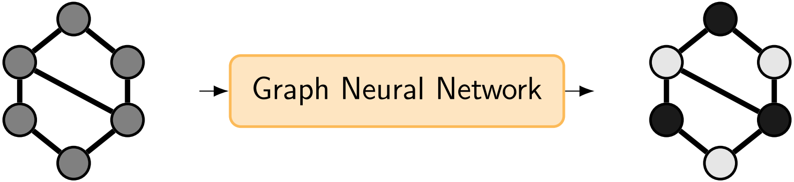
Neural Combinatorial Optimization

Learn heuristics for combinatorial optimization with Graph Neural Networks:



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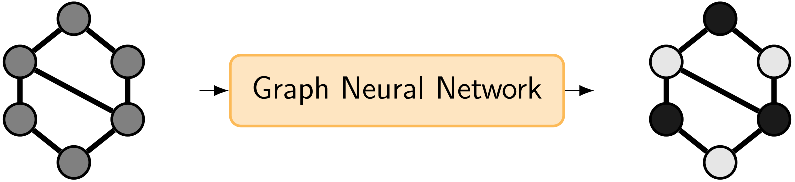

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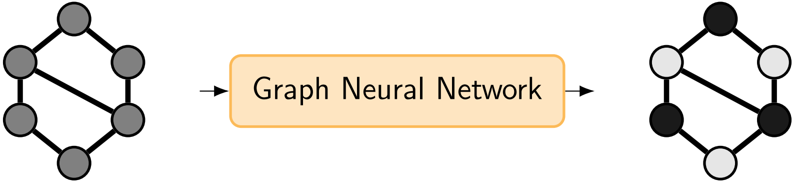

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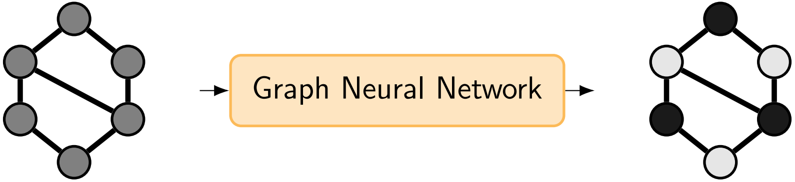

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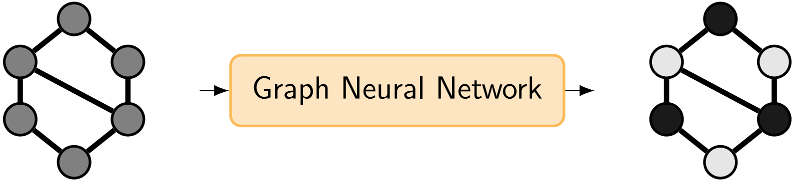

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Constraint Satisfaction Problems

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$$\alpha \models C \iff (\alpha(X_1^C), \dots, \alpha(X_\ell^C)) \in R^C$$

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Quality of assignment α for instance $\mathcal{I} = (\mathcal{X}, \mathcal{C}, \mathcal{D})$:

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Instance + Assignment

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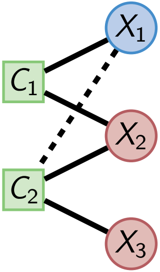
$\longrightarrow$



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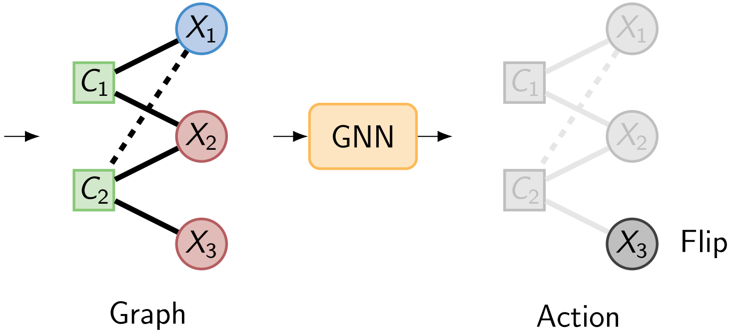

Related Work

Overview: (Cappart et al., 2021)

SAT:

- RLSAT (Yolcu and Póczos, 2019)
- PDP (Amizadeh et al., 2019)

MaxCut:

- S2V (Khalil et al., 2017)
- ECO-DQN (Barrett et al., 2020)
- ECORD (Barrett et al., 2022)

Binary CSPs:

- RUNCSP (Tönshoff et al., 2021)

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- Utilizes a global search action space.

Constraint Value Graph

CSP Instance $\mathcal{I}$:

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

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

$C_1 : X \leq Y$
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Assignment $\alpha = (2, 1, 2)$

Constraint Value Graph

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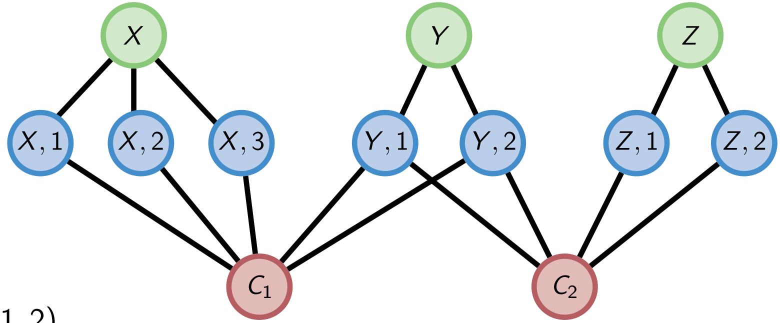

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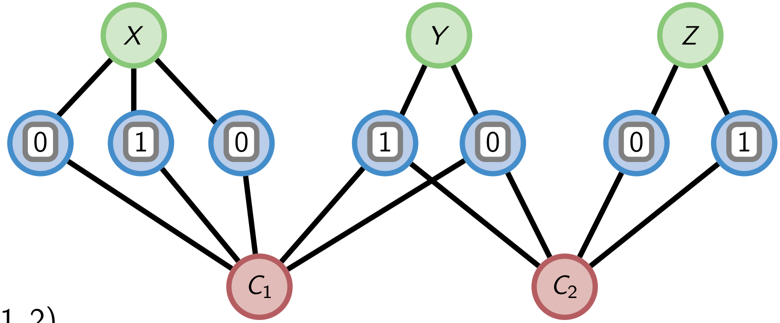

$L_{\mathcal{D}}(v) = 1 \iff \alpha(X_v) = v$

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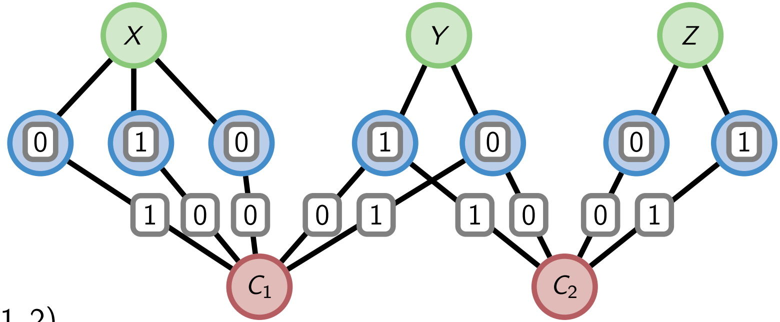

$L_{\mathcal{C}}(v, C) = 1 \iff \alpha[X_v = v] \models C$

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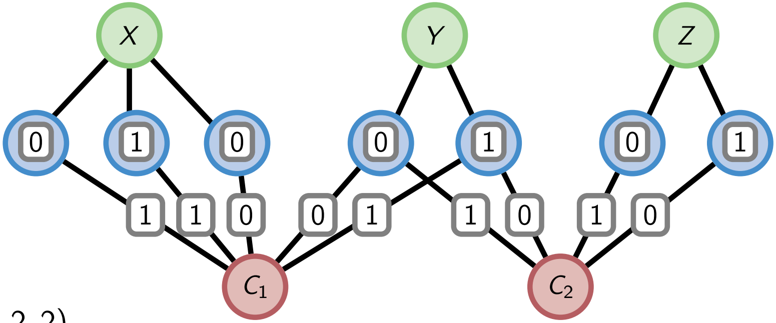

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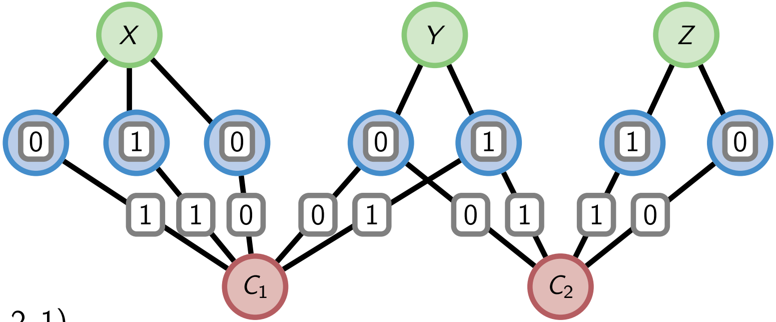

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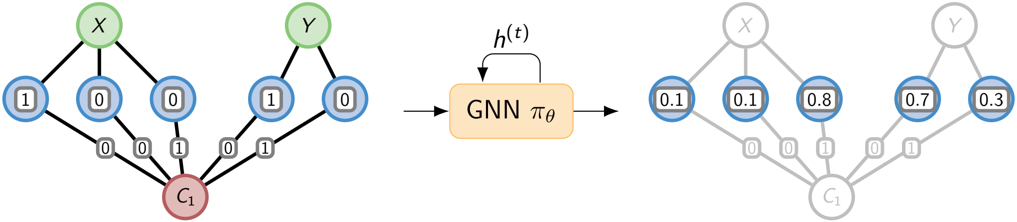

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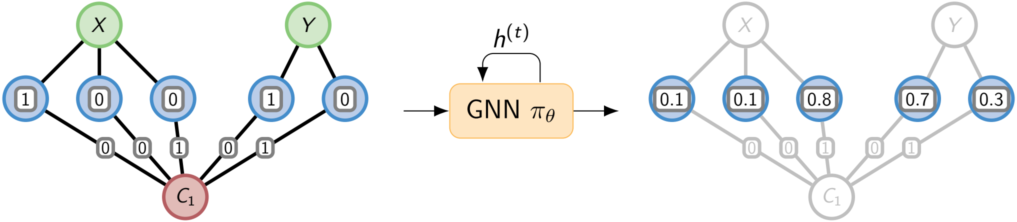

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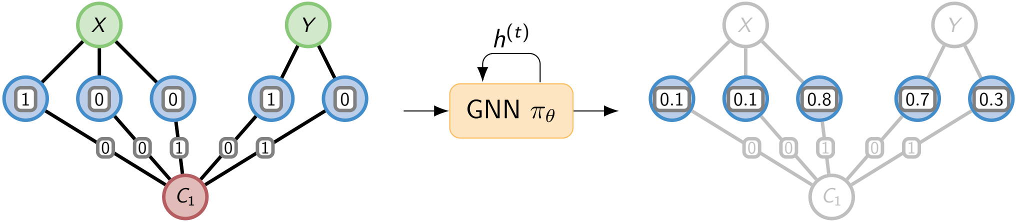

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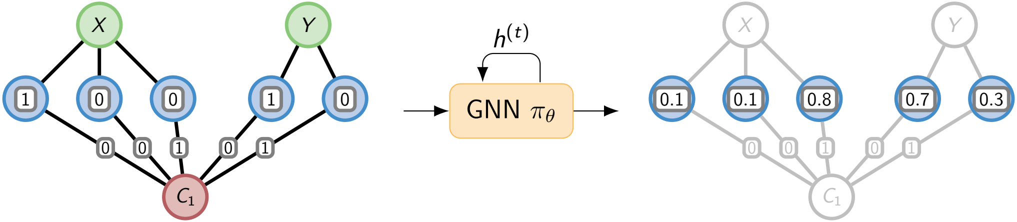

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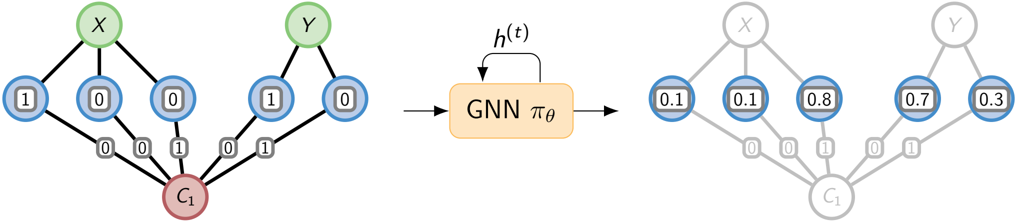

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- Next assignment: $\alpha^{(t+1)} \sim \varphi^{(t+1)}$

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Input: CSP instance $\mathcal{I}$, number of iterations T.

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$$\alpha^{(0)}$$

$$h^{(0)}$$

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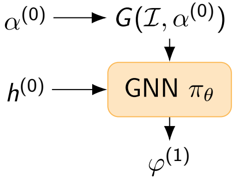

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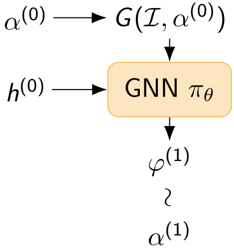

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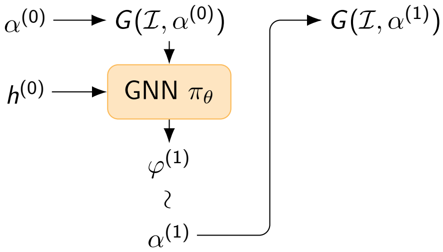

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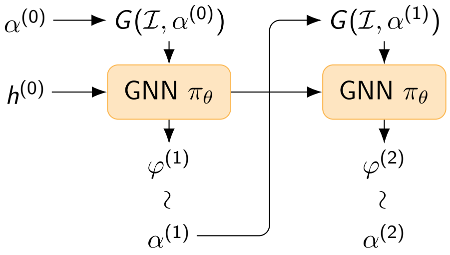

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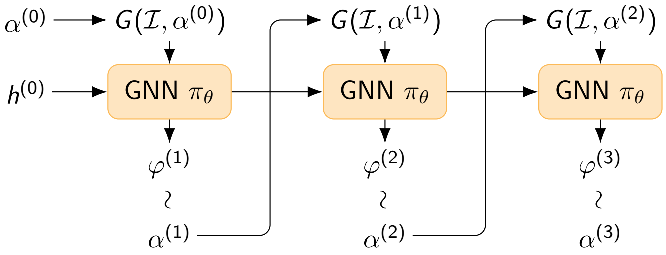

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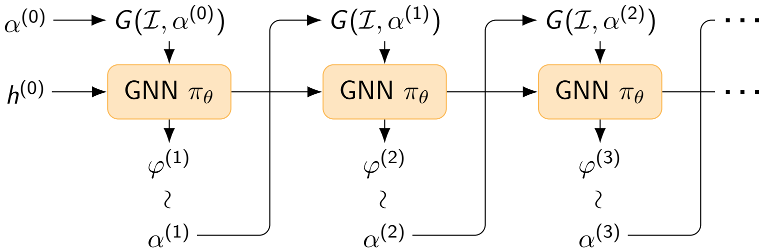

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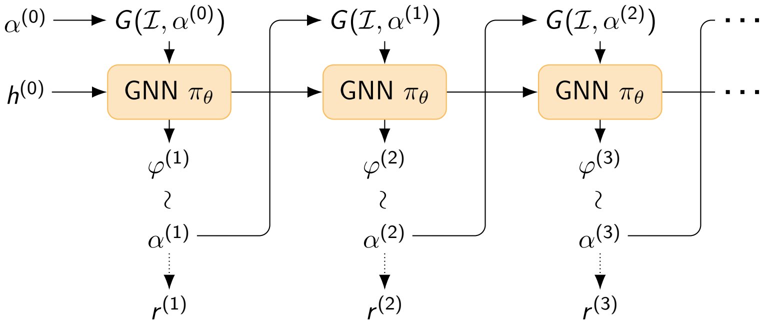

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For the total reward after T iterations we observe:

$$\sum_{t=1}^{T} r^{(t)} = q^{(T+1)} - Q_{\mathcal{I}}(\alpha^{(0)}) \tag{3}$$

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$$\theta^* = \arg\max_{\theta} \mathop{\mathbf{E}}_{\substack{\mathcal{I}\sim\Omega \\ \boldsymbol{\alpha}\sim\pi_\theta(\mathcal{I})}} \left[\sum_{t=1}^{T} \lambda^{t-1} r^{(t)} \right] \tag{4}$$

We use REINFORCE (Williams, 1992) to learn network parameters θ with SGD:

$$\mathcal{L}(\mathcal{I}, \boldsymbol{\alpha}, \boldsymbol{\varphi}_\theta) = -\sum_{t=1}^{T} G_t \log \mathbf{P}(\alpha^{(t)} | \varphi_\theta^{(t)}), \qquad G_t = \sum_{k=t}^{T} \lambda^{k-t} r^{(k)} \tag{5}$$

Training

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Policy Gradient methods allow us to handle very large action spaces.

Experiments

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We train heuristics for the following CSPs:

- Model RB ($\Omega_{\mathbf{RB}}$)
- Graph Coloring ($\Omega_{\mathbf{COL}}$)
- MaxCut ($\Omega_{\mathbf{MCUT}}$)
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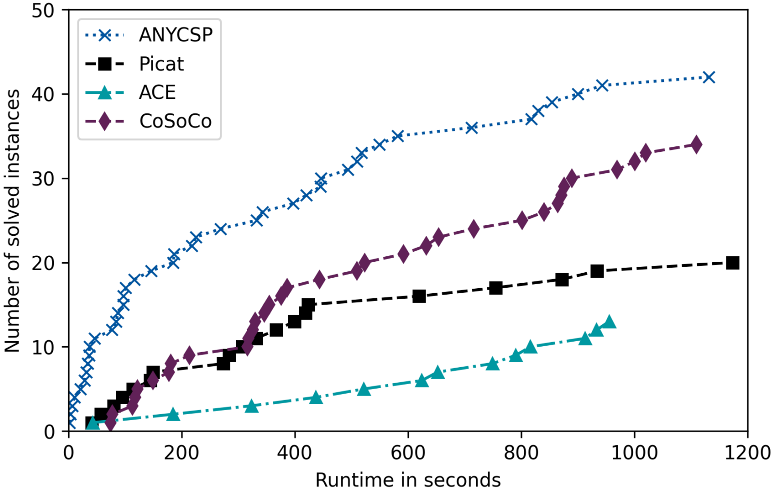
- Train for 500K steps of SGD ($\sim$48h) and batch size 25.

Model RB Benchmarks



MaxCut

Instances: (Unweighted) GSet graphs

Metric: Mean absolute deviation from known optimum 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**

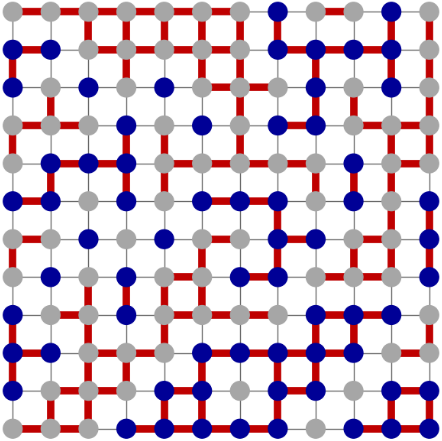
Graph Colouring

Instances: Structured k-Colouring instances ($4 \leq k \leq 73$, $|V| \leq 2000$, $|E| \leq 20000$)

Metric: Number of optimally coloured graphs.

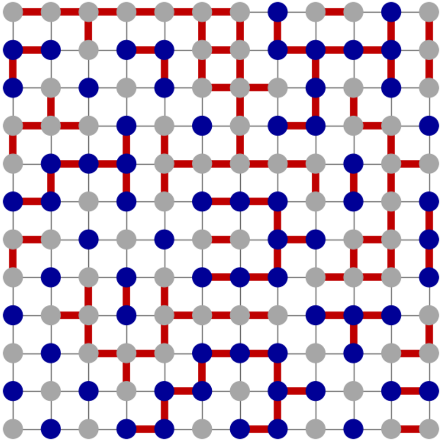
METHOD	$COL_{<10}$	$COL_{\geq 10}$
RUNCSP	33	-
COSOCO	49	33
PICAT	49	38
GREEDY	16	15
DSATUR	38	28
HYBRIDEA	**50**	**40**
ANYCSP	**50**	**40**

Graph Colouring



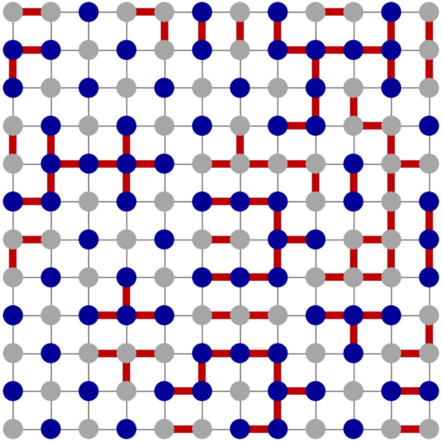
$t = 0$

Graph Colouring



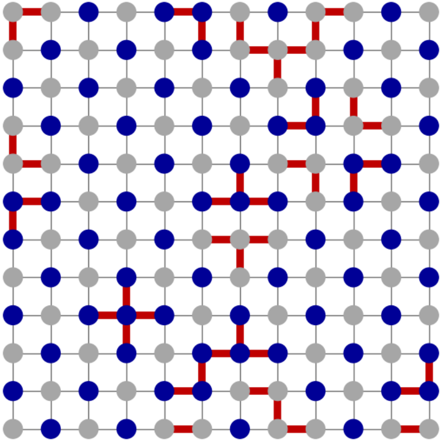
$t = 1$

Graph Colouring



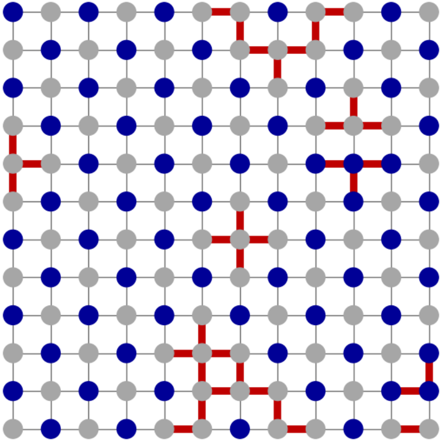
$t = 2$

Graph Colouring



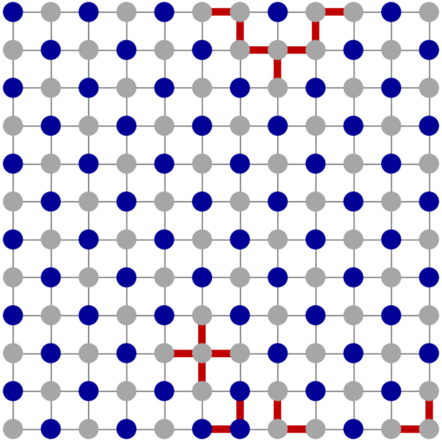
$t = 3$

Graph Colouring



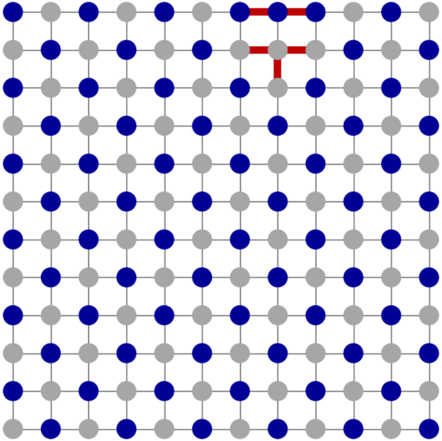
$t = 4$

Graph Colouring



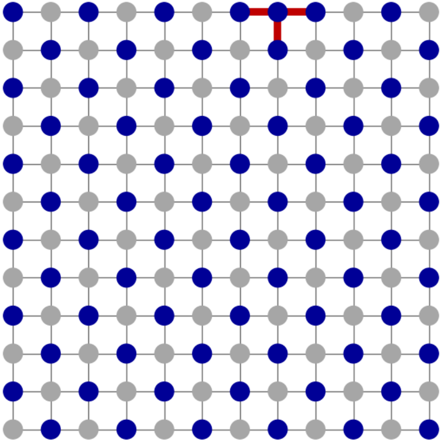
$t = 5$

Graph Colouring



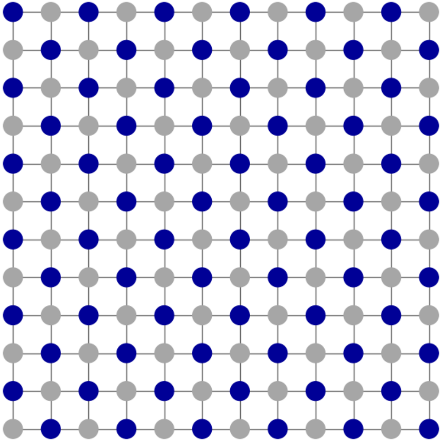
$t = 6$

Graph Colouring



$t = 7$

Graph Colouring



$t = 8$

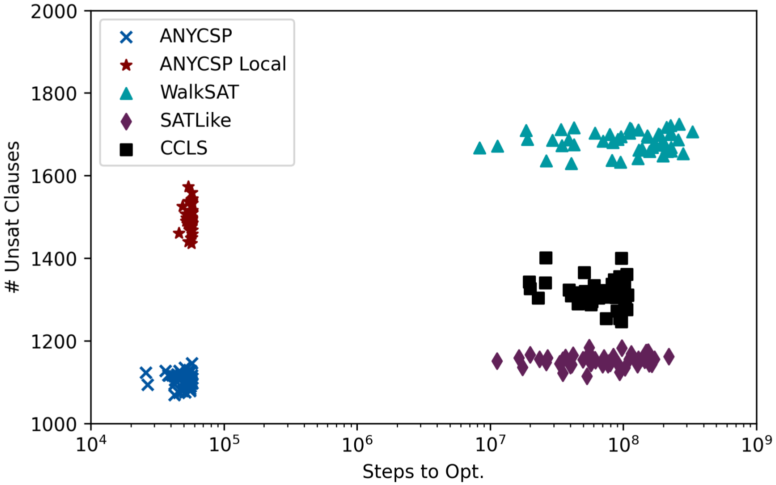
SAT

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-5-SAT



2000
1800
1600
1400
1200
1000
Unsat Clauses
10^4
10^5
10^6
10^7
10^8
10^9
Steps to Opt.
ANYCSP
ANYCSP Local
WalkSAT
SATLike
CCLS

Conclusion

ANYCSP:

- Constraint Value Graphs: A generic and compact representation for CSPs.
- REINFORCE 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 heuristic.

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Max-k-SAT

Instances: CNF formulas with 10K variables and 75K-300K clauses.

Metric: Mean number of unsatisfied clauses.

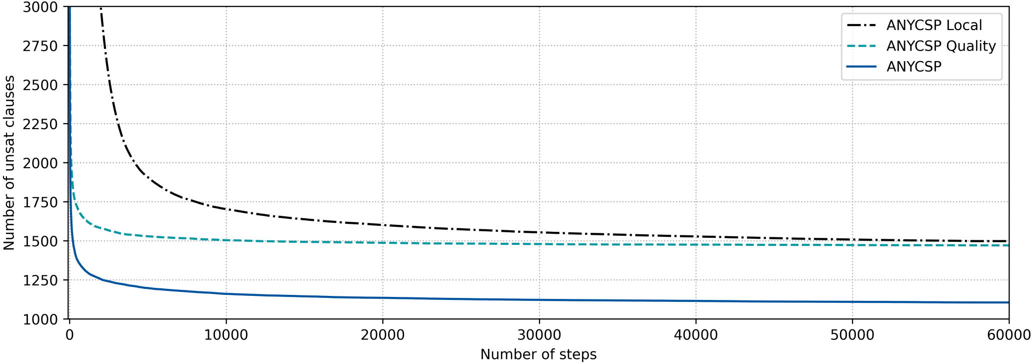
Method	3CNF	4CNF	5CNF
WalkSAT	2145.28	1556.68	1685.10
CCLS	1567.24	1323.14	1315.96
SATLike	1595.86	1188.56	1152.88
ANYCSP	**1537.46**	**1126.44**	**1103.14**

Cross-Comparison

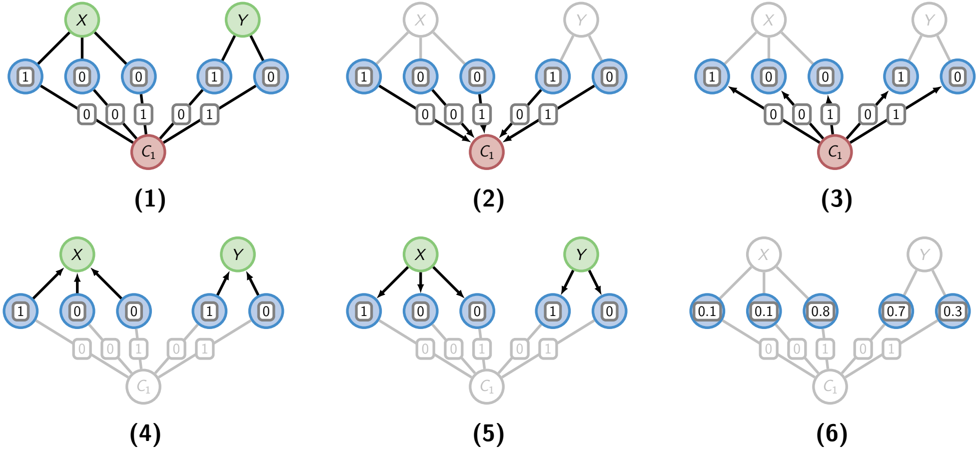
Training Distribution Ω vs Test CSPs:

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


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

π_θ: Message Passing Scheme



Markov Decision Process

The formal Markov Decision Process of ANYCSP:

- State at time t: $s^{(t)} = (G(\mathcal{I}, \alpha^{(t)}), q^{(t)})$, with $q^{(t)} = \max_{t'<t} Q_{\mathcal{I}}(\alpha^{(t')})$.
- Initial assignment $\alpha^{(0)}$ is drawn uniformly, $q^{(0)} = 0$.
- Action space $\mathcal{A}$: Set of all assignments of $\mathcal{I}$.
- Transition function: $(s^{(t)}, \alpha^{(t+1)}) \mapsto (G(\mathcal{I}, \alpha^{(t+1)}), \max\{q^{(t)}, Q_{\mathcal{I}}(\alpha^{(t)})\})$.
- Reward: $r^{(t)} = \max\{0, Q_{\mathcal{I}}(\alpha^{(t)}) - q^{(t)}\}$