Random Search Neural Networks for Efficient and Expressive Graph Learning

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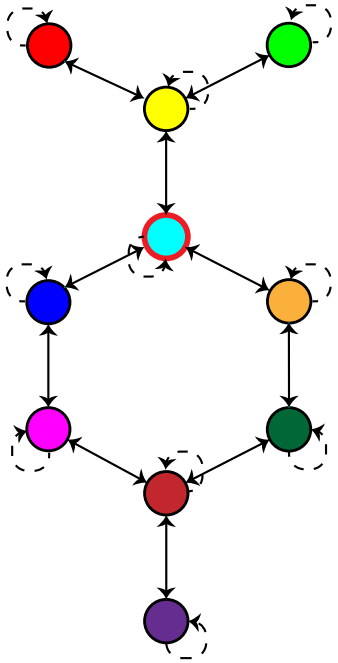
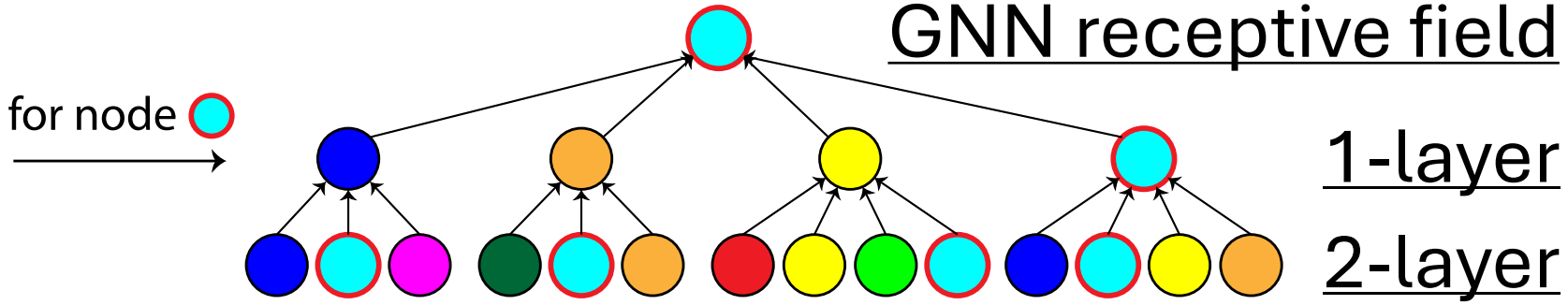
Limitations of Message-passing GNNs

- **Message-passing GNNs** are popular models for learning on graphs
  - Limited in **expressive power**[1]
  - Struggle with **oversmoothing**[2] and **oversquashing**[3]



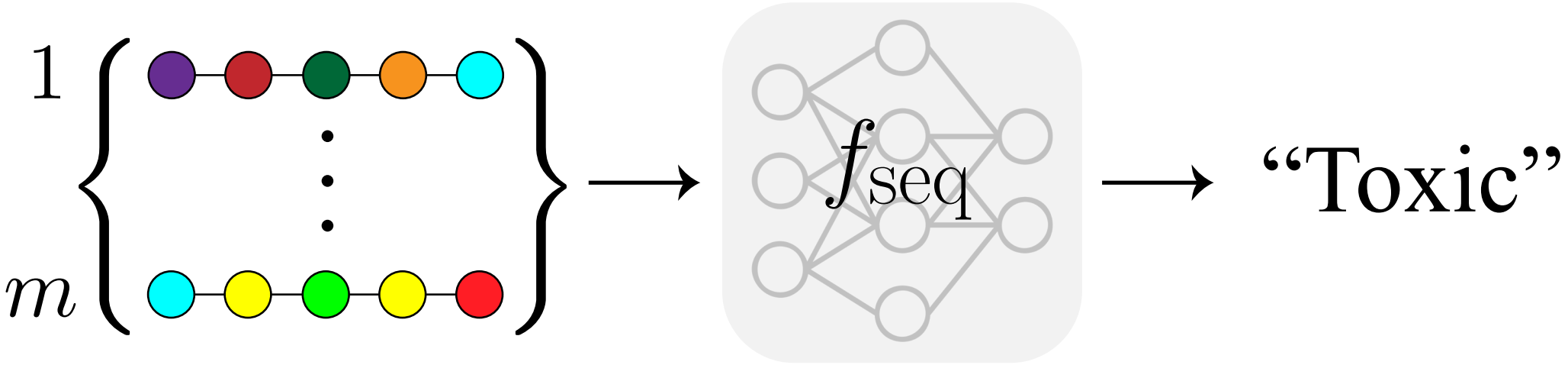
$$\mathbf{h}^{(l+1)}(i) = \text{Aggregate}(\{\mathbf{h}^{(l)}(j) : j \in \mathcal{N}(i)\})$$



[1. Xu et al., 2019, 2. Li et al., 2018, 3. Alon and Yahov 2020]

Random Walk Neural Networks (RWNNs)

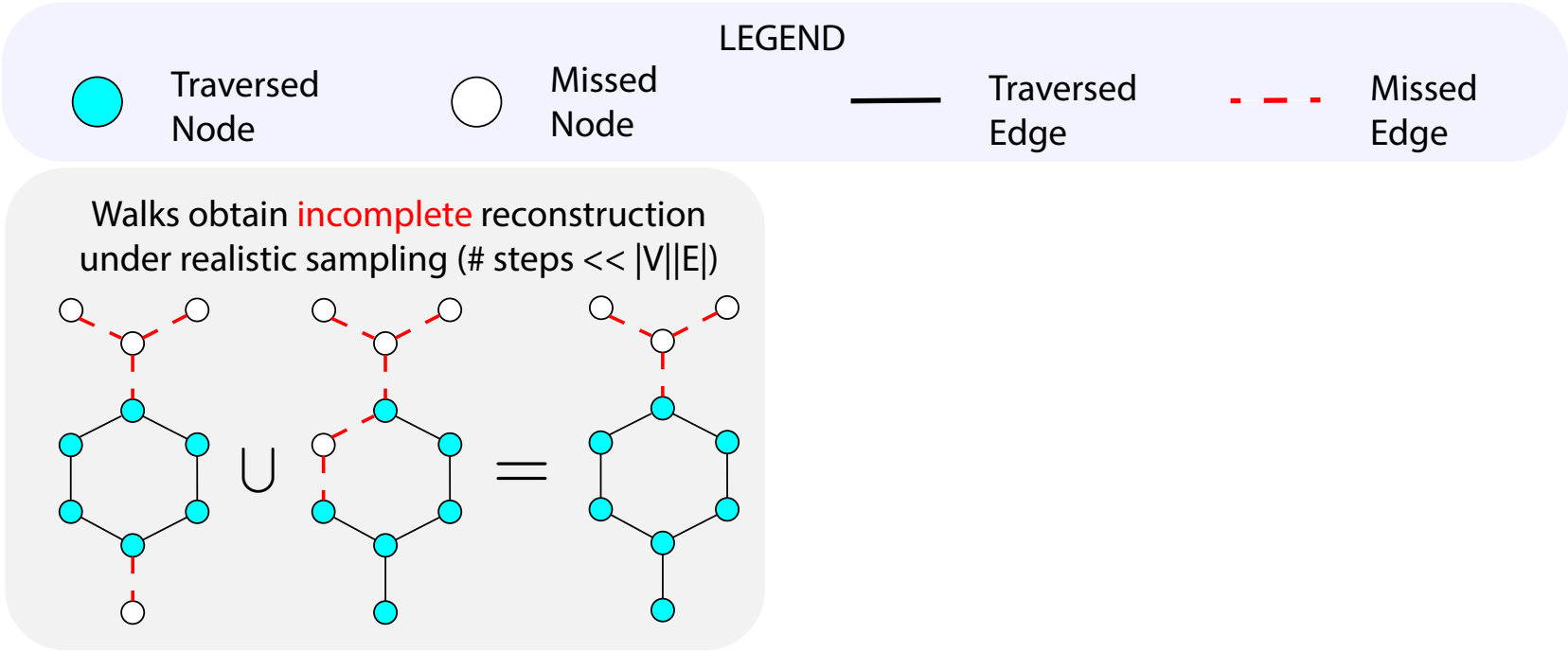
- **Random walk neural networks**[4,5,6] are a promising alternative GNN
  1. Sample random walks from the graph
  2. Process walks with powerful sequence models
  3. Aggregate walks for the final graph-level prediction



[4. Wang and Cho 2024 , 5. Kim et al., 2025, 6. Chen et al., 2025]

Gap: RWNNs are limited by coverage

- **RWNNs** are limited under **partial node and edge coverage**

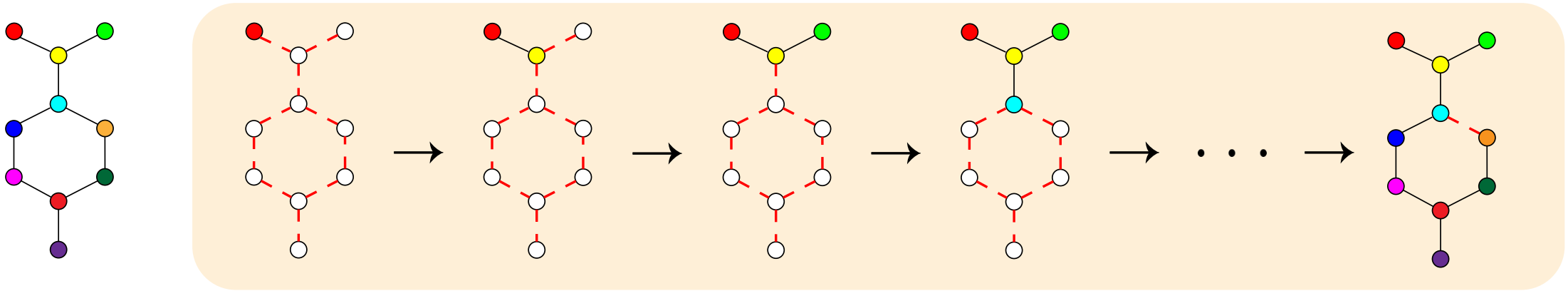


Our Approach: Random Search Neural Networks (RSNNs)

- We replace random walks entirely with **random depth first searches**
  1. Sample start node uniformly at random
  2. Visit neighbors uniformly at random

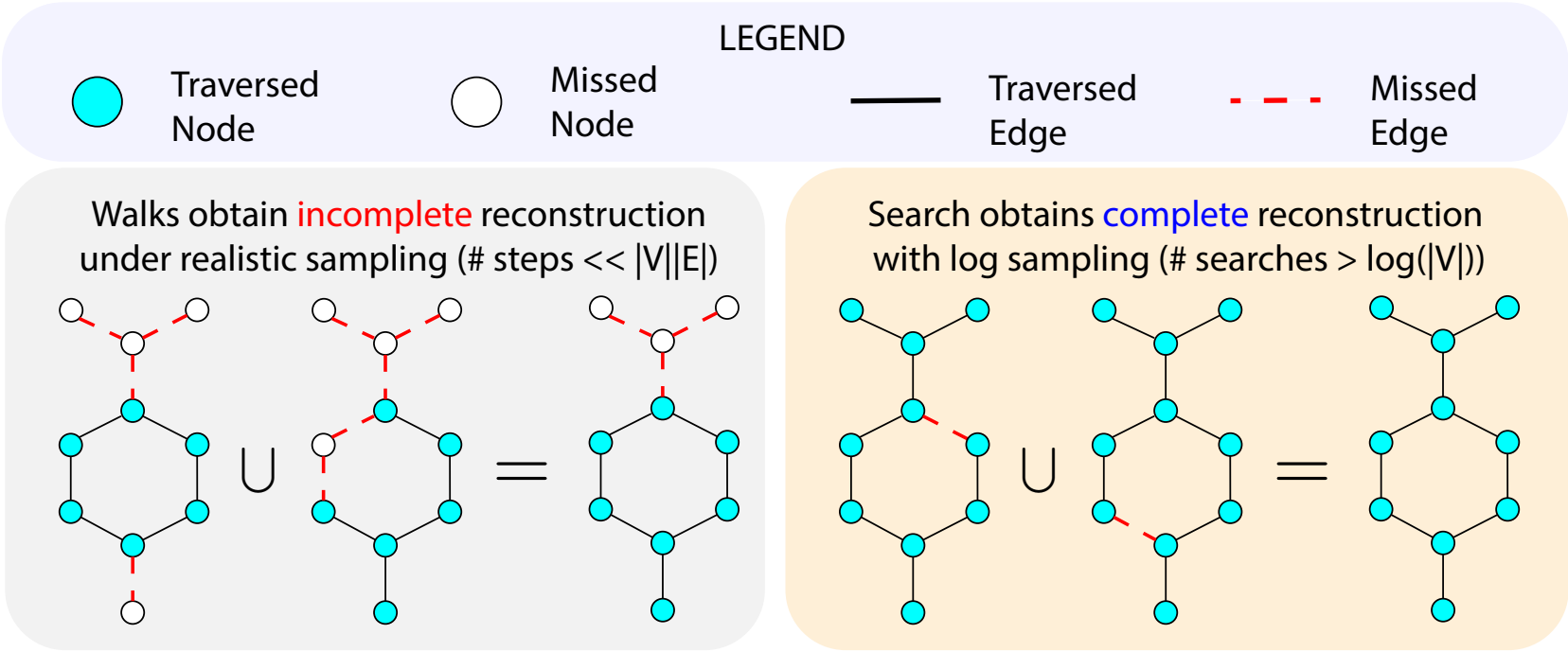
Original Graph

Random Depth First Search on G:

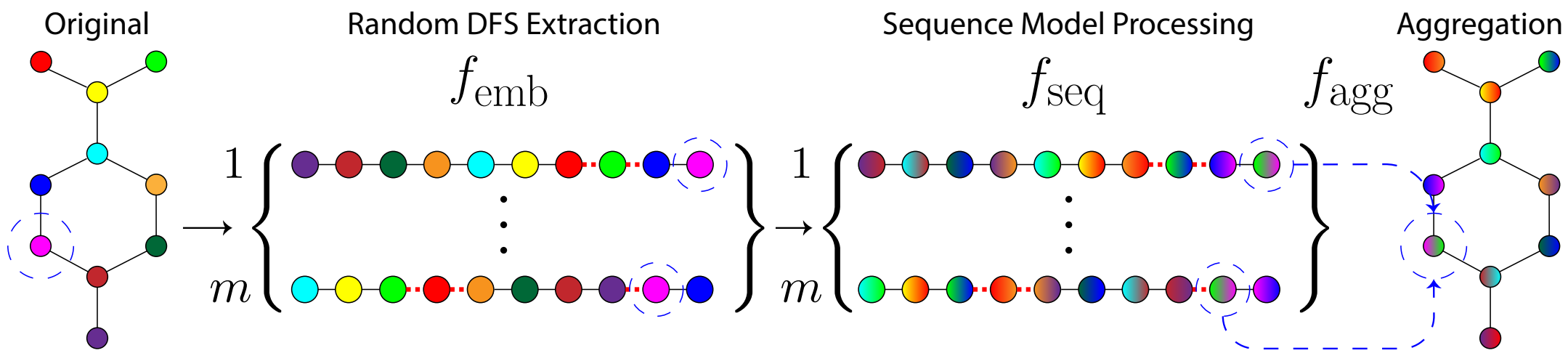


RSNN Node and Edge Coverage

- **RWNNs** are limited under **partial node and edge coverage**
- **Random Search NNs** **significantly improve graph coverage** vs RWNNs



RSNN efficient coverage and universality



- Theoretical guarantees
  - RSNNs require **logarithmic searches in $|V|$** for complete edge coverage on sparse bounded-degree graphs
  - Full coverage RSNNs are **universal approximators** of graph functions

RSNN Discriminative Performance

Table 1: Median (min, max) of performance across test splits.

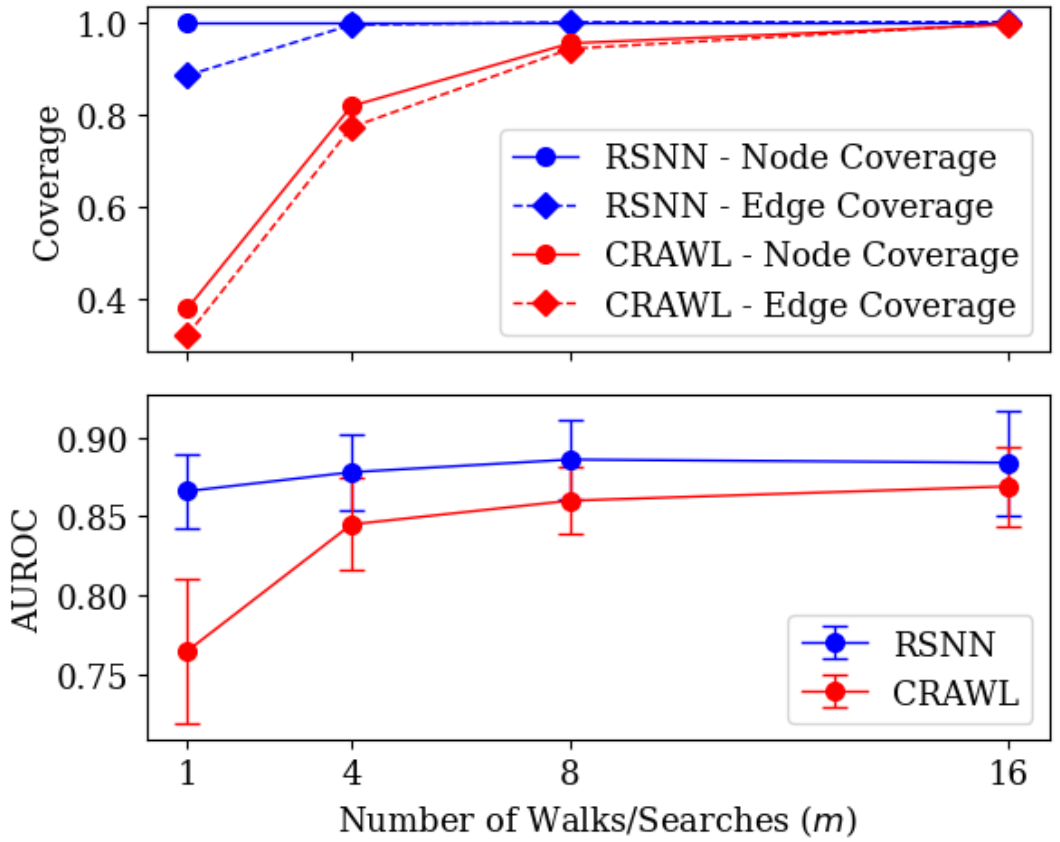
		MoleculeNet	ProteinShake
		Clintox	**Structural Class**
	# Graphs	1.5K	10K
	Avg. $\lvert V\rvert$	26.1	217.5
	Avg. $\lvert E\rvert$	55.5	593.8
	Metric	AUC ↑	ACC ↑
NA	**SMILES**	62.5 (45.7, 68.6)	—
NA	**GT (full)**	57.1 (46.5, 73.5)	—
NA	**GCN**	62.4 (56.9, 74.7)	68.0 (67.9, 69.2)
$m = 1$	**RWNN**	71.0 (54.9, 79.5)	45.4 (41.5, 45.9)
$m = 1$	**CRAWL**	70.0 (64.6, 73.6)	53.0 (50.7, 53.4)
$m = 1$	**RSNN (ours)**	**88.1 (84.9, 91.5)**	**62.2 (60.0, 65.6)**
$m = 8$	**RWNN**	85.0 (82.6, 88.7)	57.0 (55.5, 58.5)
$m = 8$	**CRAWL**	86.5 (83.6, 91.4)	72.7 (71.7, 73.3)
$m = 8$	**RSNN (ours)**	**88.3 (80.1, 91.3)**	**74.4 (74.1, 75.4)**

- RSNNs outperform popular **graph learning baselines** on molecular and protein graph classification tasks
- RSNNs outperform **RWNNs** across **all budgets of walks/searches m**

RSNN Node and Edge Coverage

- RWNNs (CRAWL) require $m = 16$ walks of length $|V|$ for full node and edge coverage
- RSNNs obtain full node and high edge coverage with just a single search. At $m = 4$ searches, RSNNs obtain full edge coverage

BBBP Molecule Graphs



Contributions

- We characterize RWNN limitations due to partial node and edge coverage
- Propose RSNN, a new approach operating on random searches
- Establish efficient coverage, universality, and invariance guarantees
- Demonstrate RSNNs consistently outperform RWNNs

Link to Paper