GLEMOS: Benchmark for Instantaneous Graph Learning Model Selection

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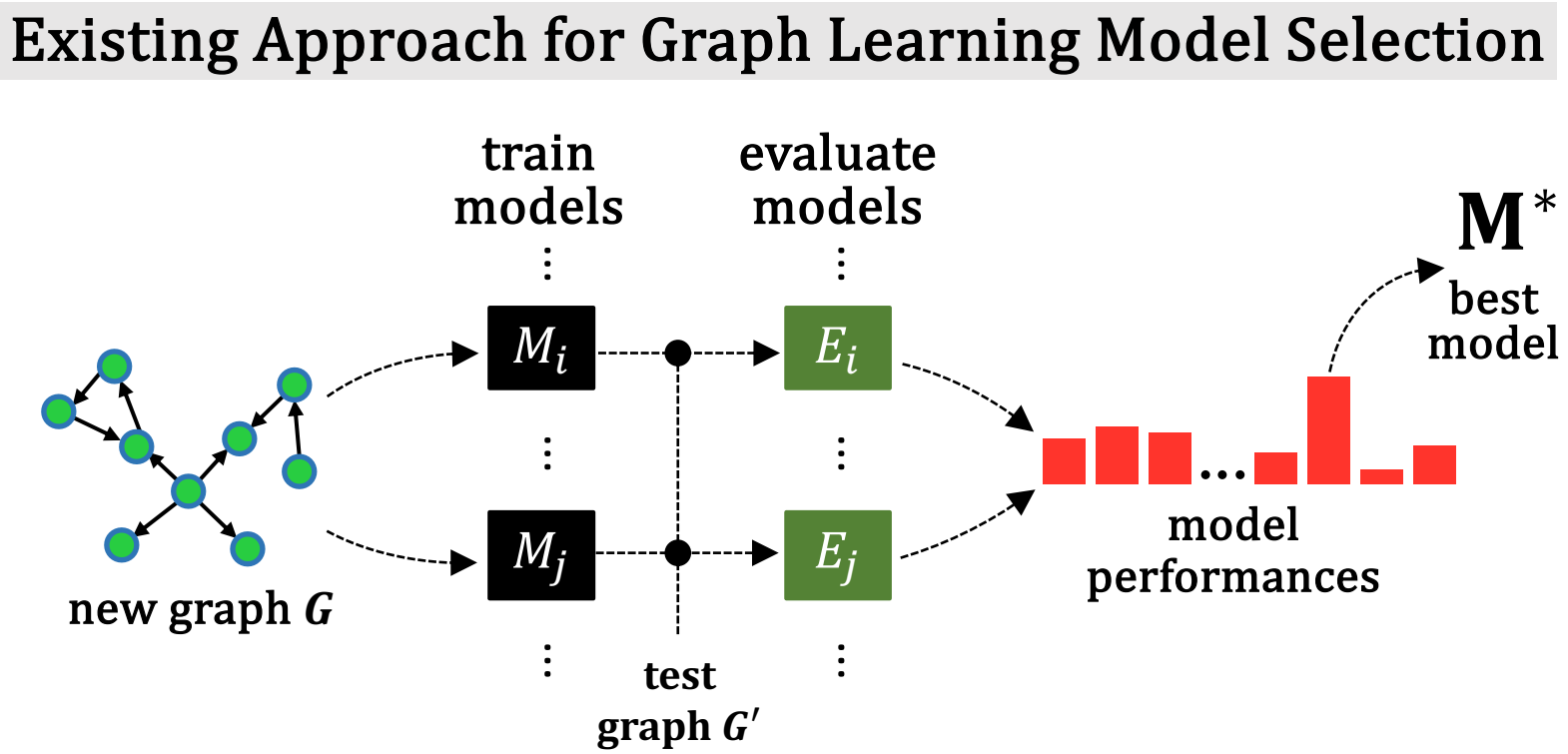
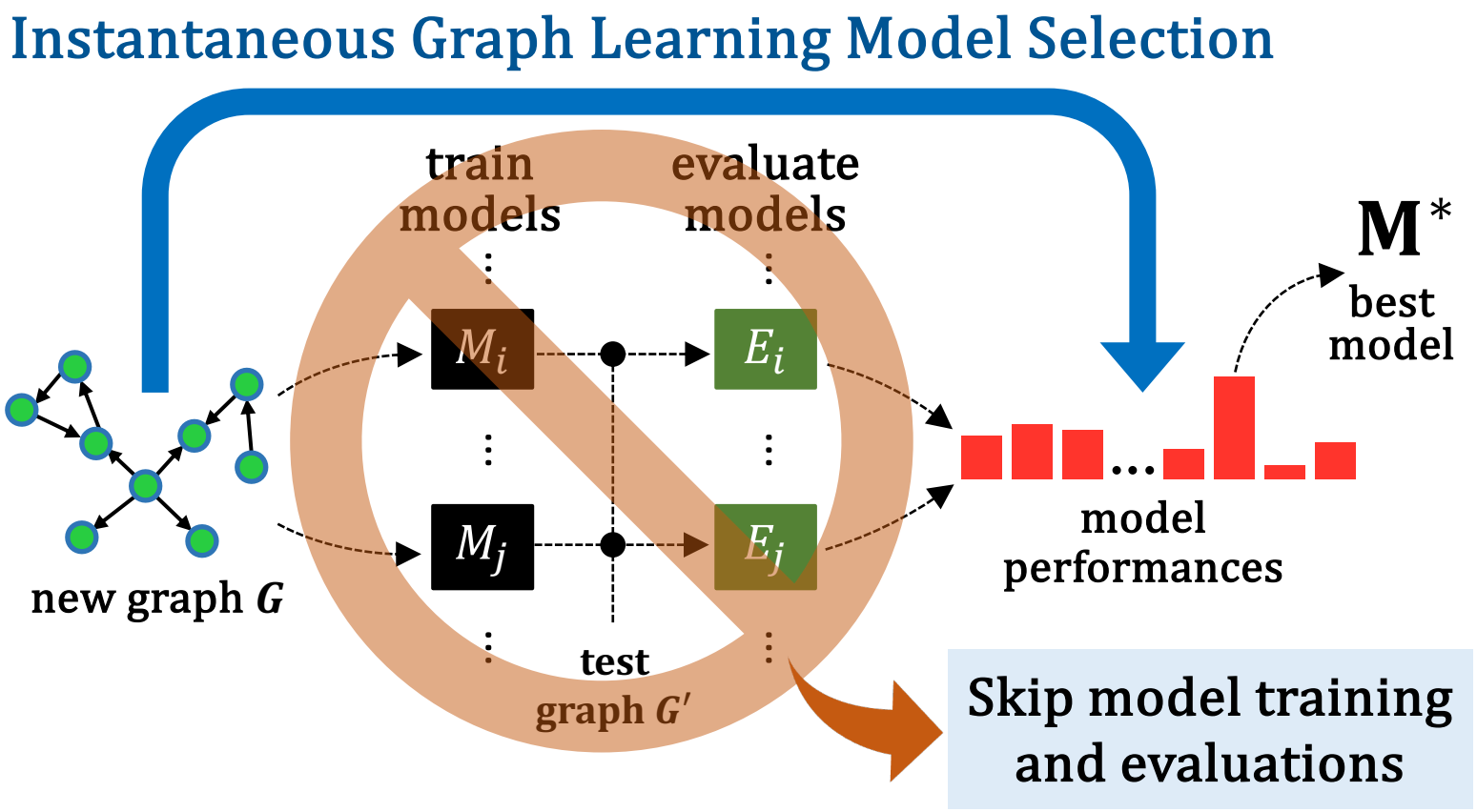
Graph Learning (GL) Model Selection



Graph Learning Model Selection



Existing Data Banks of GNNs

	Benchmark Testbeds	Instantaneous Selection Algorithms	Meta-Graph Features	Graph Learning Models	# Graph Datasets	Graph Size (max # nodes)	# Data Domains
GNN-Bank-101 (ICLR '23)	✗	✗	✗	GNNs	12	34k	5
NAS-Bench-Graph (NeurIPS '22)	✗	✗	✗	GNNs	9	170k	4
GraphGym (NeurIPS '20)	✗	✗	✗	GNNs	32	34k	7

Contributions of The Proposed GLEMOS

- Extensive Benchmark Data with Multiple GL Tasks

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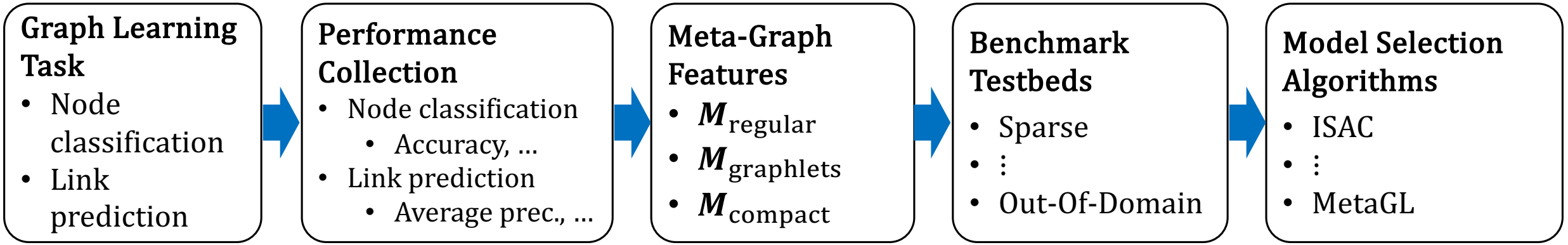
GLEMOS (Ours)	✓	✓	✓	**GNNs & Non-GNNs**	**457**	**496k**	**37**

Contributions of The Proposed GLEMOS

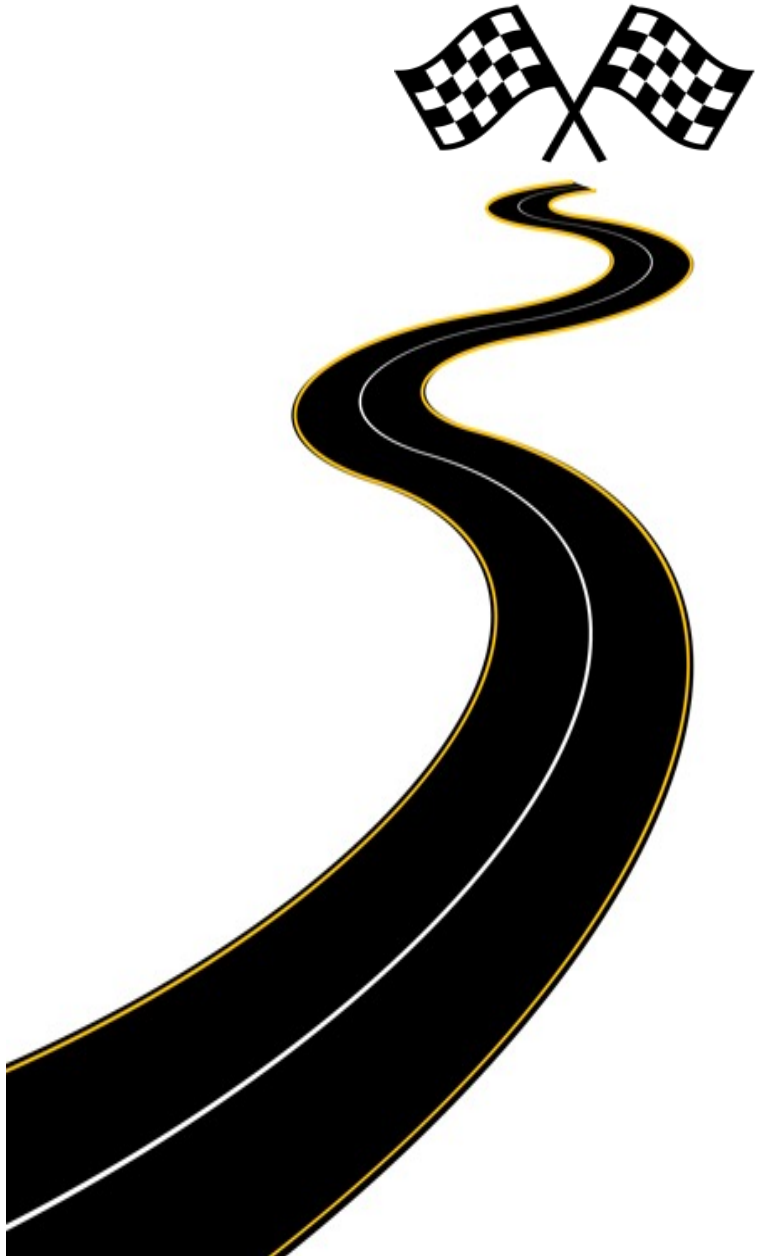
- Extensive Benchmark Data with Multiple GL Tasks
- Comprehensive Evaluation Testbeds
- Extensible Benchmark Environment
- Future Research Directions

Overview of GLEMOS

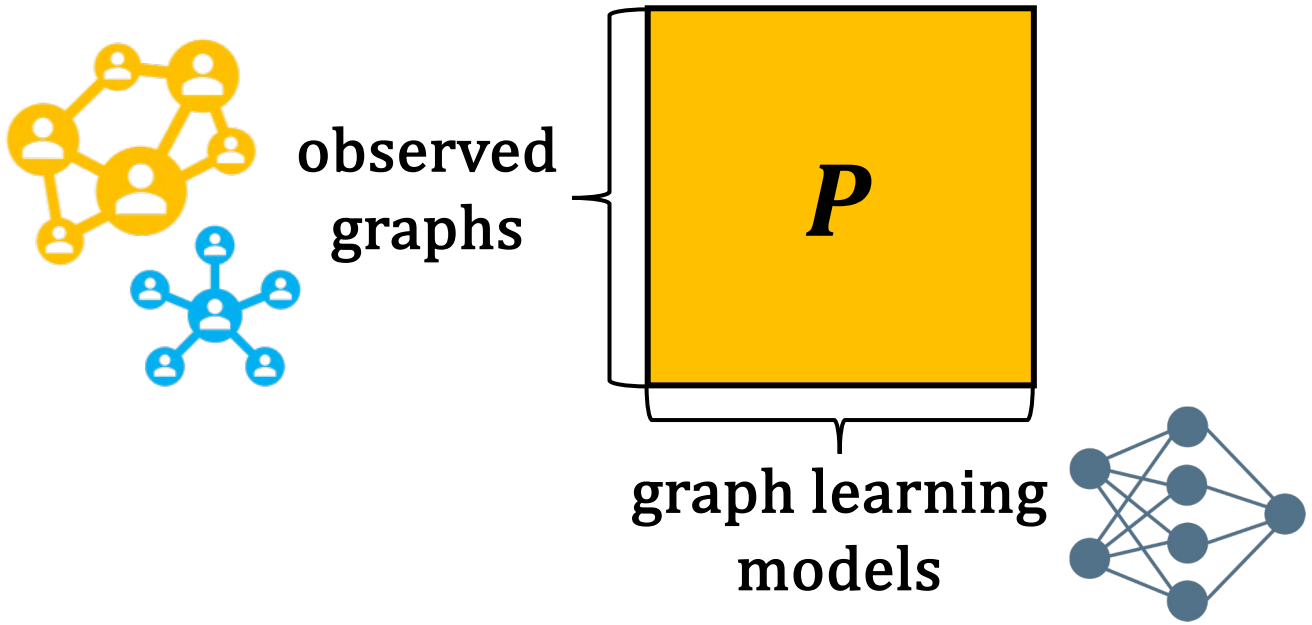


Roadmap

- Introduction
- **Performance Collection**
- Meta-Graph Features
- Benchmark Testbeds & Algorithms
- Future Directions & Conclusion

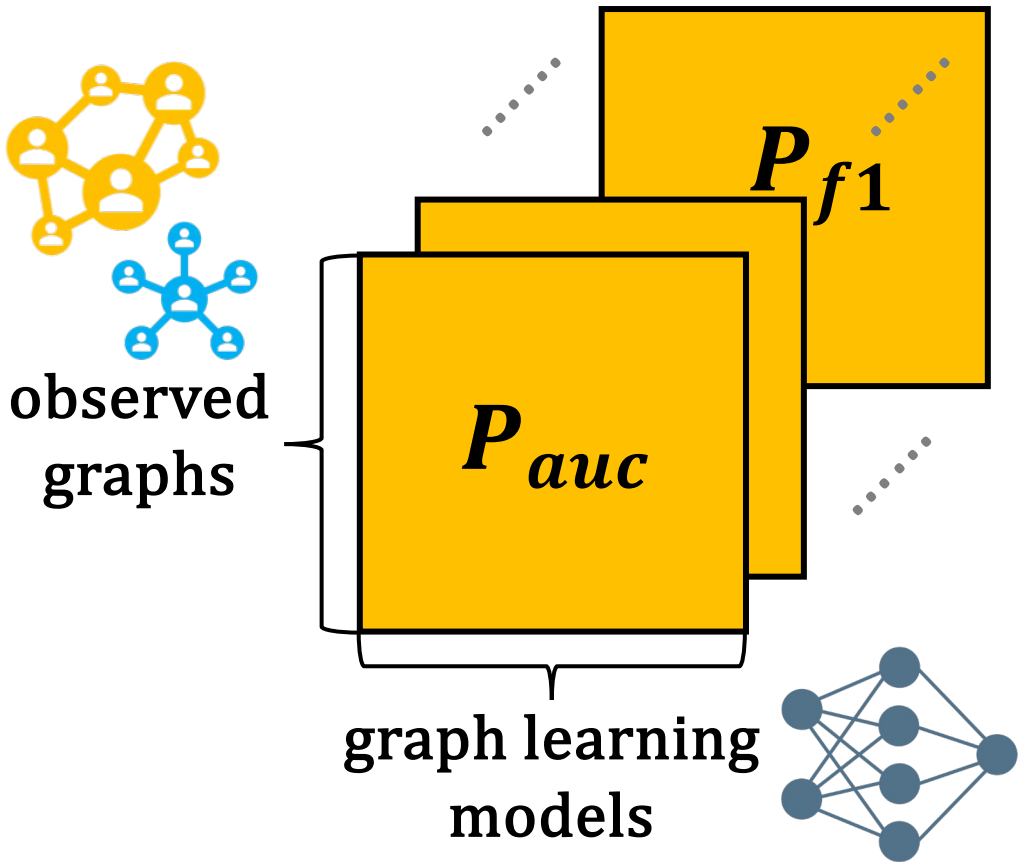


Performance Collection

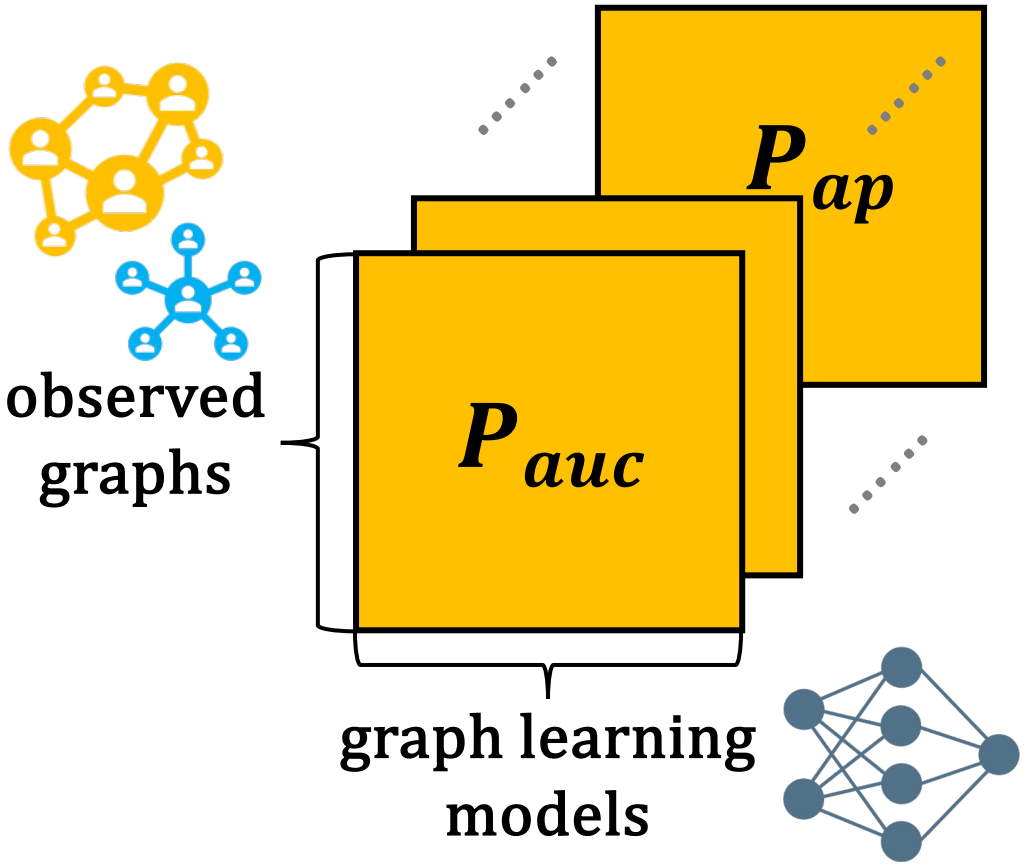


Performance Matrix P

Performance Collection



Node Classification Perfs.

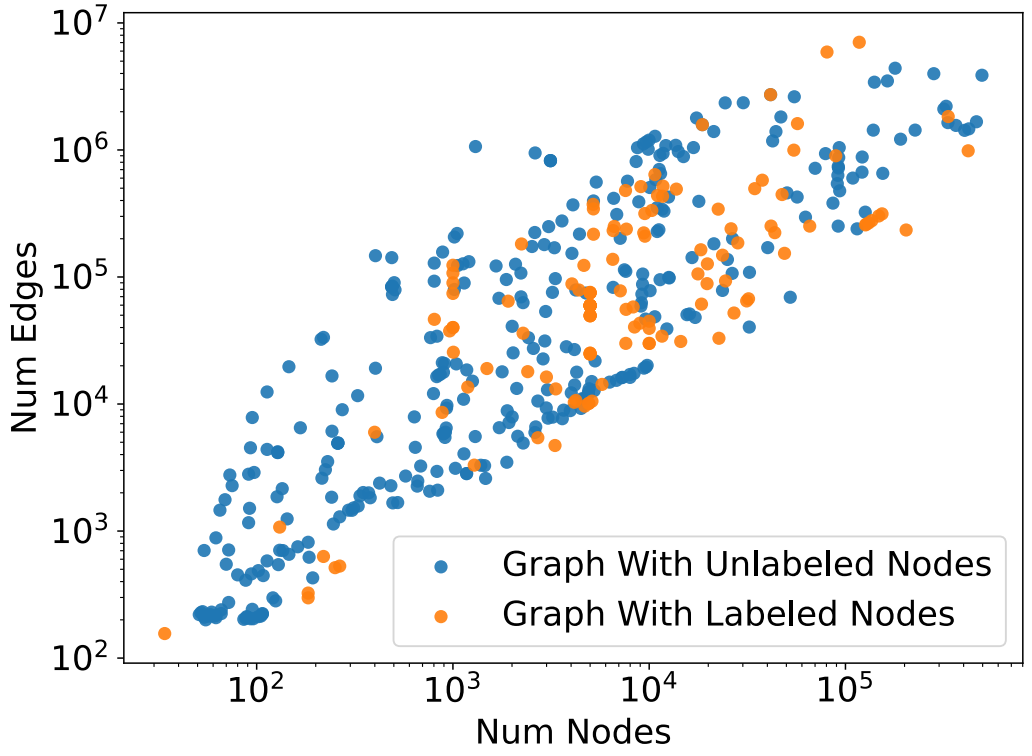


Link Prediction Perfs.

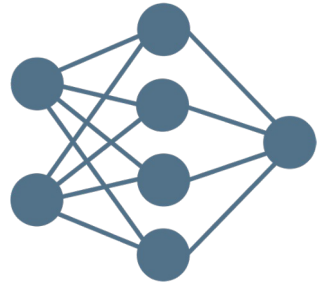
Performance Collection: Graphs

GLEMOS covers representative and diverse graph datasets

	Node Classification	Link Prediction
Total graphs	128	457
• # nodes	34–422k	34–496k
• # edges	156–7M	156–7M
• # node feats	2–61k	2–61k
• # node classes	2–195	N/A
• # data domains	25	37



Performance Collection: Models



GLEMOS covers representative and diverse GL models

Method	NC	LP	Count	Method	NC	LP	Count
GCN	✓	✓	30	GraRep	✓	✓	6
GraphSAGE	✓	✓	24	DGI	✓	✓	24
GAT	✓	✓	40	node2vec	✓	✓	72
GIN	✓	✓	10	Label Prop.	✓		16
EGC	✓	✓	28	Jaccard's Coeff		✓	1
SGC	✓	✓	10	Resource Alloc.		✓	1
ChebNet	✓	✓	27	Adamic/Adar		✓	1
PNA	✓	✓	32	SEAL		✓	36
Spectral Emb.	✓	✓	8				
				Total Count			**366**

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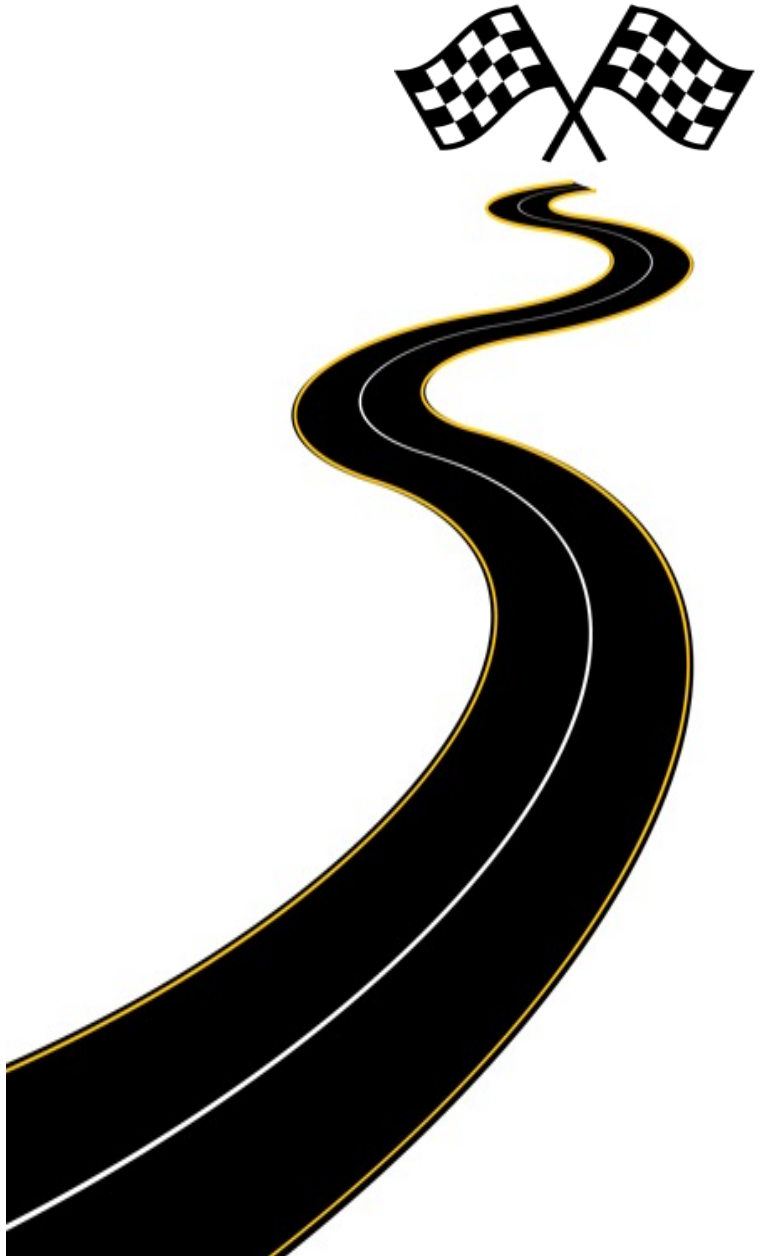
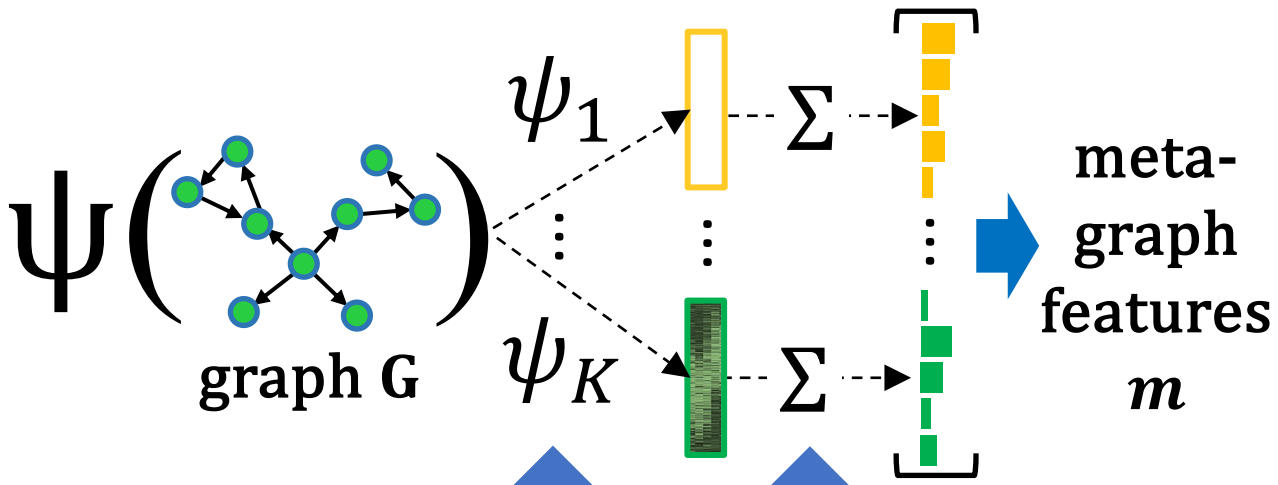


Meta-Graph Features: Feature Generation



Step 1—Structural Feature Extraction

Step 2—Statistical Feature Summarization

Meta-Graph Features: Collections

Predefined sets of meta-graph features

- $\boldsymbol{M_{regular}}$: 318 features
- $\boldsymbol{M_{graphlets}}$: 756 features
- $\boldsymbol{M_{compact}}$: 58 features
- $\boldsymbol{M_{reg+raphlets}}$: 1,074 features

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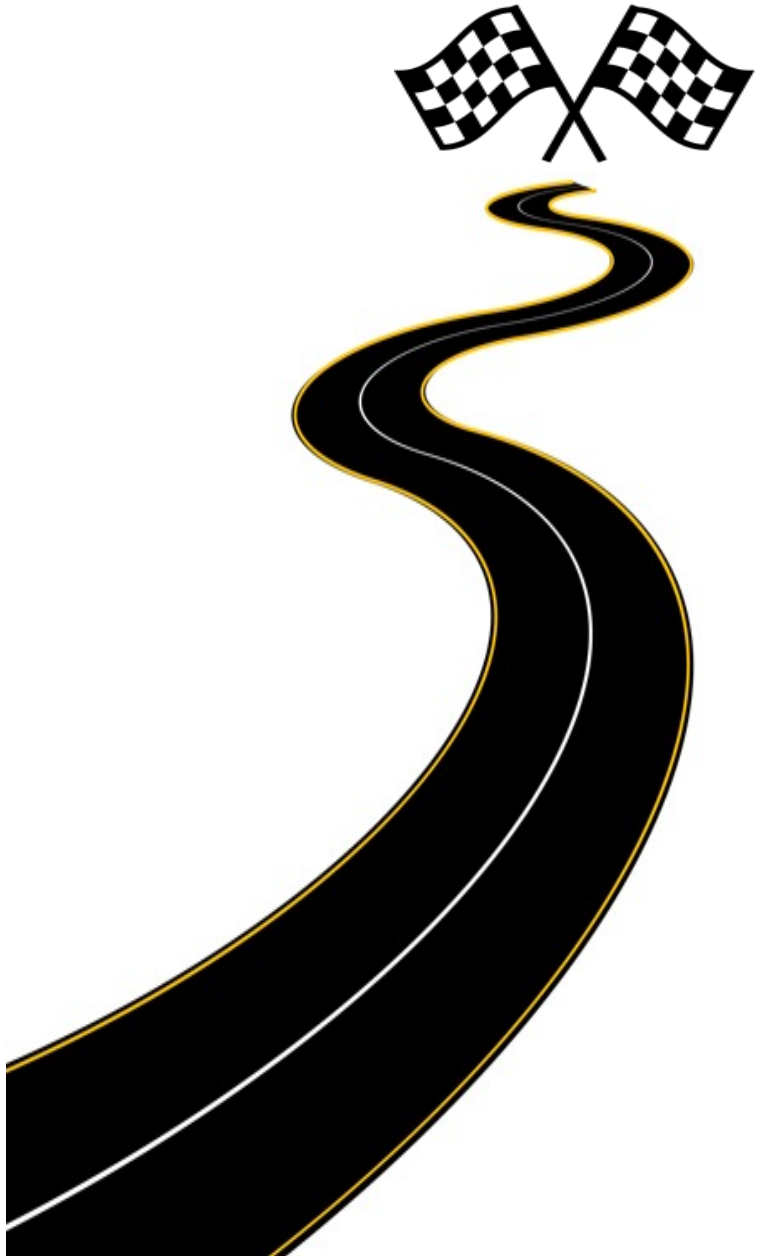
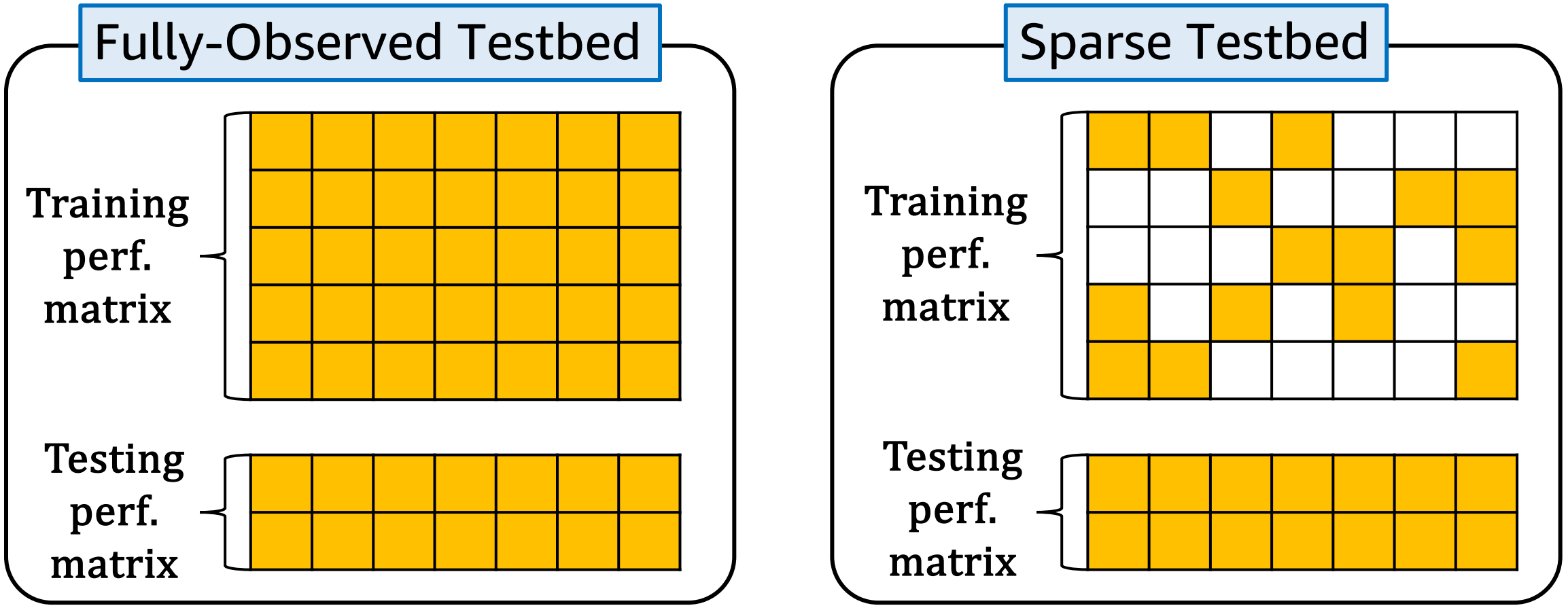
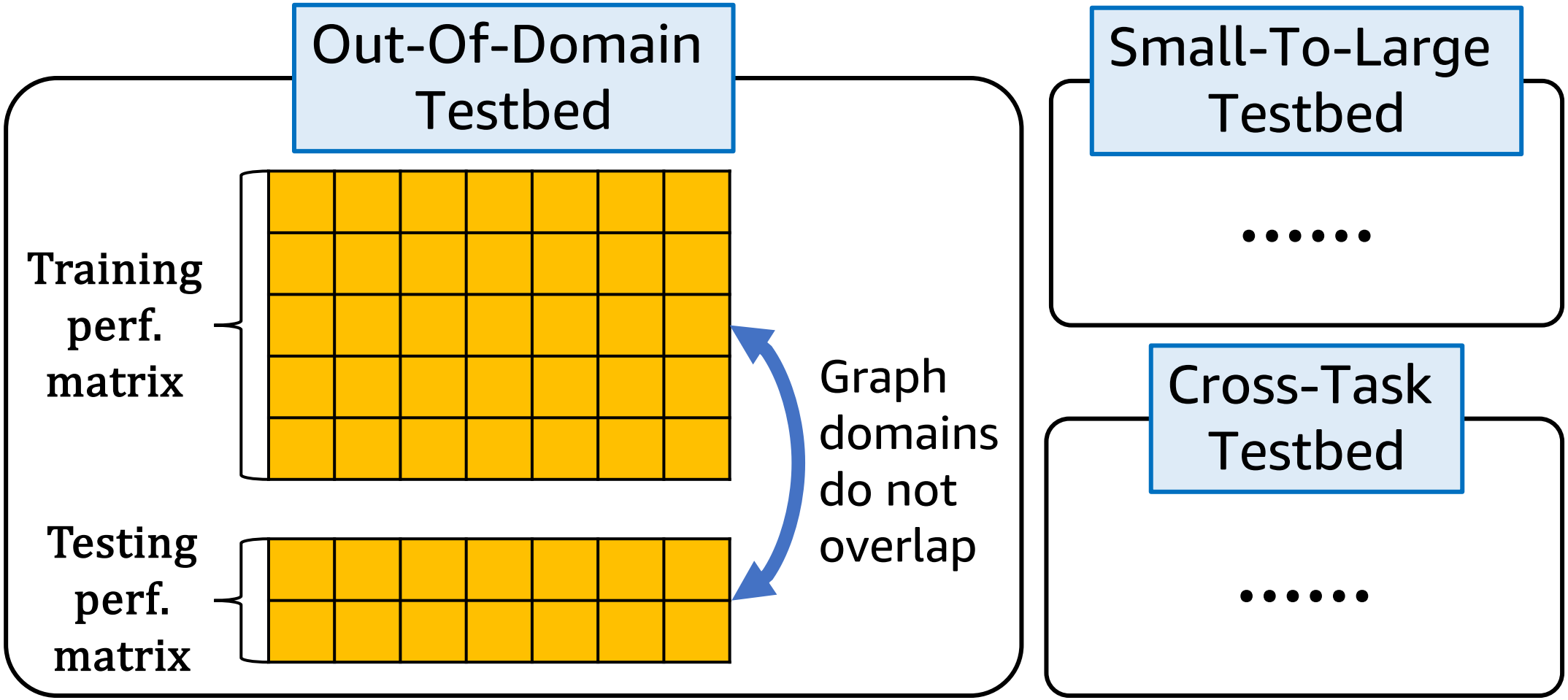


Benchmark Testbeds



Benchmark Testbeds



Instantaneous Model Selection Algorithms

Algorithm	C1. Use meta-features	C2. Use prior performances	C3. Optimizable
Random Selection			
GB-Avg. Perf		✓	
GB-Avg. Rank		✓	
ISAC	✓	✓	
AS	✓	✓	
Supervised Surrogates	✓	✓	✓
ALORS	✓	✓	✓
NCF	✓	✓	✓
MetaOD	✓	✓	✓
MetaGL	✓	✓	✓

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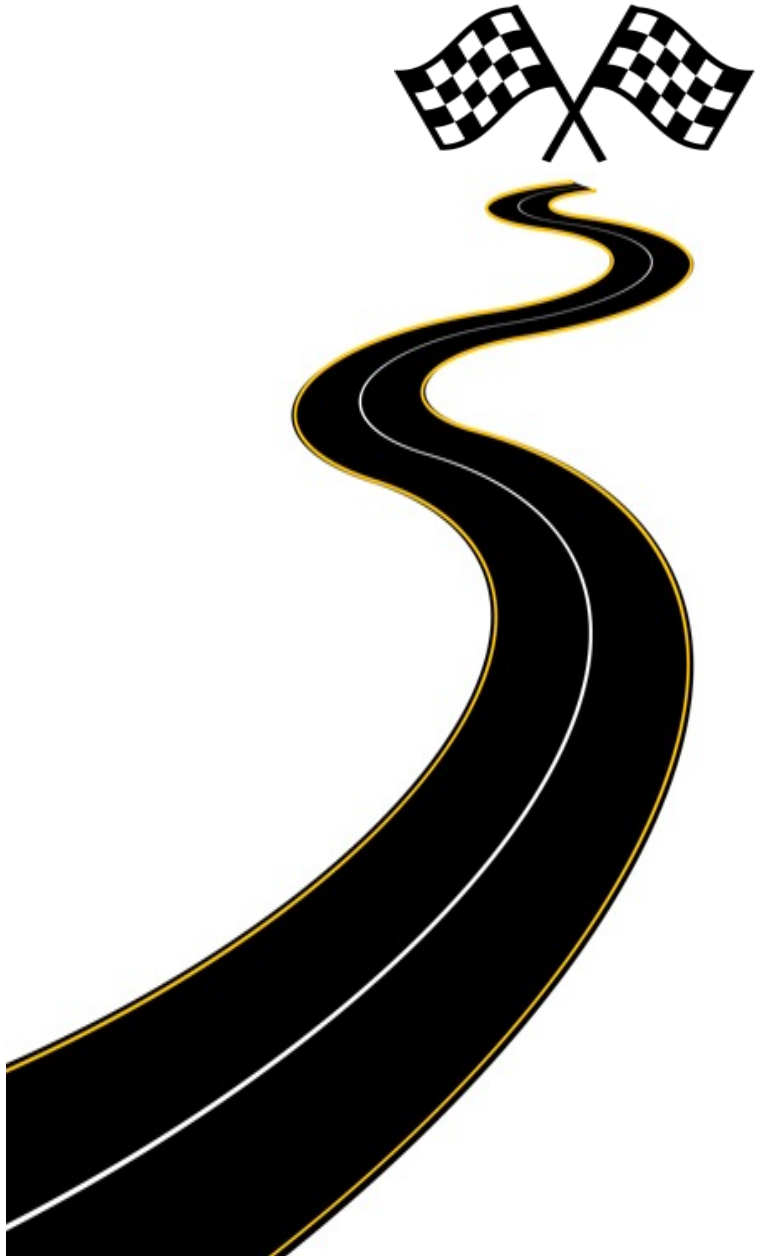


Future Directions

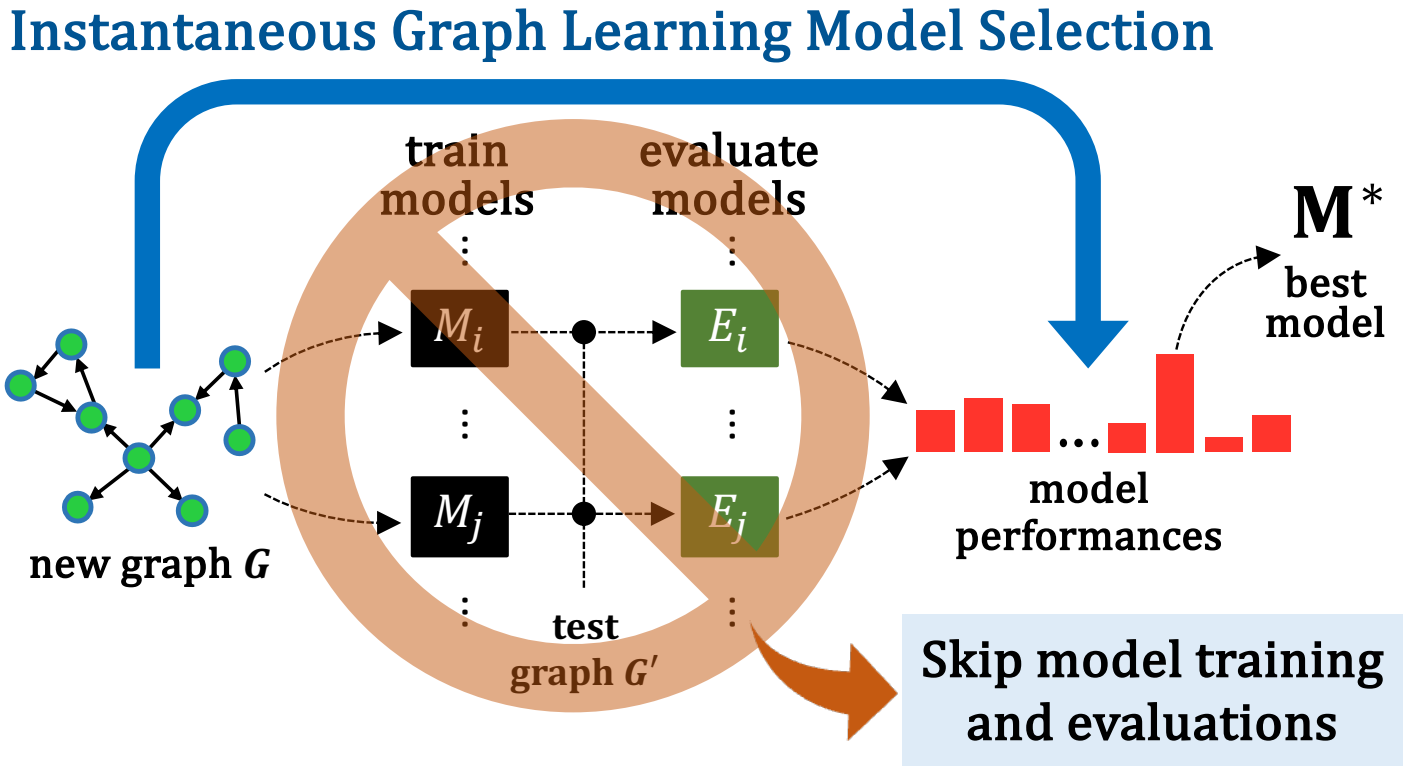
- D1: Enabling the use of additional graph data
- D2: Developing data augmentation techniques
- D3: Handling out-of-distribution settings
- D4: Collecting performance more efficiently

Conclusion

Extensive Benchmark Data

Model Selection Algorithms

Evaluation Testbeds



Extensible Benchmark Environment