GLEMOS: Benchmark for Instantaneous Graph Learning Model Selection

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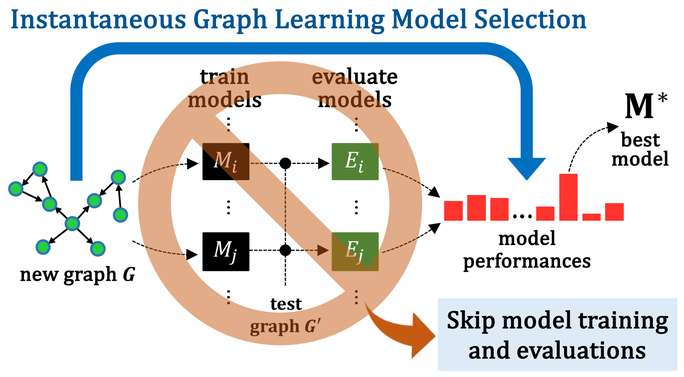
NEURAL INFORMATION PROCESSING SYSTEMS

Introduction

The choice of a graph learning (GL) model (i.e., a GL algorithm and its hyperparameter settings) has a significant impact on the performance of downstream tasks. However, selecting the right GL model becomes increasingly difficult and time consuming as more and more GL models are developed. Accordingly, it is of great significance and practical value to equip users of GL with the ability to perform a near-instantaneous selection of an effective GL model without manual intervention. Despite the recent attempts to tackle this important problem, there has been no comprehensive benchmark environment to evaluate the performance of GL model selection methods. To bridge this gap, we present GLEMOS, a comprehensive benchmark for instantaneous GL model selection, which makes the following contributions.

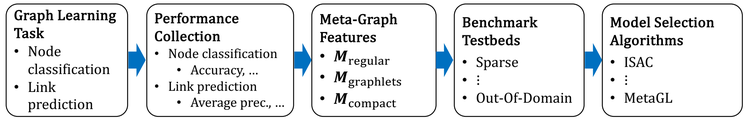
- **Extensive Benchmark Data with Multiple GL Tasks.** GLEMOS provides extensive benchmark data, including the performances of 366 models on 457 graphs over fundamental GL tasks, i.e., link prediction and node classification.
- **Comprehensive Evaluation Testbeds.** GLEMOS designs multiple evaluation settings, and assesses how effectively representative model selection techniques perform in these different settings.
- **Extensible Open Source Environment.** GLEMOS is designed to be easily extended with new models, new graphs, and new performance records.
- **Future Research Directions.** We discuss the limitations of existing model selection methods and highlight future research directions.

Instantaneous Graph Learning Model Selection



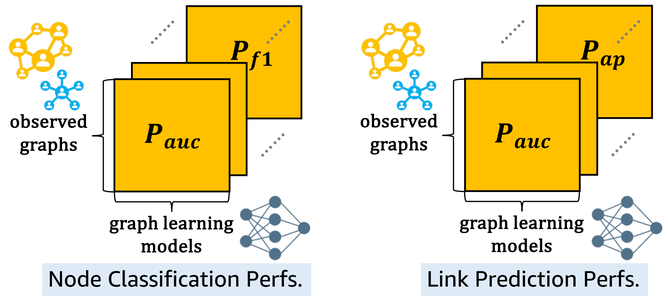
Via instantaneous graph learning model selection, the best model to deploy on the new graph can be found without performing computationally expensive model training and evaluations.

Overview of GLEMOS



GLEMOS provides a comprehensive benchmark environment, covering the steps required to achieve effective instantaneous GL model selection, with multiple options for major building blocks.

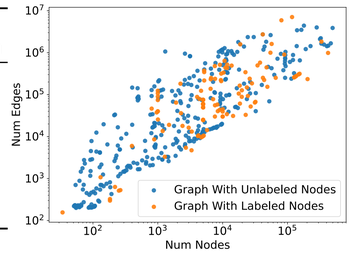
Performance Collection



GLEMOS covers representative and diverse sets of graphs and GL models.

Graphs

	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

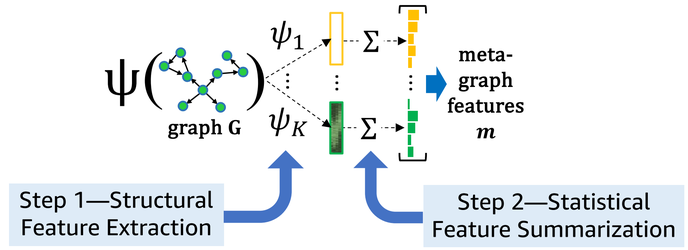


Models

NC: Applicable for node classification. LP: Applicable for link prediction.

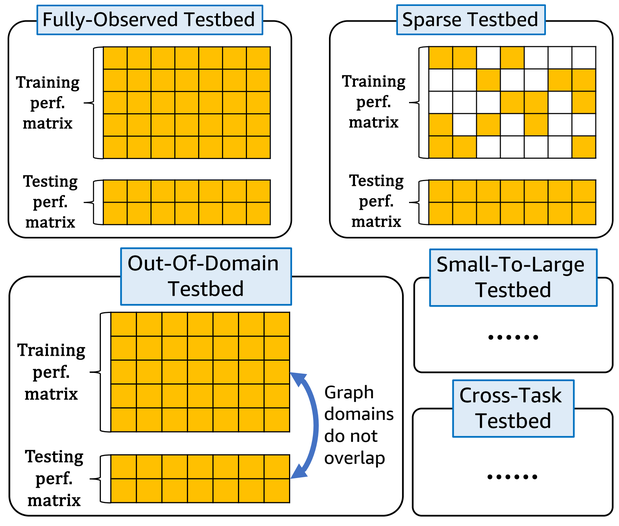
Method	NC	LP	Count	Method	NC	LP	Count
GCN	✓	✓	30	GraRep	✓	✓	6
GraphSAGE	✓	✓	24	DGI	✓	✓	24
GAT	✓	✓	40	node2vec	✓	✓	72
GIN	✓	✓	10	Label Prop.	✓		16
EGC	✓	✓	28	Jaccard's Coeff		✓	1
SGC	✓	✓	10	Resource Alloc.		✓	1
ChebNet	✓	✓	27	Adamic/Adar		✓	1
PNA	✓	✓	32	SEAL		✓	36
Spectral Emb.	✓	✓	8				
				Total Count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

Meta-Graph Features



- GLEMOS provides multiple predefined sets of meta-graph features, with the largest one having more than 1,000 features.

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	✓	✓	✓