METAGL: EVALUATION-FREE SELECTION OF GRAPH LEARNING MODELS VIA META-LEARNING

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ABSTRACT

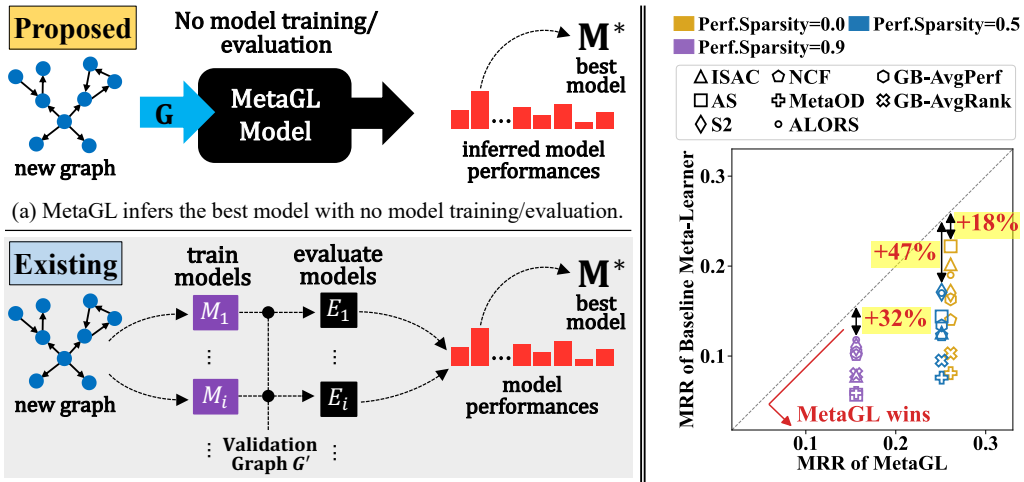
Given a graph learning task, such as link prediction, on a new graph, how can we select the best method as well as its hyperparameters (collectively called a model) without having to train or evaluate any model on the new graph? Model selection for graph learning has been largely ad hoc. A typical approach has been to apply popular methods to new datasets, but this is often suboptimal. On the other hand, systematically comparing models on the new graph quickly becomes too costly, or even impractical. In this work, we develop the *first meta-learning approach for evaluation-free graph learning model selection*, called METAGL, which utilizes the prior performances of existing methods on various benchmark graph datasets to automatically select an effective model for the new graph, *without* any model training or evaluations. To quantify similarities across a wide variety of graphs, we introduce specialized meta-graph features that capture the structural characteristics of a graph. Then we design G-M network, which represents the relations among graphs and models, and develop a graph-based meta-learner operating on this G-M network, which estimates the relevance of each model to different graphs. Extensive experiments show that using METAGL to select a model for the new graph greatly outperforms several existing meta-learning techniques tailed for graph learning model selection (up to *47%* better), while being extremely fast at test time ($\sim$*1 sec*).

1 INTRODUCTION

Given a graph learning (GL) task, such as link prediction, for a new graph dataset, how can we select the best method as well as its hyperparameters (HPs) (collectively called a model) *without performing any model training or evaluations on the new graph*? GL has received increasing attention recently (Xia et al., 2021; Zhang et al., 2022), achieving successes across a large array of applications, such as recommendation and ranking (Fan et al., 2019; Park et al., 2020), traffic forecasting (Jiang & Luo, 2021), bioinformatics (Su et al., 2020; Li et al., 2017a), anomaly detection (Cai et al., 2021), and question answering (Park et al., 2022). However, as GL methods continue to be developed for various tasks, it becomes increasingly difficult to determine which model to use for the given graph.

Model selection (*i.e.*, selecting a method and its configuration such as HPs) for graph learning has been largely ad hoc to date. A typical approach, called "no model selection", is to simply apply popular methods to new graphs, often with the default HP values. However, it is well known that there is no universal learning algorithm that performs best on *all* problem instances (Wolpert & Macready, 1997), and such consistent model selection is often suboptimal. At the other extreme lies "naive model selection" (Fig. 1b), where all candidate models are trained on the new graph, evaluated on a hold-out validation graph, and then the best performing model for the new graph is selected. This approach is very costly as all candidate models are trained when a new graph arrives. Recent methods on neural architecture search (NAS) and hyperparameter optimization (HPO) of GL methods, which we review in Section 3, adopt smarter, more efficient strategies, such as Bayesian optimization (Snoek et al., 2012; Tu et al., 2019), which carefully choose a relatively small number of HP settings to evaluate. However, they still need to evaluate multiple configurations of each GL method on the new graph.

Evaluation-free model selection is yet another paradigm, which aims to tackle the limitations of the above approaches by attempting to simultaneously achieve the speed of no model selection and the accuracy of exhaustive model selection. Recently, a seminal work by Zhao et al. (2021) proposed a technique for outlier detection (OD) model selection, which carries over the observed performance of OD methods on benchmark datasets for selecting OD methods. However, it does not address the



(a) MetaGL infers the best model with no model training/evaluation.

(b) Existing model selection methods train/evaluate multiple models.

(c) MetaGL consistently performs the best.

Figure 1: (a) Given an unseen graph G and a large space $\mathcal{M}$ of models to search over, METAGL efficiently infers the best model $M^* \in \mathcal{M}$ without having to train a single model from $\mathcal{M}$ on the new graph G. (b) Existing approaches, by contrast, need to train and evaluate multiple models $M_i \in \mathcal{M}$ to be able to select the best one. (c) Given observed performance with varying sparsity levels, METAGL consistently outperforms existing meta-learners, with up to 47% better model selection performance.

unique challenges of GL model selection, and cannot be directly used to solve the problem. Inspired by this work, we systematically tackle the model selection problem for graph learning, especially link prediction. We choose link prediction as it is a key task for graph-structured data: It has many applications (*e.g.*, recommendation, knowledge graph reasoning, and entity resolution), and several inference and learning tasks can be cast as a link prediction problem (*e.g.*, Fadaee & Haeri (2019)). In this work, we develop METAGL, *the first meta-learning framework for evaluation-free selection of graph learning models*, which finds an effective GL model to employ for a new graph *without* training or evaluating any GL model on the new graph, as Figure 1a illustrates. METAGL satisfies all of desirable features for GL model selection listed in Table 1, while no existing paradigms satisfy all.

The high-level idea of meta-learning based model selection is to estimate a candidate model's performance on the new graph based on its observed performances on *similar* graphs. Our meta-learning problem for graph data presents a unique challenge of how to model graph similarities, and what characteristic features (*i.e.*, meta-features) of a graph to consider. Note that this step is often not needed for traditional meta-learning problems on non-graph data, as features for non-graph objects (*e.g.*, location, age of users) are often readily available. Also, the high complexity and irregularity of graphs (*e.g.*, different number of nodes and edges, and widely varying connectivity patterns among different graphs) makes the task even more challenging. To handle these challenges, we design specialized *meta-graph features* that can characterize major structural properties of real-world graphs.

Then to estimate the performance of a candidate model on a given graph, METAGL learns to embed models and graphs in the shared latent space such that their embeddings reflect the graph-to-model affinity. Specifically, we design a multi-relational graph called *G-M network*, which captures multiple types of relations among models and graphs, and develop a meta-learner operating on this G-M network, based on an attentive graph neural network that is optimized to leverage meta-graph features and prior model performance into producing model and graph embeddings that can be effectively used to estimate the best performing model for the new graph. METAGL greatly outperforms existing meta-learners in GL model selection (Fig. 1c). In sum, the key contributions of this work are as follows.

- **Problem Formulation.** We formulate the problem of selecting effective GL models in an evaluation-free manner (*i.e.*, without ever having to train/evaluate any model on the new graph), To the best of our knowledge, we are the first to study this important problem.
- **Meta-Learning Framework and Features.** We propose METAGL, the first meta-learning framework for evaluation-free GL model selection. For meta-learning on various graphs, we design meta-graph features that quantify graph similarities by capturing structural characteristics of a graph.
- **Effectiveness.** Using METAGL for GL model selection greatly outperforms existing meta-learning techniques (up to *47%* better, Fig. 1c), with negligible runtime overhead at test time ($\sim$*1 sec*).

Benchmark Data/Code: To facilitate further research on this important new problem, we release code and data, including performances of 400+ models on 300+ graphs, and 300+ meta-graph features.

Table 1: The proposed METAGL wins on features in comparison to existing graph learning (GL) model selection (MS) paradigms, all of which fail to satisfy some of desirable properties for GL MS.

Desiderata for Graph Learning (GL) MS \ GL Model Selection (MS) Paradigms	No model selection	Naive model selection (Fig. 1b)	Graph HPO/NAS (*e.g.*, AutoNE, AGNN; See Sec 3 and Fig. 1b)	METAGL (Ours, Fig. 1a)
Evaluation-free GL model selection	✓			✓
Capable of MS from among multiple GL algorithms		✓		✓
Capitalizing on graph similarities for GL MS				✓
Estimating model performance based on past observations			✓	✓

2 PROBLEM FORMULATION

Given a new unseen graph, our goal is to select the best model from a heterogeneous set of graph learning models, without requiring any model evaluations and user intervention. In comparison to traditional meta-learning problems where a model denotes a single method and its hyperparameters, a model in the graph meta-learning problem is more broadly defined to be

$$\text{model } M = \{(\text{graph embedding method}, \text{hyperparameters}), (\text{predictor}, \text{hyperparameters})\}, \quad (1)$$

as graph learning tasks usually involve two steps: (1) embedding the graph using a graph representation learning method, and (2) providing node embeddings to the predictor of a downstream task like link prediction. Both steps require learning a method with specific hyperparameters. Thus, there can be many models with the same embedding method and predictor, which have different hyperparameters. Also, the set $\boldsymbol{\mathcal{M}}$ of models may contain many different graph representation learning methods (*e.g.*, node2vec (Grover & Leskovec, 2016), GraphSAGE (Hamilton et al., 2017), DeepGL (Rossi et al., 2020) to name a few), as well as multiple task-specific predictors, making $\boldsymbol{\mathcal{M}}$ *heterogeneous*.

Given a training meta-corpus of n graphs $\boldsymbol{\mathcal{G}} = \{G_i\}_{i=1}^n$, and m models $\boldsymbol{\mathcal{M}} = \{M_j\}_{j=1}^m$ for GL tasks, we derive performance matrix $\mathbf{P} \in \mathbb{R}^{n \times m}$ where P_{ij} is the performance (*e.g.*, accuracy) of model j on graph i. Our meta-learning problem for evaluation-free GL model selection is defined as follows.

Problem 1 (Evaluation-Free Graph Learning Model Selection)**.**

Given
- an unseen test graph $G_{\text{test}} \notin \boldsymbol{\mathcal{G}}$, and
- a potentially sparse performance matrix $\mathbf{P} \in \mathbb{R}^{n \times m}$ of m *heterogeneous* graph learning models $\boldsymbol{\mathcal{M}} = \{M_1, \ldots, M_m\}$ on n graphs $\boldsymbol{\mathcal{G}} = \{G_1, \ldots, G_n\}$,

Select
- the best model $M^* \in \boldsymbol{\mathcal{M}}$ to employ on G_{test} *without* evaluating any model in $\boldsymbol{\mathcal{M}}$ on G_{test}.

3 RELATED WORK

A majority of works on GL focus on developing new algorithms for certain graph tasks and applications (Xia et al., 2021; Zhang et al., 2022). In comparison, there exist relatively few recent works that address the GL model selection problem (Zhang et al., 2021). They mainly focus on neural architecture search (NAS) and hyperparameter optimization (HPO) for GL models, especially graph neural networks (GNNs). Toward efficient and effective NAS and HPO in GL, they investigated several approaches, such as Bayesian optimization (AutoNE by Tu et al. (2019)), reinforcement learning (GraphNAS by Gao et al. (2020), AGNN by Zhou et al. (2019), Policy-GNN by Lai et al. (2020)), hypernets (ST-GCN by Zhu et al. (2021)), and evolutionary algorithms (Bu et al. (2021)), as well as techniques like subgraph sampling (AutoNE by Tu et al. (2019)), graph coarsening (JITuNE by Guo et al. (2021)), and hierarchical evaluation (HESGA by Yuan et al. (2021)). However, as summarized in Table 1, these methods cannot perform evaluation-free GL model selection (Problem 1), since they need to evaluate multiple configurations of each GL method on the new graph for model selection. Further, they are limited to finding the best configuration of a single algorithm, and thus cannot select a model from a heterogeneous model set $\boldsymbol{\mathcal{M}}$ with various GL models, as Problem 1 requests. An earlier work on GNN design space (You et al., 2020) is somewhat relevant, as it proposes an approach to quantify graph similarities, which can be used to find an observed graph similar to the test graph, and select a model that performed best on it. However, their approach evaluates a set of anchor models on all graphs, and computes similarities between two graphs based on anchor models' performance on them. As it needs to run anchor models on the new graph, it is inapplicable to Problem 1. For the first time, METAGL enables evaluation-free model selection from a heterogeneous set of GL models.

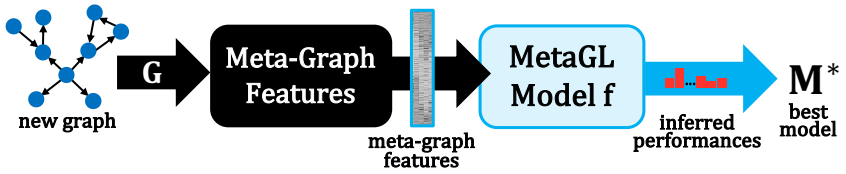


Figure 2: Given a new graph G, METAGL extracts meta-graph features, and applies a meta-learned model to them, which efficiently infers the best model $M^* \in \boldsymbol{\mathcal{M}}$ for G, with no model evaluation.

4 FRAMEWORK

In this section, we present METAGL, our meta-learning based framework that solves Problem 1 by leveraging prior performances of existing methods. METAGL consists of two phases: (1) *offline meta-training* phase (Section 4.1) that trains a meta-learner using observed graphs $\boldsymbol{\mathcal{G}}$ and model performances $\mathbf{P}$, and (2) *online model prediction* phase (Section 4.2), which selects the best model for the new graph. A summary of notations used in this work is provided in Table 3 in the Appendix.

4.1 OFFLINE META-TRAINING

Meta-learning leverages prior experience from related learning tasks to do a better job on the new task. When the new task is similar to some historical learning tasks, then the knowledge from those similar tasks can be transferred and applied to the new task. Thus effectively capturing the similarity between an input task and observed ones is fundamentally important for successful meta-learning. In meta-learning, the similarity between learning tasks is modeled using *meta-features*, *i.e.*, characteristic features of the learning task that can be used to quantify the task similarity.

Meta-Graph Features. Given the graph learning model selection problem (where new graphs correspond to new learning tasks), METAGL captures the graph similarity by extracting *meta-graph features* such that they reflect the structural characteristics of a graph. Notably, since graphs have irregular structure, with different number of nodes and edges, METAGL designs meta-graph features to be of the same size for any arbitrary graph such that they can be easily compared using meta-graph features. We use the symbol $\mathbf{m} \in \mathbb{R}^d$ to denote the fixed-size meta-graph feature vector of graph G. We defer the details of how METAGL computes $\mathbf{m}$ to Section 4.3.

Model Performance Estimation. To estimate how well a model would perform on a given graph, METAGL represent models and graphs in the latent k-dimensional space, and captures the graph-to-model affinity using the dot product similarity between the two representations $\mathbf{h}_{G_i}$ and $\mathbf{h}_{M_j}$ of the i-th graph G_i and j-th model M_j, respectively, such that $p_{ij} \approx \langle \mathbf{h}_{G_i}, \mathbf{h}_{M_j} \rangle$ where p_{ij} is the performance of model M_j on graph G_i. Then to obtain the latent representation $\mathbf{h}$, we design a learnable function $f(\cdot)$ that takes in relevant information on models and graphs from the meta-graph features $\mathbf{m}$ and the prior knowledge (*i.e.*, model performances $\mathbf{P}$ and observed graphs $\boldsymbol{\mathcal{G}}$). Below in this section, we focus on the inputs to the function $f(\cdot)$, and defer the details of $f(\cdot)$ to Section 4.4.

We first factorize performance matrix $\mathbf{P}$ into latent graph factors $\mathbf{U} \in \mathbb{R}^{n \times k}$ and model factors $\mathbf{V} \in \mathbb{R}^{m \times k}$, and take the model factor $\mathbf{V}_j \in \mathbb{R}^k$ (the j-th row of $\mathbf{V}$) as the input representation of model M_j. Then, METAGL obtains the latent embedding $\mathbf{h}_{M_j}$ of model M_j by $\mathbf{h}_{M_j} = f(\mathbf{V}_j)$. For graphs, more information is available since we have both meta-graph features $\mathbf{m}$ and meta-train graph factors $\mathbf{U}$. However, while we have the same number of models during training and inference, we observe new graphs during inference, and thus cannot obtain the graph factor $\mathbf{U}_{\text{test}}$ for the test graph as for the train graphs since matrix factorization (MF) is transductive by construction (*i.e.*, existing models' performance on the test graph is needed to get latent factors for the test graph directly via MF). To handle this issue, we learn an estimator $\phi : \mathbb{R}^d \mapsto \mathbb{R}^k$ that maps the meta-graph features $\mathbf{m}$ into the latent factors of meta-train graphs obtained via MF above (*i.e.*, for graph G_i with $\mathbf{m}$, $\phi(\mathbf{m}) = \widehat{\mathbf{U}}_i \approx \mathbf{U}_i$) and use this estimated graph factor. We then combine both inputs ($[\mathbf{m}; \phi(\mathbf{m})] \in \mathbb{R}^{d+k}$), and apply linear transformation to make the input representation of graph G_i to be of the same size as that of model M_j, obtaining the latent embedding of graph G_i to be $\mathbf{h}_{G_i} = f(\mathbf{W}[\mathbf{m}; \phi(\mathbf{m})])$ where $\mathbf{W} \in \mathbb{R}^{k \times (d+k)}$ is a weight matrix. Thus in METAGL, the performance p_{ij} of model M_j on graph G_i with meta-graph features $\mathbf{m}$ is estimated as

$$p_{ij} \approx \widehat{p}_{ij} = \langle f(\mathbf{W}[\mathbf{m}; \phi(\mathbf{m})]), f(\mathbf{V}_j) \rangle. \tag{2}$$

Meta-Learning Objective. For tasks where the goal is to estimate real values, such as accuracy, the mean squared error (MSE) is a typical choice for the loss function. While MSE is easy to optimize and

effective for regression, it does not directly take the ranking quality into account. By contrast, in our problem setup, accurately ranking models for each graph dataset is more important than estimating the performance itself, which makes MSE a suboptimal choice. In particular, Problem 1 focuses on finding the model with the best performance on the given graph. Therefore, we consider rank-based learning objectives, and among them, we adapt the top-1 probability to the proposed Problem 1 as follows. Let $\widehat{\mathbf{P}}_i \in \mathbb{R}^m$ be the i-th row of $\widehat{\mathbf{P}}$ (*i.e.*, estimated performance of all m models on graph G_i). Given $\widehat{\mathbf{P}}_i$, the top-1 probability $p_{\text{top1}}^{\widehat{\mathbf{P}}_i}(j)$ of j-th model M_j in the model set $\boldsymbol{\mathcal{M}}$ is defined to be

$$p_{\text{top1}}^{\widehat{\mathbf{P}}_i}(j) = \frac{\pi(\widehat{p}_{ij})}{\sum_{k=1}^{m} \pi(\widehat{p}_{ik})} = \frac{\exp(\widehat{p}_{ij})}{\sum_{k=1}^{m} \exp(\widehat{p}_{ik})} \tag{3}$$

where $\pi(\cdot)$ is an increasing, strictly positive function, which we define to be an exponential function.

Theorem 1 (Cao et al. (2007))**.** Given the performance $\widehat{\mathbf{P}}_i$ of all models on graph G_i, $p_{\text{top1}}^{\widehat{\mathbf{P}}_i}(j)$ represents the probability of model M_j to be ranked at the top of the list (*i.e.*, all models in $\boldsymbol{\mathcal{M}}$). Top-1 probabilities $p_{\text{top1}}^{\widehat{\mathbf{P}}_i}(j)$ for all $j = 1, \ldots, m$ form a probability distribution over m models.

Based on Theorem 1, we obtain two probability distributions by applying top-1 probability to the true performance $\mathbf{P}_i$ and estimated performance $\widehat{\mathbf{P}}_i$ of m models, and optimize METAGL such that the distance between the two resulting distributions gets decreased. Using the cross entropy as the distance metric, we obtain the following loss over all n meta-train graphs $\boldsymbol{\mathcal{G}}$:

$$L(\mathbf{P}, \widehat{\mathbf{P}}) = -\sum_{i=1}^{n} \sum_{j=1}^{m} p_{\text{top1}}^{\mathbf{P}_i}(j) \log \left(p_{\text{top1}}^{\widehat{\mathbf{P}}_i}(j) \right) \tag{4}$$

When $\mathbf{P}$ is sparse, meta-training can be performed via slightly modified Eqs. (3) and (4) in App. G.2.

4.2 ONLINE MODEL PREDICTION

In the meta-training phase, METAGL learns estimators $f(\cdot)$ and $\phi(\cdot)$, as well as weight matrix $\mathbf{W}$ and latent model factors $\mathbf{V}$. Given a new graph G_{test}, METAGL first computes the meta-graph features $\mathbf{m}_{\text{test}} \in \mathbb{R}^d$ as we discuss in Section 4.3. Then $\mathbf{m}_{\text{test}}$ is regressed to obtain the (approximate) latent graph factors $\widehat{\mathbf{U}}_{\text{test}} = \phi(\mathbf{m}_{\text{test}}) \in \mathbb{R}^k$. Recall that the model factors $\mathbf{V}$ learned in the meta-training stage can be directly used for model prediction. Then model M_j's performance on test graph G_{test} can be estimated by applying Equation (2) with $\mathbf{m}_{\text{test}}$ and $\phi(\mathbf{m}_{\text{test}})$. Finally, the model that has the highest estimated performance is selected by METAGL as the best model M^*, *i.e.*,

$$M^* \leftarrow \underset{M_j \in \boldsymbol{\mathcal{M}}}{\arg\max} \left\langle f(\mathbf{W}[\mathbf{m}_{\text{test}}; \phi(\mathbf{m}_{\text{test}})]), f(\mathbf{V}_j) \right\rangle \tag{5}$$

Note that model selection using Equation (5) depends only on the meta-graph features $\mathbf{m}_{\text{test}}$ of the test graph and other pretrained estimators and latent factors that METAGL learned in the meta-training phase. As no model training or evaluation is involved, model prediction by METAGL is much faster than training and evaluating different models multiple times, as our experiments show in Section 5.4. Further, model prediction process is fully automatic it does not require users to choose or fine-tune any values at test time. Figure 2 shows an overview of the model prediction process, and Algorithm 1 in the Appendix lists steps for offline meta-training and online model prediction.

4.3 STRUCTURAL META-GRAPH FEATURES

Meta-graph features are a crucial component of our meta-learning approach METAGL since they capture important structural characteristics of an arbitrary graph. Meta-graph features enable METAGL to quantify graph similarities, and utilize prior experience with observed graphs for GL model selection. It is important that a sufficient and representative set of meta-graph features are used to capture the important structural properties of graphs from a wide variety of domains, including biological, technological, information, and social networks to name a few.

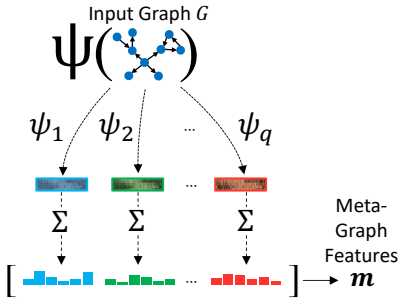


Figure 3: Meta-graph features in METAGL are derived in two steps. See Section 4.3 for details.

In this work, we are not able to leverage the commonly used simple statistical meta-features used by previous work on model selection-based meta-learning, as they cannot be used directly

over irregular and complex graph data. To address this problem, we introduce the notion of meta-graph features and develop a general framework for computing them on any arbitrary graph.

Meta-graph features in METAGL are derived in two steps, which is shown in Figure 3. First, we apply a set of structural meta-feature extractors $\Psi = \{\psi_1, \ldots, \psi_q\}$ to the input graph G, obtaining $\Psi(G) = \{\psi_1(G), \ldots, \psi_q(G)\}$. Applying $\psi \in \Psi$ to G yields a vector or a distribution of values for the nodes (or edges) in the graph, such as degree distribution and PageRank scores. That is, in Figure 3, ψ_1 can be a degree distribution, ψ_2 can be PageRank scores of all nodes, and so on. Specifically, we use both local and global structural feature extractors. To capture the local structural properties around a node or an edge, we compute node degree, number of wedges, triangles centered at each node, and also frequency of triangles for every edge. To capture global structural properties of a node, we derive eccentricity, PageRank score, and k-core number of each node. Appendix D summarizes meta-feature extractors used in this work.

Let ψ denote the local structural extractors for nodes. Given a graph $G_i = (V_i, E_i)$ and ψ, we obtain an $|V_i|$-dimensional node vector $\psi(G_i)$. Since any two graphs G_i and G_j are likely to have a different number of nodes and edges, the resulting structural feature matrices $\psi(G_i)$ and $\psi(G_j)$ for these graphs are also likely to be of different sizes as the rows of these matrices correspond to nodes or edges of the corresponding graph. Thus, in general, these structural feature-based representations of the graphs cannot be used directly to derive similarity between graphs.

Now, to address this issue, we apply the set Σ of *global* statistical meta-graph feature extractors to every $\psi_i(G)$, $\forall i = 1, \ldots, q$, which summarizes each $\psi_i(G)$ to a fixed-size vector. Specifically, $\Sigma(\psi_i(G))$ applies each of the statistical functions in Σ (*e.g.*, mean, kurtosis, etc) to the distribution $\psi_i(G)$, which computes a real number that summarizes the given feature distribution $\psi_i(G)$ from different statistical point of view, producing a vector $\Sigma(\psi_i(G)) \in \mathbb{R}^{|\Sigma|}$. Then we obtain the meta-graph feature vector $\mathbf{m}$ of graph G by concatenating the resulting meta-graph feature vectors:

$$\mathbf{m} = [\Sigma(\psi_1(G)) \ \cdots \ \Sigma(\psi_q(G))] \in \mathbb{R}^d. \tag{6}$$

Table 5 in Appendix D lists the global statistical functions Σ used in this work to derive meta-graph features. Further, in addition to the node- and edge-level structural features, we also compute global graph statistics (scalars directly derived from the graph, *e.g.*, density and degree assortativity coefficient), and append them to $\mathbf{m}$, *i.e.*, the node- or edge-level structural features obtained above.

Most importantly, given any arbitrary graph G', the proposed approach is guaranteed to output a fixed d-dimensional meta-graph feature vector characterizing G'. Hence, the structural similarity of any two graphs G and G' can be quantified using a similarity function over $\mathbf{m}$ and $\mathbf{m}'$, respectively.

4.4 EMBEDDING MODELS AND GRAPHS

Given an informative context (*i.e.*, input features) of models and graphs that METAGL learns from model performances $\mathbf{P}$ and meta-graph features $\mathbf{M}$ (Sections 4.1 and 4.3), how can we use it to effectively learn model and graph embeddings that capture graph-to-model affinity? We note that similar entities can make each other's context more accurate and informative. For instance, in our problem setup, similar models tend to have similar performance distributions over graphs, and likewise similar graphs are likely to exhibit similar affinity to different models. With this consideration, we model the task as a graph representation learning problem, where we construct a graph called *G-M network* that connects similar graphs and models, and learn the graph and model embeddings over it.

G-M Network. We define G-M network to be a multi-relational graph with two types of nodes (*i.e.*, models and graphs) where edges connect similar model nodes and graph nodes. To measure similarity among graphs and models, we utilize the latent graph and model factors ($\mathbf{U}$ and $\mathbf{V}$, respectively) obtained by factorizing $\mathbf{P}$, as well as the meta-graph features $\mathbf{M}$. More precisely, we use the estimated graph factor $\widehat{\mathbf{U}}$ instead of $\mathbf{U}$ to let the same graph construction process work for new graphs. Note that this gives us two types of features for graph nodes (*i.e.*, $\widehat{\mathbf{U}}$ and $\mathbf{M}$), and one type of features for model nodes (*i.e.*, $\mathbf{V}$). To let different features influence the embedding step differently as needed, we connect graph nodes and model nodes using five type of edges: M-g2g, P-g2g, P-m2m, P-g2m, P-m2g where g and m denote the type of nodes that an edge connects (graph and model, respectively), and M and P denote that the edge is based on meta-graph features and model performance, respectively. For example, M-g2g and P-g2g edges connect two graph nodes that are similar in terms of $\mathbf{M}$ and $\widehat{\mathbf{U}}$, respectively. Then for each edge type, we construct a k-NN graph by connecting nodes to their top-k similar nodes, where node-to-node similarity is defined as the cosine similarity between the

corresponding node features. For instance, for P-g2m edge type, graph nodes and model nodes are linked based on the similarity between $\widehat{\mathbf{U}}$ and $\mathbf{V}$. Fig. 7 in the Appendix illustrates the G-M network.

Learning Over G-M Network. Given the G-M network $\mathcal{G}_{\text{train}}$ with meta-train graphs and models, graph neural networks (GNNs) provide an effective framework to embed models and graphs via (weighted) neighborhood aggregation over $\mathcal{G}_{\text{train}}$. However, since the structure of G-M network is induced by simple k-NN search, some of the neighbors may not provide the same amount of information as others, or may even provide noisy information. We found it helpful to perform attentive neighborhood aggregation, so more informative neighbors can be given more weights. To this end, we choose to use attentive GNNs designed for multi-relational networks, and specifically use HGT (Hu et al., 2020). Then the embedding function $f(\cdot)$ in Section 4.1 is defined to be $f(\mathbf{x}) = \text{HGT}(\mathbf{x}, \mathcal{G}_{\text{train}})$ during training, which transforms the input node feature $\mathbf{x}$ into an embedding via attentive neighborhood aggregation over $\mathcal{G}_{\text{train}}$. Further details of HGT are provided in Appendix G.4.

Inference Over G-M Network. For inference at test time, we extend $\mathcal{G}_{\text{train}}$ to be a larger G-M network $\mathcal{G}_{\text{test}}$ that additionally contains test graph nodes, and edges between test graph nodes, and existing graphs and models in $\mathcal{G}_{\text{train}}$. The extension is done in the same way as in the training phase, by finding top-k similar nodes. Then the embedding at test time can be done by $f(\mathbf{x}) = \text{HGT}(\mathbf{x}, \mathcal{G}_{\text{test}})$.

5 Experiments

5.1 Experimental Settings

Models and Evaluation. A model in our problem (Eqn. 1) consists of two components. The first component performs graph representation learning (GRL), and the other component leverages the learned embeddings for a downstream task of interest. In this work, we focus on link prediction, which is a key task for graph-structured data as we discuss in Section 1. We evaluate the performance of selecting a link prediction model for new graphs *without any model evaluation*. For the first component, we use 12 popular GRL methods, and for the second component for link scoring, we use a simple estimator that computes the cosine similarity between two node embeddings. This results in a model set $\boldsymbol{\mathcal{M}}$ with 423 models. The full list of models is given in Table 4 in Appendix C.

For evaluation, we create a testbed containing benchmark graphs, meta-graph features, and a performance matrix. We construct the performance matrix by evaluating each link prediction model in $\boldsymbol{\mathcal{M}}$ on the graphs in the testbed, in terms of mean average precision score. Then we evaluate MetaGL and baselines via 5-fold cross validation where the benchmark graphs are split into meta-train $\boldsymbol{\mathcal{G}}_{\text{train}}$ and meta-test $\boldsymbol{\mathcal{G}}_{\text{test}}$ graphs for each fold, and meta-learners trained over the meta-train graph data are evaluated using the meta-test graph datasets. Thus, model performances over the meta-test graphs $\boldsymbol{\mathcal{G}}_{\text{test}}$ and the meta-graph features of $\boldsymbol{\mathcal{G}}_{\text{test}}$ were unseen during training, but used only for testing.

Since model selection aims to accurately predict the best model for a new graph, we evaluate the top-1 prediction performance in terms of MRR (Mean Reciprocal Rank), AUC, and NDCG (Normalized Discounted Cumulative Gain). To apply MRR and AUC, we label models such that the top-1 model (*i.e.*, the model with the best performance for the given graph) is labeled as 1, while all others are labeled as 0. For NDCG, we report NDCG@1, which evaluates the relevance of top-1 predicted model. All metrics range from 0 to 1, with larger values indicating better performance.

Table 2: The proposed MetaGL outperforms existing meta-learners, given fully observed performance matrix. **Best** results are in bold, and second best results are underlined. "MetaGL_Baseline" notation (*e.g.*, MetaGL_S2) indicate that the baseline meta-learner uses MetaGL's meta-graph features.

	Method	MRR	AUC	NDCG@1
	Random Selection	0.011	0.490	0.745
Simple	Global Best-AvgPerf	0.163	0.877	0.932
	Global Best-AvgRank	0.103	0.867	0.930
	MetaGL_AS	0.222	0.905	0.947
	MetaGL_ISAC	0.215	0.891	0.941
Optimization-based	MetaGL_S2	0.128	0.861	0.933
	MetaGL_ALORS	0.120	0.868	0.921
	MetaGL_NCF	0.132	0.875	0.931
	MetaGL_MetaOD	0.075	0.599	0.889
	MetaGL	**0.261**	**0.941**	**0.962**

Baselines. Being the first work for evaluation-free model selection in GL, we do not have immediate baselines for comparison. Instead, we adapt baselines used for OD model selection (Zhao et al., 2021) and collaborative filtering for our problem setting. In Appendix A, we describe baselines in detail. Baselines are grouped into two categories: (a) ***Simple meta-learners*** select a model that performs generally well, either globally or locally: **Global Best (GB)-AvgPerf**, **GB-AvgRank**, **ISAC** (Kadioglu et al., 2010), and **ARGOSMART (AS)** (Nikolić et al., 2013); (b) ***Optimization-based meta-***

learners learn to estimate the model performance by modeling the relation between meta features and model performances: **Supervised Surrogates (S2)** (Xu et al., 2012), **ALORS** (Misir & Sebag, 2017), **NCF** (He et al., 2017), and **MetaOD** (Zhao et al., 2021). We also include **Random Selection (RS)** as a baseline to see how these methods compare to random scoring.

Note that, except the simplest meta-learners RS and GB, no baselines can handle graph data, and thus they cannot estimate model performance on the new graph on their own. In that sense, they are not direct competitors of METAGL. We enable them to be used for GL model selection by providing the proposed meta-graph features. MetaOD, which was originally designed for OD model selection, is also given the same meta-graph features to perform GL model selection. We denote baselines either by combining METAGL with their names (*e.g.*, METAGL_S2) to clearly show that they use METAGL's meta-graph features, or using their name alone (*e.g.*, S2) for simplicity.

5.2 MODEL SELECTION ACCURACY

Fully Observed Performance Matrix. In this setup, meta-learners are trained using a full performance matrix $\mathbf{P}$ with no missing entries. The model selection accuracy of all meta-learners in this setup is reported in Table 2, where METAGL achieves the best performance in all metrics, with *18%* higher MRR than the best baseline (AS).

- Among simple meta-learners, Global Best meta-learners, which simply average model performance or rank over all observed graphs, are outperformed by more sophisticated meta-learners AS and ISAC, which leverage dataset similarities for model selection using meta-graph features.
- For optimization-based meta-learners, it is important to be aware of how models and graphs relate to each other, and have high flexibility to capture that complex relationship. In methods like ALORS and MetaOD, relations between models and datasets (*i.e.*, relative position of models and datasets in the embedding subspace) are learned rather indirectly via reconstructing the performance matrix.
- METAGL, in contrast, directly captures graph-to-model affinity by modeling their relations via employing flexible GNNs over the G-M network, as well as reconstructing the performance matrix. As a result, METAGL consistently outperforms other optimization-based meta-learners.

Partially Observed Performance Matrix. In this setup, meta-learners are trained using a sparse performance matrix $\mathbf{P}$, obtained by randomly masking out a full $\mathbf{P}$. Figure 4 reports results obtained with varying sparsity, ranging up to 0.9. In this more challenging setup, METAGL consistently performs the best across all levels of sparsity, achieving up to *47%* higher MRR than the best baseline.

- With increased sparsity, nearly all meta-learners perform increasingly worse, as one might expect.
- While AS was the best baseline given a full $\mathbf{P}$, its accuracy decreased rapidly as sparsity increased. Since AS selects a model based on the 1NN meta-train graph, it is highly sensitive to $\mathbf{P}$'s sparsity.
- Baselines such as the Global Best baselines are more stable as they average across multiple graphs.
- Optimization-based methods like METAGL and S2 perform favorably to simple meta-learners in sparse settings as they learn to reconstruct $\mathbf{P}$ by modeling the relation between graphs and models.

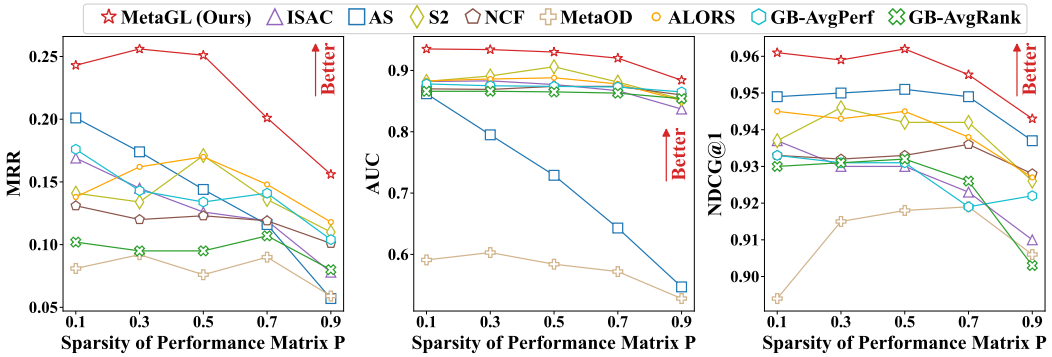


Figure 4: METAGL consistently performs the best, as the sparsity of performance matrix $\mathbf{P}$ varies. METAGL and all baseline meta-learners used the same meta-graph features proposed in this work.

5.3 EFFECTIVENESS OF META-GRAPH FEATURES

In Figure 5, we evaluate how the performance of meta-learners obtained with the proposed meta-graph feature (Section 4.3) compares to that obtained with existing graph-level embedding (GLE) techniques, GL2Vec (Chen & Koga, 2019), Graph2Vec (Narayanan et al., 2017), and GraphLoG (Xu et al., 2021).

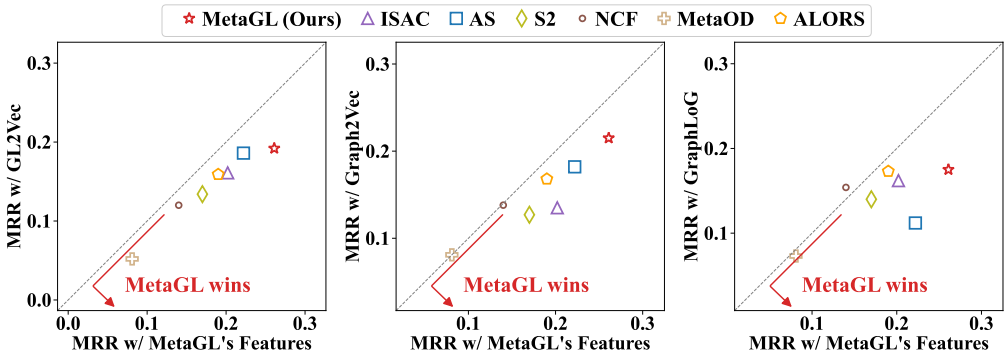


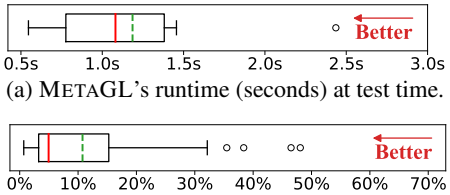
Figure 5: Using the proposed meta-graph features (Section 4.3), all meta-learners nearly consistently perform better (*i.e.*, points are below the diagonal) than with existing graph-level embedding methods.

Figure 8 in App. I.1 provides results for three other GLE methods, WaveletCharacteristic (Wang et al., 2021), SF (de Lara & Pineau, 2018), and LDP (Cai & Wang, 2019).

- Most points are below the diagonal in Figure 5, *i.e.*, all meta-learners nearly consistently perform better when they use METAGL's meta-graph features than when they use existing GLE methods. This shows the effectiveness of METAGL's features for the proposed task of GL model selection.
- METAGL performs the best, whether METAGL's features or existing GLE methods are used.

5.4 MODEL SELECTION EFFICIENCY

To evaluate how efficient METAGL's model selection is, we measure its runtime (*i.e.*, the time to create meta-graph features for the new graph at test time, plus the time to predict the best model), and compare it with the time to train a GL model. Figure 6 shows the distribution in box plots, where red and green lines denote the median and mean, respectively.



(a) METAGL's runtime (seconds) at test time.

(b) METAGL's runtime / Time to train GL models for 5% of their potential settings (in pct.).

Figure 6: METAGL is fast (∼1 sec.), and incurs negligible overhead. Red and green lines denote the median and mean, respectively.

Results show that METAGL is fast, and incurs negligible runtime overhead: its runtime is just around 1 seconds or less in most cases (Figure 6a). Notably, compared to training each GL model for only 5% of its available model configurations, METAGL takes considerably less time, *i.e.*, a median of 5% and a mean of 11% of the time required for model training (Figure 6b). Given large-scale test graphs in practice, the speed-up enabled by METAGL will be greater than that reported in Figure 6b, due to the increased training time on such graphs. Also, METAGL's model selection process can be further streamlined, *e.g.*, by parallelizing meta-feature generation process. We provide additional results on the runtime of METAGL and naive model selection in Appendix I.2.

5.5 ABLATION STUDY

We present ablation study in App. I.3, which shows the effectiveness of METAGL's proposed components, *i.e.*, the meta-learning objective, G-M network, and the graph encoder used by METAGL.

6 CONCLUSION

As more and more GL models are developed, selecting which one to use is becoming increasingly hard. Toward near-instantaneous, automatic GL model selection, we make the following contributions.

- **Problem Formulation.** We present the first problem formulation to select effective GL models in an evaluation-free manner (*i.e.*, without ever having to train/evaluate any model on the new graph).
- **Meta-Learning Framework and Features.** We propose METAGL, the first meta-learning framework for evaluation-free GL model selection, and meta-graph features to quantify graph similarities.
- **Effectiveness.** Using METAGL for model selection greatly outperforms existing meta-learning techniques (up to *47%* better), while incurring negligible runtime overhead at test time (∼*1 sec*).

Benchmark Data/Code: To facilitate further research on this crucial new problem, we release code and data, including performances of 400+ models on 300+ graphs, and 300+ meta-graph features.

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In Appendix, we provide a description of the baselines (Appendix A), notations used in this work (Appendix B), and the model set (Appendix C), and present a summary of meta-graph features (Appendix D), details of graph datasets in the testbed (Appendix E), and experimental details (Appendix F). We then provide additional details of METAGL (Appendix G), *e.g.*, the G-M network and the embedding function $f(\cdot)$ discussed in Section 4.4, as well as additional results (Appendix I), *e.g.*, ablation studies.

A BASELINES

Being the first work for evaluation-free model selection in graph learning (GL), we do not have immediate baselines for comparison. Instead, we adapt baselines used in MetaOD (Zhao et al., 2021) for outlier detection (OD) model selection as well as collaborative filtering for our problem setting. The baselines used in experiments can be organized into the following two categories.

(a) ***Simple meta-learners*** select a model that performs generally well, either globally or locally.

- **Global Best (GB)-AvgPerf** selects the model that has the largest average performance over all meta-train graphs.
- **Global Best (GB)-AvgRank** computes the rank of all models (in percentile) for each graph, and selects the model with the largest average ranking over all meta-train graphs.
- **ISAC** (Kadioglu et al., 2010) first clusters meta-train datasets using meta-graph features, and at test time, finds the cluster closest to the test graph, and selects the model with the largest average performance over all graphs in that cluster.
- **ARGOSMART (AS)** (Nikolić et al., 2013) finds the meta-train graph closest to the test graph (*i.e.*, 1NN) in terms of meta-graph feature similarity, and selects the model with the best result on the 1NN graph.

(b) ***Optimization-based meta-learners*** learn to estimate the model performance by modeling the relation between meta-graph features and model performances.

- **Supervised Surrogates (S2)** (Xu et al., 2012) learns a surrogate model (a regressor) that maps meta-graph features to model performances.
- **ALORS** (Misir & Sebag, 2017) factorizes the performance matrix into latent factors on graphs and models, and estimates the performance to be the dot product between the two factors, where a non-linear regressor maps meta-graph features into the latent graph factors.
- **NCF** (He et al., 2017) replaces the dot product used in ALORS with a more general neural architecture that estimates performance by combining the linearity of matrix factorization and non-linearity of deep neural networks.
- **MetaOD** (Zhao et al., 2021) pioneered the field of unsupervised OD model selection by designing meta-features specialized to capture the outlying characteristics of datasets, as well as improving upon ALORS with the adoption of an NDCG-based meta-training objective. We enable MetaOD to be applicable to our problem setting, by applying our proposed meta-graph features to MetaOD.

In addition, we also include **Random Selection (RS)** as a baseline, to see how meta-learners perform in comparison to random scoring. Note that among the above approaches, only GB-AvgPerf and GB-AvgRank do not rely on meta-features for model selection. All other meta-learners make use of the proposed meta-graph features to estimate model performances on an unseen test graph.

B NOTATIONS

Table 3 provides a list of notations frequently used in this work.

C MODEL SET

A model in the model set $\mathcal{M}$ refers to a graph representation learning (GRL) method along with its hyperparameters settings, and a predictor that makes a downstream task-specific prediction given the node embeddings from the GRL method. In this work, we use a link predictor which scores a given link by computing the cosine similarity between the two nodes' embeddings. Table 4 shows the

Table 3: Summary of notations.

$\boldsymbol{\mathcal{G}}$	set of graphs $\{G_1, \ldots, G_n\}$ in the training set
n	number of graphs in training set $n = \lvert\boldsymbol{\mathcal{G}}\rvert$
G_{test}	new unseen test graph $G_{\text{test}} \notin \boldsymbol{\mathcal{G}}$
$\boldsymbol{\mathcal{M}}$	model set $\{M_1, \ldots, M_m\}$ to search over
m	number of models to search over $m = \lvert\boldsymbol{\mathcal{M}}\rvert$
Ψ	set of structural meta-node/edge feature extractors
Σ	set of meta-graph feature extractors
$\mathbf{M}$	meta-graph feature matrix where $\mathbf{M} \in \mathbb{R}^{n \times d}$
d	number of meta-graph features
$\mathbf{m}_{\text{test}}$	meta-graph feature vector for the new unseen test graph G_{test}
k	embedding size
$\mathbf{P}$	performance matrix of m models on n graphs
$\mathbf{U}$	latent graph factors obtained by factorizing $\mathbf{P}$ ($\mathbf{P} \approx \mathbf{U}\mathbf{V}^\intercal$)
$\mathbf{V}$	latent model factors obtained by factorizing $\mathbf{P}$ ($\mathbf{P} \approx \mathbf{U}\mathbf{V}^\intercal$)
$f(\cdot)$	learnable embedding function for models and graphs

Table 4: Graph representation learning (GRL) models and their hyperparameter settings, which collectively comprise the model set $\boldsymbol{\mathcal{M}}$ with 423 unique GRL models. For details of the hyperparameters, please refer to the cited paper.

Methods	**Hyperparameter Settings**	**Count**
SGC (Wu et al., 2019a)	# (number of) hops $k \in \{1, 2, 3\}$	3
GCN (Kipf & Welling, 2017)	# layers $L \in \{1, 2, 3\}$, # epochs $N \in \{1, 10\}$	6
GraphSAGE (Hamilton et al., 2017)	# layers $L \in \{1, 2, 3\}$, # epochs $N \in \{1, 10\}$, aggregation functions $f \in \{\text{mean}, \text{gcn}, \text{lstm}\}$	18
node2vec (Grover & Leskovec, 2016)	$p, q \in \{1, 2, 4\}$	9
role2vec (Ahmed et al., 2018)	$p, q \in \{0.25, 1, 4\}$, $\alpha \in \{0.01, 0.1, 0.5, 0.9, 0.99\}$, motif combinations $\mathcal{H} \in \{\{H_1\}, \{H_2, H_3\}, \{H_2, H_3, H_4, H_6, H_8\}, \{H_1, H_2, \ldots, H_8\}\}$	180
GraRep (Cao et al., 2015)	$k \in \{1, 2\}$	2
DeepWalk (Perozzi et al., 2014)	$p = 1, q = 1$	1
HONE (Rossi et al., 2018)	$k \in \{1, 2\}$, $D_{\text{local}} \in \{4, 8, 16\}$, variant $v = \{1, 2, 3, 4, 5\}$	30
node2bits (Jin et al., 2019)	walk num $w_n \in \{5, 10, 20\}$, walk len $w_l \in \{5, 10, 20\}$, log base $b \in \{2, 4, 8, 10\}$, feats $f \in \{16\}$	36
DeepGL (Rossi et al., 2020)	$\alpha \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$, motif size $\in \{4\}$, eps tolerance $t \in \{0.01, 0.05, 0.1\}$, relational aggr. $\in \{\{m\}, \{p\}, \{s\}, \{v\}, \{m, p\}, \{m, v\}, \{s, m\}, \{s, p\}, \{s, v\}\}$ where m, p, s, v denote mean, product, sum, var	135
LINE (Tang et al., 2015)	# hops/order $k \in \{1, 2\}$	2
Spectral Emb. (Luo et al., 2003)	tolerance $t \in \{0.001\}$	1
Total Count		**423**

complete list of 12 popular GRL methods and their specific hyperparameter settings, which compose 412 unique models in the model set $\boldsymbol{\mathcal{M}}$. Note that the link predictor is omitted from Table 4 since we employ the same link predictor based on cosine similarity to all GRL methods.

D META-GRAPH FEATURES

Structural Meta-Feature Extractors. To capture the local structural properties around a node or an edge, we compute the distribution of node degrees, number of wedges, triangles centered at each node, as well as the frequency of triangles for each edge. To capture the global structural properties of a node, we derive the eccentricity, PageRank score, and k-core number of each node. We also capture the global graph-level statistics (*i.e.*, different from local node/edge-level structural properties), such

as the density of $\mathbf{A}$ and $\mathbf{A}\mathbf{A}^T$ where $\mathbf{A}$ is the adjacency matrix, and also the degree assortativity coefficient r.

Global Statistical Functions. For each of the structural property distributions (degree, k-core numbers, and so on) derived by the above structural meta-feature extractors, we apply the set Σ of global statistical functions (Table 5) over it to obtain a fixed-length vector representation for the node/edge/graph-level structural feature distribution.

After obtaining a set of meta-graph features, we concatenate all of them together to create the final meta-graph feature vector $\mathbf{m}$ for the graph.

Table 5: Summary of the global statistical functions Σ for deriving a set of meta-graph features from a graph invariant (*e.g.*, k-core numbers, node degrees, and so on). Let $\mathbf{x}$ denote an arbitrary graph invariant vector for some graph $G_i = (V_i, E_i)$ and $\pi(\mathbf{x})$ is the sorted vector of $\mathbf{x}$. Note $\mathbf{x}$ can be any representation, *e.g.*, node degree vector (value for each node in G_i) or a degree distribution vector.

Name	**Equation**
Num. unique values	$\mathsf{card}(\mathbf{x})$
Density	$\mathsf{nnz}(\mathbf{x})/\lvert\mathbf{x}\rvert$
Q_1, Q_3	median of the $\lvert\mathbf{x}\rvert/2$ smallest (largest) values
IQR	$Q_3 - Q_1$
Outlier LB $\alpha \in \{1.5, 3\}$	$\sum_i \mathbb{I}(x_i < Q_1 - \alpha IQR)$
Outlier UB $\alpha \in \{1.5, 3\}$	$\sum_i \mathbb{I}(x_i > Q_3 + \alpha IQR)$
Total outliers $\alpha \in \{1.5, 3\}$	$\sum_i \mathbb{I}(x_i < Q_1 - \alpha IQR) + \sum_i \mathbb{I}(x_i > Q_3 + \alpha IQR)$
(α-std) outliers $\alpha \in \{2, 3\}$	$\mu_{\mathbf{x}} \pm \alpha\sigma_{\mathbf{x}}$
Spearman (ρ, p-val)	$\mathsf{spearman}(\mathbf{x}, \pi(\mathbf{x}))$
Kendall (τ, p-val)	$\mathsf{kendall}(\mathbf{x}, \pi(\mathbf{x}))$
Pearson (r, p-val)	$\mathsf{pearson}(\mathbf{x}, \pi(\mathbf{x}))$
Min, max	$\min(\mathbf{x})$, $\max(\mathbf{x})$
Range	$\max(\mathbf{x}) - \min(\mathbf{x})$
Median	$\mathsf{med}(\mathbf{x})$
Geometric Mean	$\lvert\mathbf{x}\rvert^{-1} \prod_i x_i$
Harmonic Mean	$\lvert\mathbf{x}\rvert / \sum_i \frac{1}{x_i}$
Mean, Stdev, Variance	$\mu_{\mathbf{x}}$, $\sigma_{\mathbf{x}}$, $\sigma^2_{\mathbf{x}}$
Skewness	$\mathbb{E}(\mathbf{x}-\mu_{\mathbf{x}})^3/\sigma^3_{\mathbf{x}}$
Kurtosis	$\mathbb{E}(\mathbf{x}-\mu_{\mathbf{x}})^4/\sigma^4_{\mathbf{x}}$
Quartile Dispersion Coeff.	$\frac{Q_3-Q_1}{Q_3+Q_1}$
Median Absolute Deviation	$\mathsf{med}(\lvert\mathbf{x} - \mathsf{med}(\mathbf{x})\rvert)$
Avg. Absolute Deviation	$\frac{1}{\lvert\mathbf{x}\rvert}\mathbf{e}^T\lvert\mathbf{x} - \mu_{\mathbf{x}}\rvert$
Coeff. of Variation	$\sigma_{\mathbf{x}}/\mu_{\mathbf{x}}$
Efficiency ratio	$\sigma^2_{\mathbf{x}}/\mu^2_{\mathbf{x}}$
Variance-to-mean ratio	$\sigma^2_{\mathbf{x}}/\mu_{\mathbf{x}}$
Signal-to-noise ratio (SNR)	$\mu^2_{\mathbf{x}}/\sigma^2_{\mathbf{x}}$
Entropy	$H(\mathbf{x}) = -\sum_i x_i \log x_i$
Norm. entropy	$H(\mathbf{x})/\log_2\lvert\mathbf{x}\rvert$
Gini coefficient	$-$
Quartile max gap	$\max(Q_{i+1} - Q_i)$
Centroid max gap	$\max_{ij} \lvert c_i - c_j\rvert$
Histogram prob. dist.	$\mathbf{p}_h = \frac{\mathbf{h}}{\mathbf{h}^T\mathbf{e}}$ (with fixed # of bins)

E GRAPH DATASETS

The testbed used in this work comprises 301 graphs that have widely varying structural characteristics. Table 6 provides a list of all graph datasets in the testbed. All graph data are from (Rossi & Ahmed, 2015); they are publicly available under the Creative Commons Attribution-ShareAlike License.

Table 6: Summary of the 301 graph datasets that comprise the testbed.

	Graph	# Nodes	# Edges		Graph	# Nodes	# Edges
1	BA-1_10_60	804	46410	152	enzymes_g297	121	149
2	BA-1_11_40	917	35860	153	enzymes_g349	64	118
3	BA-1_12_10	827	8215	154	enzymes_g355	66	112
4	BA-1_13_10	1043	10375	155	enzymes_g504	66	120
5	BA-1_14_40	829	32340	156	enzymes_g523	48	111
6	BA-1_16_40	1126	44220	157	enzymes_g526	58	110
7	BA-1_17_10	895	8895	158	enzymes_g527	57	107
8	BA-1_18_40	1141	44820	159	enzymes_g532	74	120
9	BA-1_1_10	862	8565	160	enzymes_g575	51	110
10	BA-1_20_10	830	8245	161	enzymes_g578	60	103
11	BA-1_22_10	1094	10885	162	enzymes_g594	52	114
12	BA-1_24_40	946	37020	163	enzymes_g597	52	116
13	BA-1_3_40	1017	39860	164	enzymes_g598	55	100
14	BA-1_4_40	970	37980	165	enzymes_g8	88	133
15	BA-1_5_10	1050	10445	166	ER-1_11_5	917	20841
16	BA-1_6_60	803	46350	167	ER-1_14_5	829	17092
17	BA-1_7_40	832	32460	168	ER-1_15_5	826	17099
18	BA-1_8_10	1040	10345	169	ER-1_24_5	946	22383
19	bio-CE-GN	2220	53683	170	ER-1_4_5	970	23747
20	bio-CE-GT	924	3239	171	ER-2_6_5	8115	16868
21	bio-CE-HT	2617	2985	172	inf-euroroad	1174	1417
22	bio-CE-LC	1387	1648	173	inf-openflights	2939	15677
23	bio-CE-PG	1871	47754	174	KPGM-log10-10-trial1	845	7194
24	bio-DM-CX	4040	76717	175	KPGM-log10-10-trial2	830	7265
25	bio-DM-HT	2989	4660	176	KPGM-log10-10-trial3	837	7251
26	bio-DM-LC	658	1129	177	KPGM-log10-12-trial1	845	8467
27	bio-DR-CX	3289	84940	178	KPGM-log10-12-trial2	864	8339
28	bio-grid-fission-yeast	2026	12637	179	KPGM-log10-12-trial3	856	8393
29	bio-HS-CX	4413	108818	180	KPGM-log10-14-trial2	885	9405
30	bio-HS-HT	2570	13691	181	KPGM-log10-8-trial1	824	6055
31	bio-HS-LC	4227	39484	182	KPGM-log10-8-trial2	796	6040
32	bio-SC-CC	2223	34879	183	KPGM-log10-8-trial3	813	6052
33	bio-SC-GT	1716	33987	184	KPGM-log8-10-trial1	220	1502
34	bio-SC-HT	2084	63027	185	KPGM-log8-10-trial2	220	1518
35	bio-SC-LC	2004	20452	186	KPGM-log8-10-trial3	224	1520
36	bio-SC-TS	636	3959	187	KPGM-log8-12-trial1	224	1729
37	biogrid-human	2005	3959	188	KPGM-log8-12-trial2	229	1756
38	biogrid-mouse	1450	1636	189	KPGM-log8-12-trial3	230	1761
39	biogrid-plant	523	838	190	KPGM-log8-14-trial1	229	1947
40	biogrid-worm	1930	3576	191	KPGM-log8-14-trial2	233	1950
41	biogrid-yeast	836	1049	192	KPGM-log8-14-trial3	230	1943
42	bn-cat-mixed-species-brain1	65	730	193	KPGM-log8-16-trial1	232	2117
43	bn-fly-drosophila-medulla1	1781	9016	194	KPGM-log8-16-trial2	230	2152
44	bn-macaque-rhesus-brain1	242	3054	195	KPGM-log8-16-trial3	235	2178
45	bn-macaque-rhesus-brain2	91	582	196	KPGM-log8-8-trial1	223	1324
46	bn-macaque-rhesus-cerebral-cortex1	91	1401	197	KPGM-log8-8-trial2	218	1312
47	bn-macaque-rhesus-interareal-cortical2	93	2262	198	KPGM-log8-8-trial3	215	1303
48	bn-mouse-brain1	213	16242	199	nci1_g1677	102	106
49	bn-mouse-kasthuri-v4	1029	1559	200	nci1_g1863	107	111
50	bn-mouse-visual-cortex2	193	214	201	nci1_g1893	96	102
51	ca-AstroPh	17903	196972	202	nci1_g1894	104	108
52	ca-CondMat	21363	91286	203	nci1_g2079	88	103
53	ca-cora	2708	5278	204	nci1_g2082	86	101
54	ca-CSphd	1882	1740	205	nci1_g2172	106	107
55	ca-DBLP-kang	2879	11326	206	nci1_g2228	92	98
56	ca-Erdos992	5094	7515	207	nci1_g2229	92	98
57	ca-GrQc	4158	13422	208	nci1_g2443	91	97
58	ca-HepPh	11204	117619	209	nci1_g2455	90	96
59	ca-netscience	379	914	210	nci1_g3139	107	112
60	ca-sandi-auths	86	123	211	nci1_g3141	92	98
61	CL-1000-1d7-trial1	928	4653	212	nci1_g3145	91	97
62	CL-1000-1d7-trial2	932	4888	213	nci1_g3444	93	102
63	CL-1000-1d7-trial3	938	4840	214	nci1_g3449	95	99
64	CL-1000-1d8-trial1	925	3776	215	nci1_g3585	105	107
65	CL-1000-1d8-trial2	930	4136	216	nci1_g3700	111	119

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Table 6 – *Continued from the previous page*

	Graph	# Nodes	# Edges		Graph	# Nodes	# Edges
66	CL-1000-1d8-trial3	925	3714	217	nci1_g3711	89	106
67	CL-1000-1d9-trial1	928	3510	218	nci1_g3901	93	102
68	CL-1000-1d9-trial2	912	3053	219	nci1_g3990	90	105
69	CL-1000-1d9-trial3	932	3278	220	nci1_g4094	90	98
70	CL-1000-2d0-trial1	909	2795	221	power-1138-bus	1138	2596
71	CL-1000-2d0-trial2	899	2941	222	power-494-bus	494	1080
72	CL-1000-2d0-trial3	916	3010	223	power-662-bus	662	1568
73	CL-1000-2d1-trial1	903	2430	224	power-685-bus	685	1967
74	CL-1000-2d1-trial2	911	2734	225	power-bcspwr09	1723	4117
75	CL-1000-2d1-trial3	915	2782	226	power-eris1176	1176	9864
76	DD_g1	327	899	227	rec-amazon	91813	125704
77	DD_g10	146	328	228	rec-movielens-tag-movies-10m	16528	71081
78	DD_g100	349	1005	229	road-chesapeake	39	170
79	DD_g1000	183	408	230	road-ChicagoRegional	1467	1298
80	DD_g1001	88	203	231	road-euroroad	1174	1417
81	DD_g1002	104	255	232	road-luxembourg-osm	114599	119666
82	DD_g1003	53	116	233	road-minnesota	2642	3303
83	DD_g1004	94	230	234	road-usroads-48	126146	161950
84	DD_g1005	370	903	235	rt-retweet	96	117
85	DD_g1006	246	568	236	rt-twitter-copen	761	1029
86	DD_g1007	309	732	237	rt_alwefaq	4171	7063
87	DD_g1008	109	304	238	rt_assad	2139	2788
88	DD_g1009	129	272	239	rt_bahrain	4676	7979
89	DD_g101	306	728	240	rt_barackobama	9631	9775
90	DD_g1010	157	363	241	rt_damascus	3052	3869
91	DD_g1011	47	136	242	rt_dash	6288	7436
92	DD_g1012	146	365	243	rt_gmanews	8373	8721
93	DD_g1013	93	211	244	rt_gop	4687	5529
94	DD_g1014	119	273	245	rt_http	8917	10314
95	DD_g1015	102	244	246	rt_islam	4497	4616
96	DD_g1016	113	291	247	rt_israel	3698	4165
97	DD_g1017	162	376	248	rt_lebanon	3961	4436
98	DD_g1018	296	680	249	rt_libya	5067	5541
99	DD_g1019	131	353	250	rt_lolgop	9765	10075
100	DD_g102	561	1422	251	rt_obama	3212	3423
101	DD_g1020	228	541	252	rt_occupy	3225	3944
102	DD_g1021	329	787	253	rt_occupywallstnyc	3609	3833
103	DD_g1022	294	730	254	rt_oman	4904	6230
104	DD_g1023	172	425	255	rt_onedirection	7987	8103
105	DD_g1024	59	160	256	rt_p2	4902	6018
106	DD_g1025	88	205	257	rt_saudi	7252	8061
107	DD_g1026	247	578	258	rt_tcot	4547	5503
108	DD_g1027	108	223	259	rt_tlot	3665	4475
109	DD_g1028	72	137	260	rt_uae	5248	6387
110	DD_g1029	99	215	261	rt_voteonedirection	2280	2464
111	DD_g103	265	647	262	sc-nasasrb	54870	1311227
112	DD_g1030	136	351	263	soc-advogato	6551	43427
113	DD_g104	372	999	264	soc-dolphins	62	159
114	DD_g105	423	1192	265	soc-firm-hi-tech	33	91
115	DD_g106	574	1355	266	soc-gplus	23628	39194
116	DD_g107	130	292	267	soc-hamsterster	2426	16630
117	DD_g108	483	1137	268	soc-highschool-moreno	70	274
118	DD_g109	132	315	269	soc-physicians	241	923
119	DD_g11	312	761	270	soc-sign-bitcoinalpha	3783	14124
120	DD_g110	394	1137	271	soc-student-coop	185	311
121	DD_g111	483	1520	272	soc-wiki-Vote	889	2914
122	DD_g112	266	631	273	socfb-Amherst	2235	90954
123	DD_g113	347	853	274	socfb-Bowdoin47	2252	84387
124	DD_g114	334	761	275	socfb-Caltech	769	16656
125	DD_g115	336	946	276	socfb-Hamilton46	2314	96394
126	eco-everglades	69	885	277	socfb-Haverford76	1446	59589
127	eco-florida	128	2075	278	socfb-nips-ego	2888	2981
128	eco-foodweb-baydry	128	2106	279	socfb-Oberlin44	2920	89912
129	eco-foodweb-baywet	128	2075	280	socfb-Reed98	962	18812
130	eco-mangwet	97	1446	281	socfb-Simmons81	1518	32988
131	eco-stmarks	54	353	282	socfb-Smith60	2970	97133
132	email-dnc-corecipient	906	10429	283	socfb-Swarthmore42	1659	61050
133	email-dnc-leak	1891	4465	284	socfb-Trinity100	2613	111996
134	email-enron-only	143	623	285	socfb-USFCA72	2682	65252
135	email-EU	32430	54397	286	socfb-Vassar85	3068	119161
136	email-radoslaw	167	3251	287	socfb-Villanova62	7772	314989
137	email-univ	1133	5451	288	socfb-Wellesley22	2970	94899
138	enzymes_g103	59	115	289	socfb-Williams40	2790	112986
139	enzymes_g118	95	121	290	tech-routers-rf	2113	6632

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Table 6 – *Continued from the previous page*

	Graph	# Nodes	# Edges		Graph	# Nodes	# Edges
140	enzymes_g123	90	127	291	tech-routers-rf	2113	6632
141	enzymes_g199	62	108	292	web-BerkStan	12305	19500
142	enzymes_g204	57	105	293	web-edu	3031	6474
143	enzymes_g209	57	101	294	web-EPA	4271	8909
144	enzymes_g215	48	104	295	web-google	1299	2773
145	enzymes_g224	54	105	296	web-indochina-2004	11358	47606
146	enzymes_g279	60	107	297	web-polblogs	643	2280
147	enzymes_g291	62	104	298	web-spam	4767	37375
148	enzymes_g292	60	100	299	web-webbase-2001	16062	25593
149	enzymes_g293	96	109	300	web-wiki-chameleon	2277	31421
150	enzymes_g295	123	139	301	web-wiki-crocodile	11631	170918
151	enzymes_g296	125	141				

F EXPERIMENTAL DETAILS

F.1 EXPERIMENTAL SETTINGS

Software. We used PyTorch[1] for implementing the training and inference pipeline, and used the DGL's implementation of HGT[2]. For MetaOD (Zhao et al., 2021), we used the implementation provided by the authors[3]. We used the Karate Club library (Rozemberczki et al., 2020) for the implementations of the following graph-level embedding (GLE) methods, Graph2Vec (Narayanan et al., 2017), GL2Vec (Chen & Koga, 2019), WaveletCharacteristic (Wang et al., 2021), SF (de Lara & Pineau, 2018), and LDP (Cai & Wang, 2019). For GraphLoG (Xu et al., 2021), we used the authors' implementation[4]. We used open source libraries, such as NetworkX[5] and NumPy[6], for implementing meta-graph feature extractors.

Hyperparameters. We set the embedding size k to 32 for METAGL and other meta-learners that learn embeddings of models and graphs. For METAGL, we created the G-M network by connecting nodes to their top-30 similar nodes. As an the embedding function $f(\cdot)$ in METAGL, we used HGT (Hu et al., 2020) with 2 layers and 4 heads per layer. HGT is included in the Deep Graph Library (DGL), which is licensed under the Apache License 2.0. For training, we used the Adam optimizer with a learning rate of 0.0005 and a weight decay of 0.0001. For GLE approaches, we used the default hyperparameter settings specified in the corresponding library and GitHub repository.

F.2 EVALUATION OF MODEL SELECTION ACCURACY (SECTION 5.2)

In our evaluation involving a partially observed performance matrix, we extended baseline meta-learners as follows so they can operate in the presence of missing entries in the performance matrix.

- Global Best-AvgPerf averaged observed performance entries alone, ignoring missing values. If an average performance cannot be computed for some model (which is the case when a model has no observed performance entries for all graphs), we use the mean of averaged performance for other models in its place.
- Global Best-AvgRank computed the model rankings for each graph in percentile, as the number of observed model performances may be different for different graphs, and averaged the rank percentiles for observed cases only, as in Global Best-AvgPerf.
- ISAC handled the sparse performance matrix in the same way as Global Best-AvgPerf, except that only a subset of graphs, which is similar to the test graph, is considered in ISAC.
- ARGOSMART (AS) computed the mean of observed performance entries of the 1NN graph, and used this quantity in place of missing values.
- ALORS factorized the sparse performance matrix using a missing value-aware non-negative matrix factorization algorithm.

[1] https://pytorch.org/
[2] https://www.dgl.ai/
[3] https://github.com/yzhao062/MetaOD
[4] https://github.com/DeepGraphLearning/GraphLoG
[5] https://networkx.org/
[6] https://numpy.org/

- Supervised Sur. (S2), NCF, and MetaOD performed optimization by only considering observed performance values in the loss function, while skipping over missing entries. Early stopping based on the validation performance was also done with respect to the observed performances alone.

F.3 Evaluation of Meta-Graph Features (Section 5.3)

Except for WaveletCharacteristic and GraphLoG, we applied graph-level embedding (GLE) approaches to all graphs in our testbed, and meta-learners were trained and evaluated using the representations of all graphs via 5-fold cross validation. Since WaveletCharacteristic and GraphLoG could not scale up to some of the largest graphs in the testbed (*e.g.*, due to out-of-memory error), we excluded 9% and 27% largest graphs for GraphLoG and WaveletCharacteristic, respectively, and evaluated meta-learners using the resulting subset of graphs. Note that, in these cases, MetaGL was also trained and evaluated using the same subset of graphs.

G Additional Details of MetaGL

G.1 MetaGL Algorithm

Algorithm 1 provides detailed steps of MetaGL, for both offline meta-training (top) and online model selection (bottom).

Algorithm 1: MetaGL: Offline Meta-Training (Top) and Online Model Selection (Bottom)

Input: Meta-train graph database $\boldsymbol{\mathcal{G}}$, model set $\boldsymbol{\mathcal{M}}$, embedding dimension k
Output: Meta-learner for model selection
/* (Offline) Meta-Learner Training (Sec. 4.1) */
Train & evaluate models in $\boldsymbol{\mathcal{M}}$ on graphs in $\boldsymbol{\mathcal{G}}$ to get performance matrix $\mathbf{P}$
Extract meta-graph features $\mathbf{M}$ for each graph G_i in $\boldsymbol{\mathcal{G}}$ (Sec. 4.3)
Factorize $\mathbf{P}$ to obtain latent graph factors $\mathbf{U}$ and model factors $\mathbf{V}$, *i.e.*, $\mathbf{P} \approx \mathbf{U}\mathbf{V}^\intercal$
Learn an estimator $\phi(\cdot)$ such that $\phi(\mathbf{m}) = \widehat{\mathbf{U}}_i \approx \mathbf{U}_i$
Create meta-train graph $\mathcal{G}_{\text{train}}$ (Sec. 4.4)
while *not converged*
  for $i = 1, \ldots, n$ **do**
    Get embeddings $f(\mathbf{W}[\mathbf{m}; \phi(\mathbf{m})])$ of train graph G_i on $\mathcal{G}_{\text{train}}$
    for $j = 1, \ldots, m$ **do**
      Get embeddings $f(\mathbf{V}_j)$ of each model M_j on $\mathcal{G}_{\text{train}}$
      Estimate $\widehat{p}_{ij} = \langle f(\mathbf{W}[\mathbf{m}; \phi(\mathbf{m})]), f(\mathbf{V}_j) \rangle$ (Eqn. 2)
    end
  end
  Compute meta-training loss $L(\mathbf{P}, \widehat{\mathbf{P}})$ (Eqn. 4) and optimize parameters
end

Input: new graph G_{test}
Output: selected model M^* for G_{test}
/* (Online) Model Selection (Sec. 4.2) */
Extract graph meta-features $\mathbf{m}_{\text{test}} = \psi(G_{\text{test}})$
Estimate latent factor $\widehat{\mathbf{U}}_{\text{test}} = \phi(\mathbf{m}_{\text{test}})$ for test graph G_{test}
Create meta-test graph $\mathcal{G}_{\text{test}}$ by extending $\mathcal{G}_{\text{train}}$ with new edges between test graph node and existing nodes in $\mathcal{G}_{\text{train}}$ (Sec. 4.4)
Get embeddings $f(\mathbf{W}[\mathbf{m}_{\text{test}}; \widehat{\mathbf{U}}_{\text{test}}])$ of test graph on $\mathcal{G}_{\text{test}}$
Get embeddings $f(\mathbf{V}_j)$ of each model M_j on $\mathcal{G}_{\text{test}}$
Return the best model $M^* \leftarrow \arg\max_{M_j \in \boldsymbol{\mathcal{M}}} \left\langle f(\mathbf{W}[\mathbf{m}_{\text{test}}; \widehat{\mathbf{U}}_{\text{test}}]), f(\mathbf{V}_j) \right\rangle$

G.2 META-LEARNING OBJECTIVE FOR SPARSE PERFORMANCE MATRIX

Given a sparse performance matrix $\mathbf{P}$, meta-training of METAGL can be performed by modifying the top-1 probability (Equation (3)) and the loss function (Equation (4)), such that the missing entries in $\mathbf{P}$ are ignored as follows:

$$p_{\text{top1}}^{\widehat{\mathbf{P}}_i}(j) = \frac{\mathbf{I}_{p_{ij}}(\pi(\widehat{p}_{ij}))}{\sum_{k=1}^{m} \mathbf{I}_{p_{ik}}(\pi(\widehat{p}_{ik}))} = \frac{\mathbf{I}_{p_{ij}}(\exp(\widehat{p}_{ij}))}{\sum_{k=1}^{m} \mathbf{I}_{p_{ik}}(\exp(\widehat{p}_{ik}))}, \tag{7}$$

$$L(\mathbf{P}, \widehat{\mathbf{P}}) = -\sum_{i=1}^{n}\sum_{j=1}^{m} \mathbf{I}_{p_{ij}} \left(p_{\text{top1}}^{\mathbf{P}_i}(j) \log \left(p_{\text{top1}}^{\widehat{\mathbf{P}}_i}(j) \right) \right). \tag{8}$$

where $\mathbf{I}_{p_{ij}}(\cdot)$ is defined as

$$\mathbf{I}_{p_{ij}}(x) = \begin{cases} x & \text{if } p_{ij} \text{ exists in the observed performance matrix } \mathbf{P}, \\ 0 & \text{if } p_{ij} \text{ is missing in the observed performance matrix } \mathbf{P}. \end{cases} \tag{9}$$

Thus the supervision signal for each graph comes only from the model performances observed on it. If an entire row in $\mathbf{P}$ is empty, the loss terms for the corresponding graph are dropped from Equation (8).

G.3 G-M NETWORK

Figure 7 illustrates the G-M network (graph-model network) (Section 4.4), which is a multi-relational bipartite network between graph nodes and model nodes. In the G-M network, model and graph nodes are connected via five types of edges (*e.g.*, P-m2m, P-g2m, M-g2g), which is shown as edges with distinct line styles and colors. Note that while Figure 7 shows only one edge per edge type, in the G-M network, each node is connected to its top-k similar nodes.

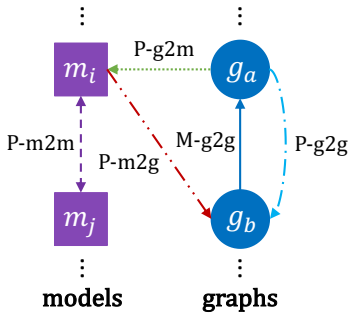


Figure 7: An illustration of the G-M network (Section 4.4), which is a multi-relational bipartite network between model nodes and graph nodes that are connected via five types of edges (*e.g.*, P-m2m, M-g2g). Note that only a subset of the edges in the G-M network is shown here for illustration purposes. See Section 4.4 for more details.

G.4 ATTENTIVE GRAPH NEURAL NETWORKS AND HETEROGENEOUS GRAPH TRANSFORMER

The embedding function $f(\cdot)$ in METAGL (Section 4.4) produces embeddings of models and graphs via weighted neighborhood aggregation over the multi-relational G-M network. Specifically, we define $f(\cdot)$ using Heterogeneous Graph Transformer (HGT) (Hu et al., 2020), which is a relation-aware graph neural network (GNN) that performs attentive neighborhood aggregation over the G-M network. Let $\mathbf{z}_t^\ell$ denote the node t's embedding produced by the ℓ-th HGT layer, which becomes the input of the $(\ell+1)$-th layer. Given L total layers, the final embedding $\mathbf{h}_t$ of node t is obtained to be the output from the last layer, *i.e.*, $\mathbf{z}_t^L$. In general, node embeddings $\mathbf{z}_t^\ell$ produced by the ℓ-th layer in an attention-based GNN, such as HGT, can be expressed as:

$$\mathbf{z}_t^\ell = \underset{\forall s \in N(t), \forall e \in E(s,t)}{\textbf{Aggregate}} \left(\textbf{Attention}(s,t) \cdot \textbf{Message}(s) \right) \tag{10}$$

where s and t are source and target nodes, respectively; $N(t)$ denotes all the source nodes of node t; and $E(s,t)$ denotes all edges from node s to t. There are three basic operators: **Attention**, which

assigns different weights to neighbors based on the estimated importance of node s with respect to target node t; **Message**, which extracts the message vector from the source node s; and **Aggregate**, which aggregates the neighborhood messages by the attention weight.

HGT effectively processes multi-relational graphs, such as the proposed G-M network, by designing all of the above three operators to be aware of node types and edge types, *e.g.*, by employing distinct set of projection weights for each type of nodes and edges, and utilizing node- and edge-type dependent attention mechanisms. We refer the reader to (Hu et al., 2020) for the details of how HGT defines the above three operators. In summary, METAGL computes the embedding function $f(\mathbf{x}_t)$ by providing node t's input features $\mathbf{x}_t$ as the initial embedding (*i.e.*, $\mathbf{z}_t^0$) to HGT, and returning $\mathbf{z}_t^L$, the output from the last layer, which is computed over the G-M network via relation-aware attentive neighborhood aggregation.

H ADDITIONAL RELATED WORK

In this section, we provide a further review of model selection in machine learning, which we group into two categories.

Evaluation-Based Model Selection: A majority of model selection methods belong to this category. Representative techniques used by these methods include grid search (Liashchynskyi & Liashchynskyi, 2019), random search (Bergstra & Bengio, 2012), early stopping-based (Golovin et al., 2017) and bandit-based (Li et al., 2017b) approaches, and Bayesian optimization (BO) (Snoek et al., 2012; Wu et al., 2019b; Falkner et al., 2018). Among them, BO methods are more efficient than grid or random search, requiring fewer evaluations of hyperparameter configurations (HCs), as they determine which HC to try next in a guided manner using prior experience from previous trials. Since these methods perform model training or evaluation multiple times using different HCs, they are much less efficient than the following group of methods.

Evaluation-Free Model Selection: Methods in this category do not require model evaluation for model selection. A simple approach (Abdulrahman et al., 2018) identifies the best model by considering the models' rankings observed on prior datasets. Instead of finding the globally best model, ISAC (Kadioglu et al., 2010) and AS (Nikolić et al., 2013) select a model that performed well on similar datasets, where the dataset similarity is modeled in the meta-feature space via clustering (Kadioglu et al., 2010) or k-nearest neighbor search (Nikolić et al., 2013). A different group of methods perform optimization-based model selection, where the model performance is estimated by modeling the relation between meta-features and model performances. Supervised Surrogates (Xu et al., 2012) learns a surrogate model that maps meta-features to model performance. Recently, MetaOD (Zhao et al., 2021) outperformed all of these methods in selecting outlier detection algorithms. As a method in this category, the proposed METAGL builds upon MetaOD and extends it for an effective and automatic GL model selection. Most importantly, METAGL selects a *graph learning* model (*e.g.*, link predictor) for the given *graph*, while MetaOD selects an *outlier detection* (OD) model for the given dataset (n-dimensional input features). To this end, METAGL designs meta features to capture the characteristics of graphs, while MetaOD designs meta features specialized for OD tasks. Further, METAGL learns latent factors of models and graphs by employing GNNs on the proposed G-M network, which are optimized via the top-1 probability; both the framework and meta-training objective of METAGL differ from those of MetaOD. Note that all of these earlier methods, except the first simple approach, rely on meta-features, and they focus on non-graph datasets. By using the proposed meta-graph features, they could be applied to the graph learning model selection task.

I ADDITIONAL RESULTS

I.1 EFFECTIVENESS OF META-GRAPH FEATURES

Figure 8 shows how accurately meta-learners can perform model selection when they use the proposed meta-graph features (Section 4.3) vs. six state-of-the-art graph-level embedding (GLE) techniques, *i.e.*, GL2Vec (Chen & Koga, 2019), Graph2Vec (Narayanan et al., 2017), GraphLoG (Xu et al., 2021), WaveletCharacteristic (Wang et al., 2021), SF (de Lara & Pineau, 2018), and LDP (Cai & Wang, 2019). As discussed in Section 5.3, all meta-learners achieve a higher model selection accuracy nearly consistently by using METAGL's meta-graph features than when they use these GLE techniques, and METAGL outperform all meta-learners, regardless of which features are used.

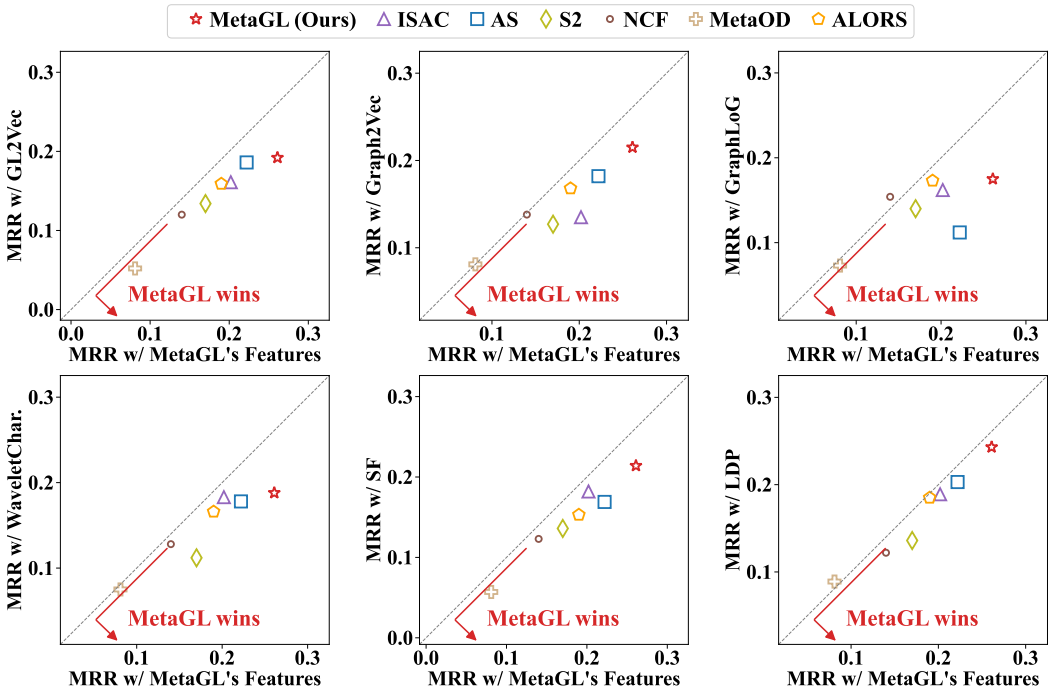


Figure 8: Using the proposed meta-graph features (Section 4.3), all meta-learners nearly consistently perform better than when they use existing graph-level embedding methods (most of the points are below the diagonal).

Table 7: METAGL is fast and incurs negligible overhead. The runtime (in secs) of naive model selection (*i.e.*, training each method using all configurations in the model set $\mathcal{M}$), versus the runtime of METAGL, *i.e.*, the time to generate meta-graph features (the penultimate row) plus the time taken for model prediction on average (the last row). Datasets are taken from (Rossi & Ahmed, 2015).

		soc-wiki-Vote	ia-reality	tech-routers-rf	ca-cora	power-US-Grid	web-EPA	socfb-Caltech	tech-pgp
line		5.45	5.85	5.40	6.47	8.23	7.28	8.19	10.15
node2vec		65.28	504.38	154.54	159.32	315.35	317.55	184.09	722.66
deepwalk		7.03	55.01	16.89	17.95	35.62	33.09	18.24	84.35
HONE		203.71	53.15	552.31	276.11	127.4	882.35	737.49	2082.06
node2bits		64.85	113.06	92.22	93.37	211.3	117.55	106.66	284.42
deepGL		145.93	633.44	331.87	504.2	1027.25	880.03	445.89	2349.3
GraphSage		272.97	1451.87	513.18	283.35	115.86	1020.30	2586.93	1171.54
GCN		26.30	57.10	45.64	52.96	57.38	66.12	94.65	163.4
METAGL	(meta feat. gen.)	0.16	0.97	0.36	0.4	1.07	0.78	0.61	2.05
	(model pred.)					0.39			

I.2 MODEL SELECTION TIME

Table 7 shows results comparing the runtime (in seconds) for naive model selection with the runtime of METAGL. Note that naive model selection requires training and evaluating each method in the model set, while in METAGL, the runtime involves only the time to generate meta-graph feature (penultimate row) and predict the best model via a forward pass (last row). Results show that METAGL is fast, and incurs negligible computational overhead.

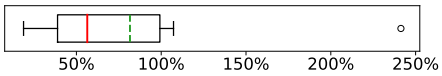
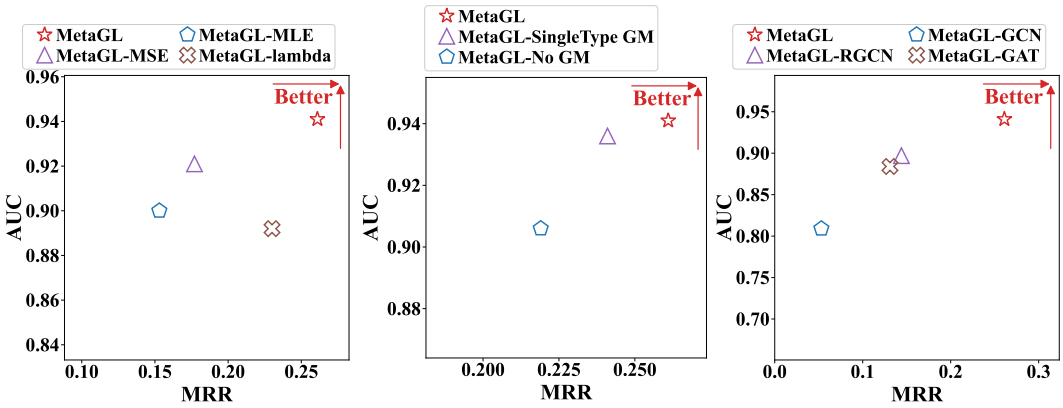


Figure 9: Distribution of the time for METAGL to make a prediction / the time to create meta-graph features (in percentage). Red and green lines denote the median and mean, respectively.

Figure 9 shows the distribution of the time taken for METAGL to predict the best model, divided by the time taken by METAGL for creating meta-graph features (in percentage). On average, it takes ∼20% less time for METAGL to make an inference than to generate meta-graph features.



(a) Meta-learning objective. (b) G-M network. (c) Graph neural networks.

Figure 10: Ablation study of METAGL on several components that METAGL uses for meta-learning. The proposed METAGL achieves the best performance, in comparison to the variants that adopt different modeling choices.

I.3 ABLATION STUDY

Figure 10 presents ablation studies on several components of METAGL for meta-learning, namely, meta-learning objective, the G-M network, and the GNN encoder. To that end, we compare METAGL against several variants that differ from METAGL only in one aspect, which we explain below. In Figure 10, METAGL refers to the proposed meta-learner as described in Section 4.

I.3.1 META-LEARNING OBJECTIVE

To optimize the framework such that it can find the best model, METAGL employs the top-1 probability as its meta-learning objective (see Section 4.1). We evaluate how METAGL's performance changes when it uses different loss functions for meta-training. **METAGL-MSE** uses mean squared error (MSE), **METAGL-MLE** employs ListMLE (Xia et al., 2008), and **METAGL-lambda** uses LambdaLoss (Wang et al., 2018). Figure 10a shows that METAGL with the top-1 probability most effectively identifies the top-performing model for the new graph, while variants that employ different learning objectives obtain suboptimal results in terms of both MRR and AUC.

I.3.2 G-M NETWORK

To learn the embeddings of models and graphs, METAGL uses a G-M network (GM), which is a multi-relational network containing multiple types of nodes and edges (see Section 4.4 and Appendix G.3). **METAGL-SingleType GM** is a variant of METAGL that uses a single-relational G-M network, where all of the nodes and edges in the original G-M network have been converted to be of the same type. **METAGL-No GM** is another variant where METAGL does not use the G-M network at all; instead, the input features of models and graphs, which are normally provided as input to the GNN in METAGL, were directly taken to be the final model and graph embeddings. Figure 10b shows that METAGL with the multi-relational G-M network is the most effective, and in utilizing the G-M network, it is helpful to be able to distinguish between the multiple types of nodes and edges. Further, in comparison to METAGL-No GM, learning the embeddings of graphs and models via the G-M network greatly improves the model selection performance.

I.3.3 GRAPH NEURAL NETWORKS

To effectively learn the embeddings of models and graphs over a multi-relational G-M network, METAGL utilizes an attentive, heterogeneous graph neural network (GNN) as its graph encoder (see Section 4.4 and appendix G.4), which can adaptively determine the aggregation weight of the neighbors (thus *attentive*), while being aware of and utilizing the multiple node and edge types in learning the embeddings (hence *heterogeneous*). To see how helpful attentive, heterogeneous GNNs

are in learning effective model and graph embeddings, here we create the following variants of METAGL, which use GNNs that are not attentive and/or not heterogeneous (*i.e.*, no mechanism to handle different node and edge types). **METAGL-RGCN** uses RGCN (Schlichtkrull et al., 2018), which is a heterogeneous GNN, but is not attentive. **METAGL-GAT** uses GAT (Velickovic et al., 2018), which is an attentive GNN, but is not heterogeneous. **METAGL-GCN** uses GCN Kipf & Welling (2017), which is neither heterogeneous nor attentive. In Figure 10c, the highest performance is achieved by METAGL that uses heterogeneous and attentive GNNs, while the lowest performance is obtained when it uses GCN, which is not attentive nor heterogeneous. Both the ability to perform attentive neighborhood aggregation, and to be able to distinguish between and utilize different node and edge types are essential in effectively capturing the complex relations between graphs and models.