AUTOGML: Fast Automatic Model Selection for Graph Machine Learning

Namyong Park
Carnegie Mellon University
namyongp@cs.cmu.edu

Ryan Rossi
Adobe Research
ryrossi@adobe.com

Nesreen Ahmed
Intel Labs
nesreen.k.ahmed@intel.com

Christos Faloutsos
Carnegie Mellon University
christos@cs.cmu.edu

Abstract
Given a graph learning task, such as link prediction, on a new graph dataset, how can we automatically select the best method as well as its hyperparameters (collectively called a model)? 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 automatic graph machine learning, called AUTOGML, which capitalizes on the prior performances of a large body of existing methods on benchmark graph datasets, and carries over this prior experience to automatically select an effective model to use for the new graph, without any model training or evaluations. To capture the similarity across graphs from different domains, we introduce specialized meta-graph features that quantify the structural characteristics of a graph. Then we design a meta-graph that represents the relations among models and graphs, and develop a graph meta-learner operating on the meta-graph, which estimates the relevance of each model to different graphs. Through extensive experiments, we show that using AUTOGML to select a method for the new graph significantly outperforms consistently applying popular methods as well as several existing meta-learners, while being extremely fast at test time.

1 Introduction
Given a graph machine learning (GML) task, such as link prediction, on a new graph dataset, how can we automatically select the best method as well as its hyperparameters (HPs) (collectively called a model), in particular, without performing any model training or evaluations on the new graph? GML (i.e., machine learning on graphs) has received increasing attention recently [44, 48], achieving successes across a large array of applications, such as recommendation [10], ranking [29, 50], traffic forecasting [18], question answering [32], explainable AI [31], bioinformatics [58, 22], and anomaly detection [6]. However, as more GML methods are developed for various tasks, it becomes increasingly difficult to determine which model to use for a given graph.

Selecting a method and its HPs (i.e., model selection) for graph learning has been largely ad hoc to date. A typical approach 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 [41], and such consistent model selection is often suboptimal. At the other extreme lies “naive model selection” (Figure 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 this new graph is selected. This approach is very costly as all candidate models are trained whenever a new graph arrives. Thus, it is impractical for real-world settings where model selection needs to be done.

Preprint. Under review.
In this work, we systematically tackle the model selection problem for graph learning, focusing on link prediction, which is a representative graph learning task. To that end, we develop AUTOGML, the first framework for automatic graph machine learning to our knowledge, which selects an effective model to employ for a new graph without any model training or evaluation, as shown in Figure 1a.

AUTOGML is a meta-learning based approach that stands on the prior performances of a large body of existing methods on extensive graph datasets. The high-level idea of AUTOGML is to estimate a candidate model’s performance on the new graph based on its performances on similar existing graphs. Once trained, AUTOGML infers the best model for any unseen graph in near-real-time (<1 second).

Our meta-learning problem for graphs requires learning similarities between graphs based on characteristic dataset features (namely meta-features). 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., gender, location, age of users) are often readily available. Even if no input features are available, the task is much more challenging for graph data than for non-graph (e.g., i.i.d., tabular) datasets, due to the high complexity and irregularity of graphs (e.g., different number of nodes and edges, as well as widely varying connectivity patterns, among different graphs). To handle these challenges, we design specialized meta-graph features that effectively characterize major structural properties of real-world graphs.

To estimate the model performance, AUTOGML 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 meta-graph, which represents the relations among models and graphs, and develop a graph meta-learner operating on this meta-graph, which is optimized to leverage meta-graph features and prior model performances into producing model and graph embeddings that can be effectively used to estimate the best performing model for the given graph.

In summary, the key contributions of this work are as follows.

- **Problem Formulation.** We formulate the problem of fast automatic model selection for graph learning, where model space includes a large array of graph learning methods and their HP settings.
- **Framework.** We propose AUTOGML, the first approach for automatic graph machine learning to our knowledge, which infers the best model for a new graph without running different models on it as in traditional model selection. AUTOGML draws on the prior performances of existing models, and can be used for different graph learning tasks, e.g., link prediction and node classification.
- **Meta-Graph Features.** We design meta-graph features for meta-learning on graphs, which can quantify graph similarities effectively by capturing the structural characteristics of a graph.
- **Effectiveness and Efficiency.** Extensive experiments show that using AUTOGML for graph model selection significantly outperforms always using popular models, as well as several existing meta-learning techniques, while incurring negligible runtime overhead (<1 second) at test time.

### 2 Problem Formulation

Given a new unseen graph, our goal is fast automatic model selection from a set of heterogeneous graph learning models, without any model evaluations and user intervention—hence fast and automatic. 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

\[ M = \{ \text{graph embedding method, hyperparameters}), \text{(predictor, hyperparameters)} \} \]

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. Hence, there can be many models that use the same embedding method and predictor, but have different hyperparameters.

Given a training meta-corpus of \( n \) graphs \( \mathcal{G} = \{ G_1, \ldots, G_n \} \), \( m \) models \( \mathcal{M} = \{ M_1, \ldots, M_m \} \) for graph learning tasks, and ground truth labels \( Y \) in the case of supervised tasks, we derive performance matrix \( P \in \mathbb{R}^{n \times m} \) where \( P_{ij} \) is the performance (e.g., accuracy, average precision) of model \( j \) on graph \( i \). Our graph meta-learning problem for fast automatic model selection is defined as follows.

**Problem 1.** Given (i) an unseen test graph \( G_{test} \not\in \mathcal{G} \), and (ii) a performance matrix \( P \in \mathbb{R}^{n \times m} \) of \( m \) models \( \mathcal{M} = \{ M_1, \ldots, M_m \} \) on \( n \) graphs \( \mathcal{G} = \{ G_1, \ldots, G_n \} \), infer the best model \( M^* \in \mathcal{M} \) to employ on \( G_{test} \) without training or evaluating any model in \( \mathcal{M} \) and requiring user intervention.

## 3 Framework

In this section, we present AUTOGML, our meta-learning based framework that solves Problem 1 by leveraging prior performances of existing methods. AUTOGML consists of the two phases: (1) **offline meta-training** phase (Sec 3.1) that trains a meta-learner using observed graphs \( \mathcal{G} \) and model performances \( P \), and (2) **online model prediction** phase (Sec 3.2), which selects the best model for the new graph. A summary of notations used in this work is provided in Table 4 in the Appendix.

### 3.1 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), AUTOGML captures the graph similarity by extracting meta-graph features such that they reflect the structural properties of the graph. Notably, since graphs have irregular structure, with different number of nodes and edges, AUTOGML 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 for graph \( G \), and defer the details of how AUTOGML computes \( \mathbf{m} \) to Section 3.3.

**Model Performance Estimation.** To estimate how well a model would perform on a given graph, AUTOGML 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 \( \mathbf{h}_G \) and \( \mathbf{h}_M \) 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 \( P \) and observed graphs \( \mathcal{G} \)). Below in this section, we focus on the inputs to the function \( f(\cdot) \), and defer the details of \( f(\cdot) \) to Section 3.4.

We first factorize performance matrix \( P \) 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, AUTOGML 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 \( \mathbf{U}_{test} \) 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). We handle this issue by learning an estimator \( \phi : \mathbb{R}^d \rightarrow \mathbb{R}^k \) 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 \( \mathbf{m}, \phi(\mathbf{m}) = \mathbf{U}_i \approx \mathbf{U}_i \), 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
Figure 2: Given a new graph $G$, AUTOGML extracts meta-graph features, and applies a meta-learned model to them, which efficiently infers the best model $M^* \in \mathcal{M}$ for $G$, with no model evaluation. $G_i$ to be of the same size as that of model $M_j$, obtaining the latent embedding of graph $G_i$ to be $h_{G_i} = f(W[m_i; \phi(m_i)])$ where $W \in \mathbb{R}^{k \times d \times k}$ is a weight matrix. Thus in AUTOGML, the performance $p_{ij}$ of model $M_j$ on graph $G_i$ with meta-graph features $m_i$ is estimated as

$$p_{ij} \approx \hat{p}_{ij} = \langle f(W[m_i; \phi(m_i)]), f(V_j) \rangle.$$  

(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 concern with the ranking quality. On the other hand, the goal of our problem setup is to accurately rank models for each graph, rather than estimating the performance itself, which makes MSE a suboptimal choice. In particular, model selection problem focuses on finding the model with the best performance on the given graph. Therefore, we consider rank-based learning objectives, and among them, we choose to employ the top-1 probability [8]. Let $\hat{P}_i \in \mathbb{R}^m$ be the $i$-th row of $\hat{P}$ (i.e., estimated performance of all $m$ models on graph $G_i$). Given $\hat{P}_i$, the top-1 probability $p_{i_{top1}}(j)$ of $j$-th model $M_j$ in the model set $\mathcal{M}$ represents the probability of $M_j$ to be ranked at the top of the list, i.e., all models in $\mathcal{M}$, given model performance $\hat{P}_i$, and is defined as

$$p_{i_{top1}}(j) = \frac{\pi(\hat{p}_{ij})}{\sum_{k=1}^m \pi(\hat{p}_{ik})} = \frac{\exp(\hat{p}_{ij})}{\sum_{k=1}^m \exp(\hat{p}_{ik})}.$$  

(3)

Here $\pi(\cdot)$ is a strictly increasing positive function, which we define to be an exponential function. Given that the top-1 probability $p_{i_{top1}}(j)$ for all $j = 1, \ldots, m$ forms a probability distribution over all $m$ models, we obtain two probability distributions by applying top-1 probability to the true performance $P_i$ and estimated performance $\hat{P}_i$ of $m$ models, and optimize AUTOGML such that the distance between the two resulting distributions gets decreased. Using the cross entropy as the distance metric, we minimize the following loss over all $n$ meta-train graphs $\mathcal{G}$:

$$L(P, \hat{P}) = -\sum_{i=1}^n \sum_{j=1}^m P_i j \log \left( \hat{P}_{i_{top1}}(j) \right)$$  

(4)

### 3.2 Online Model Prediction

In the meta-training phase, AUTOGML learns estimators $f(\cdot)$ and $\phi(\cdot)$, as well as weight matrix $W$ and latent model factors $V$. Given a new graph $G_{test}$, AUTOGML first computes the meta-graph features $m_{test} \in \mathbb{R}^k$ as we discuss in Section 3.3. Then $m_{test}$ is regressed to obtain the latent graph factors $\hat{U}_{test} = \phi(m_{test}) \in \mathbb{R}^k$. Recall that the model factors $V$ 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 $m_{test}$. Finally, the model that has the highest estimated performance is selected by AUTOGML as the best model $M^*$, i.e.,

$$M^* \leftarrow \arg \max_{M_j \in \mathcal{M}} \langle f(W[m_{test}; \phi(m_{test})]), f(V_j) \rangle$$  

(5)

Note that model selection using Equation (5) depends only on the meta-graph features $m_{test}$ of the test graph and other pretrained estimators and latent factors that AUTOGML learned in the meta-training phase. As no model training or evaluation is involved, model prediction by AUTOGML is fast, taking negligible runtime compared to the time to train the selected model as our experiments show in Section 4.3. Further, model prediction process is fully automatic it does not require users to choose or fine-tune any values at test time. Figure 3 shows an overview of model prediction process, and Algorithm 1 in the Appendix lists steps for offline meta-training and online model prediction.

### 3.3 Structural Meta-Graph Features

Meta-graph features are a crucial component of our meta-learning approach AUTOGML since they capture the important structural characteristics of an arbitrary graph dataset. Such meta-graph features
enables AUTOGML to quantify and leverage the similarity between meta-train graphs during training. It is important that a sufficient and representative set of graph meta-features are used to capture the important structural properties of graphs from a wide variety of different domains, including biological, technological, information, and social networks to name a few.

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 AUTOGML 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, \( \psi_1 \) i.e., can be a degree distribution, \( \psi_2 \) 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 \( \psi \) denote the local structural extractors for nodes. Given a graph \( G_i = (V_i, E_i) \) and \( \psi \), we obtain an \( |V_i| \)-dimensional node vector \( x_i = \psi(G_i) \). 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. 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 \( \Sigma \) of global statistical meta-graph extractors to every \( \psi_i(G), \forall i = 1, \ldots, q \), which summarizes each \( \psi_i(G) \) to a vector. Specifically, \( \Sigma(\psi_i(G)) \) applies each of the statistical functions in \( \Sigma \) (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 \( m \) of graph \( G \) by concatenating the resulting meta-graph feature vectors:

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

Table C in the Appendix lists the global statistical functions \( \Sigma \) 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 \( m \), 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 it. Hence, the structural similarity of any two graphs \( G \) and \( G' \) can be quantified using a similarity function over \( m \) and \( m' \), respectively.

### 3.4 Embedding Models and Graphs

Given the informative context (i.e., input features) of models and graphs that AUTOGML learns from model performances \( P \) and meta-graph features \( M \) (Section 3.1), 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 meta-graph that connects similar models and graphs, and learn the model and graph embeddings over it.

**Meta-Graph.** We define meta-graph 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 (\( U \) and \( V \), respectively) obtained by factorizing \( P \), as well as the meta-graph features \( M \). More precisely, we use the estimated...
graph factor \( \hat{\mathbf{U}} \) 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., \( \hat{\mathbf{U}} \) 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 types of edges: \( \mathbf{M}-\mathbf{g}2\mathbf{g} \), \( \mathbf{P}-\mathbf{g}2\mathbf{g} \), \( \mathbf{P}-\mathbf{m}2\mathbf{m} \), \( \mathbf{P}-\mathbf{g}2\mathbf{m} \), \( \mathbf{P}-\mathbf{m}2\mathbf{g} \), where \( \mathbf{g} \) and \( \mathbf{m} \) denote the type of nodes that an edge connects (graph and model, respectively), and \( \mathbf{M} \) and \( \mathbf{P} \) denote that the edge is based on meta-graph features and model performance, respectively. For example, \( \mathbf{M}-\mathbf{g}2\mathbf{g} \) and \( \mathbf{P}-\mathbf{g}2\mathbf{g} \) edges connect two graph nodes that are similar in terms of \( \mathbf{M} \) and \( \hat{\mathbf{U}} \), 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 \( \mathbf{P}-\mathbf{g}2\mathbf{m} \) edge type, graph nodes and model nodes are linked based on the similarity between \( \hat{\mathbf{U}} \) and \( \mathbf{V} \). Figure 5 in the Appendix illustrates the meta-graph.

**Learning Over Meta-Graph.** Given the meta-graph \( G_{\text{train}} \) containing meta-train graphs and models, graph neural networks (GNNs) provide an effective framework to embed models and graphs via (weighted) neighborhood aggregation. However, since the graph structure of meta-graph 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 [17] in experiments. Then the embedding function \( f(\cdot) \) in Section 3.1 is defined to be \( f(\mathbf{h}) = \text{HGT}(\mathbf{h}, G_{\text{train}}) \) during training, which transforms the input node feature \( \mathbf{h} \) into an embedding via attentive neighborhood aggregation over \( G_{\text{train}} \). Further details of HGT are provided in Appendix G.2.

**Inference Over Meta-Graph.** For inference at test time, we extend \( G_{\text{train}} \) to be a larger meta-graph \( G_{\text{test}} \) that additionally contains test graph nodes, and edges between test graph nodes and existing graphs and models in \( G_{\text{train}} \). The extension is done in the same way as for the training phase, by finding top-\( k \) similar nodes. Then the embedding for the inference can be done by \( f(\mathbf{h}) = \text{HGT}(\mathbf{h}, G_{\text{test}}) \).

4 Experiments

4.1 Experimental Settings

**Models and Evaluation.** Recall that a model in our problem (Equation (1)) typically consists of two components. The first component learns the graph representation, and the other component leverages the learned embeddings for a downstream task of interest. In this work, we evaluate our framework for automatically selecting a link prediction model for the new graph without any model evaluations.

For the first component of link prediction model, we use 12 popular graph representation learning (GRL) methods with distinct hyperparameters (HPs). 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 \( \mathcal{M} \) with 423 unique models. The full list of GRL methods and their HP settings is given in Table 5 in Appendix C.

For evaluation, we create a testbed consisting of benchmark graphs, meta-graph features, and a performance matrix \( \mathbf{P} \). We construct the performance matrix \( \mathbf{P} \) by evaluating each link prediction model in \( \mathcal{M} \) on the datasets in the testbed, in terms of the MAP (Mean Average Precision) score. Then we evaluate AUTOGLML and baselines in the testbed via 5-fold cross validation where the benchmark graphs are split into meta-train and meta-test datasets for each fold, and the performance of meta-learners trained over the meta-train data is evaluated using the meta-test dataset.

Since model selection aims to accurately predict the best model for the new graph, we evaluate the top-1 prediction results of meta-learners in terms of AUC, MAP, and NDCG (Normalized Discounted Cumulative Gain). To apply AUC and MAP, we treat the task as a binary classification problem, where only 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 concerns only the top-1 predicted model’s performance. All metrics range from 0 to 1 (larger values are better).

**Testbed Setup.** To evaluate the meta-learners in different usage scenarios, we construct two testbeds.

- **Search-within-a-model testbed** evaluates how accurately meta-learners perform in finding the best hyperparameter configuration (HC) of a specific method. Thus performance matrix \( \mathbf{P} \) contains only the performances obtained with different HCs of a single method.
- **Search-across-all-models testbed** evaluates how well meta-learners select the best model from the heterogeneous model set composed by pairing each model with its distinct HCs. Thus, this is the most general and challenging setup, where \( \mathbf{P} \) contains all models’ performance on all graphs.
Table 2: AUTOGLM achieves higher model selection accuracy than baselines in most cases on the search-within-a-model testbed. The best results are in bold, and the second best results are underlined.

| Search-within-a-model testbed | DeepGL [12] | node2vec [12] | HONE [55] | GraphSage [14] | role2vec [21] |
|-------------------------------|-------------|---------------|-----------|----------------|--------------|
| AUC                           | 0.495 0.036 | 0.867 0.485 0.303 0.972 | 0.503 0.127 | 0.826 0.516 0.195 | 0.822 0.514 0.030 0.792 |
| Global Best-Avg.              | 0.691 0.164 | 0.938 0.502 0.331 0.974 | 0.779 0.448 | 0.931 0.783 0.433 | 0.947 0.846 0.146 0.955 |
| Global Best-Rank              | 0.698 0.192 | 0.938 0.581 0.377 0.975 | 0.778 0.440 | 0.931 0.784 0.407 | 0.943 0.808 0.119 0.954 |
| ALGOSMART (AS)                | 0.770 0.210 | 0.935 0.615 0.400 0.982 | 0.786 0.422 | 0.939 0.777 0.409 | 0.947 0.812 0.124 0.951 |
| ISAC                          | 0.713 0.170 | 0.940 0.611 0.413 0.982 | 0.777 0.424 | 0.930 0.785 0.430 | 0.945 0.852 0.144 0.954 |
| ALORS                         | 0.670 0.079 | 0.929 0.566 0.382 0.981 | 0.746 0.300 | 0.924 0.797 0.426 | 0.945 0.818 0.113 0.950 |
| NCF                           | 0.695 0.144 | 0.934 0.545 0.358 0.978 | 0.767 0.392 | 0.929 0.785 0.420 | 0.945 0.844 0.126 0.951 |
| Supervised Surrogate (SS)     | 0.610 0.051 | 0.918 0.586 0.390 0.979 | 0.752 0.324 | 0.927 0.766 0.367 | 0.935 0.809 0.112 0.951 |
| AUTOGLM (Ours)                | 0.791 0.237 | 0.947 0.632 0.427 0.982 | 0.801 0.456 | 0.939 0.814 0.440 | 0.948 0.852 0.139 0.961 |

Both testbeds use a graph corpus consisting of 301 graphs from 21 domains, which have fundamentally different structural characteristics. Table 7 in Appendix shows the distribution of graphs per domain.

**Baselines.** Being the first work for automatic model selection in graph machine learning, we do not have immediate baselines for comparison. Therefore, we adapt some existing approaches for our problem setting, and also devise baselines based on simple ideas frequently used in practice.

In Appendix A we describe all baselines in detail. Briefly, baselines are grouped into three categories. (a) **No model selection** uses the same popular model for link prediction: node2vec [12] and GCN [21]; (b) **Simple meta-learners** select a model that performs generally well, either globally or locally: Global Best (GB)-Avg, Global Best (GB)-Rank, ISAC [20], and ALGOMART (AS) [28]; (c) **Optimization-based meta-learners** learn to estimate the model performance by modeling the relation between meta-graph features and model performances: Supervised Surrogates (SS) [45], ALORS [27], and NCF [15].

We also include **Random Selection (RS)** as a baseline to see how these methods compare to randomly scoring models. Note that except the simplest meta-learner GB, all of the above baseline meta-learners rely on our proposed meta-graph features to be able to estimate model performance on a new graph.

### 4.2 Model Selection Accuracy

We evaluate model selection accuracy using both testbed setups.

**Search-within-a-model Testbed.** In this setup, the goal is to select the best model from among the HCs of a single method. In Table 2 we show how effective AUTOGLM and baselines are in finding the best HC of five chosen methods, averaged over 301 graphs. Results show that AUTOGLM nearly consistently achieves the highest model selection accuracy in terms of all metrics. Among baselines, AS achieves better performance than other baselines. However, there is no consistent winner among baselines. Notably, optimization-based meta-learners, such as ALORS and SS, are mostly outperformed by simpler meta-learners like ISAC and AS, which first find similar metatrain graphs and use their observed performance directly for model selection. On the other hand, optimization-based meta-learners try to reconstruct the performance matrix via matrix factorization or regression, which is a harder task. As an optimization-based technique, AUTOGLM outperforms these baselines by more effectively capturing graph-to-model affinity via learning over meta-graph.

**Search-across-all-models Testbed.** This setup aims to identify the best model among all existing methods and their HCs. Thus, most methods focus on finding an optimal HC for a single method can not be used. Table 1 shows the results. Always using popular methods, such as GCN and node2vec, does not perform well. Although these methods perform reasonably well in comparison to other methods in the testbed, they are not often the best model. Note that these models are associated with
We investigate how different sets of meta-graph features affect the results. Among them, BO methods are more efficient than grid or random search, requiring fewer evaluations. A majority of model selection methods belong to this category. Representative techniques used by these methods include grid search [24], random search [3], early stopping-based [11] and bandit-based [23] approaches, and Bayesian optimization (BO) [37, 43, 9]. Among them, BO methods are more efficient than grid or random search, requiring fewer evaluations.

5 Related Work

Model Selection in Machine Learning. As manual model selection gets too expensive [46], automating model selection [16] becomes increasingly important, 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 [24], random search [3], early stopping-based [11] and bandit-based [23] approaches, and Bayesian optimization (BO) [37, 43, 9]. Among them, BO methods are more efficient than grid or random search, requiring fewer evaluations.
Table 3: Our proposed meta-graph features enable effective automatic model selection by AUTOGML as well as other methods that rely on meta-features. AUTOGML consistently outperforms all other meta-learners, as different sets of meta-graph features are used ($m_{small}$, $m$, and $m_{extended}$).

| Search-across-all-models tested | $m_{small}$ | $m$ | $m_{extended}$ |
|---------------------------------|-------------|-----|---------------|
|                                 | AUC         | MAP | NDCG@1        | AUC         | MAP | NDCG@1 | AUC         | MAP | NDCG@1 |
| Random Selection                | 0.513       | 0.022 | 0.742 | 0.490       | 0.011 | 0.745 | 0.490       | 0.011 | 0.745  |
| GCN                             | 0.499       | 0.002 | 0.755 | 0.499       | 0.002 | 0.755 | 0.499       | 0.002 | 0.755  |
| node2vec                        | 0.505       | 0.016 | 0.931 | 0.505       | 0.016 | 0.931 | 0.505       | 0.016 | 0.931  |
| Global Best-Avg.                | 0.877       | 0.163 | 0.932 | 0.877       | 0.163 | 0.932 | 0.877       | 0.163 | 0.932  |
| Global Best-Rank                | 0.834       | 0.205 | 0.933 | 0.834       | 0.205 | 0.933 | 0.834       | 0.205 | 0.933  |
| ALGOSMART (AS)                  | 0.889       | 0.206 | 0.946 | 0.905       | 0.222 | 0.947 | 0.911       | 0.224 | 0.952  |
| ISAC                            | 0.886       | 0.220 | 0.944 | 0.891       | 0.215 | 0.941 | 0.881       | 0.196 | 0.942  |
| ALORS                           | 0.869       | 0.159 | 0.935 | 0.868       | 0.120 | 0.921 | 0.851       | 0.096 | 0.918  |
| NCF                             | 0.873       | 0.176 | 0.932 | 0.875       | 0.132 | 0.931 | 0.877       | 0.148 | 0.935  |
| Supervised Surrogate            | 0.871       | 0.132 | 0.928 | 0.861       | 0.128 | 0.928 | 0.854       | 0.087 | 0.920  |
| AUTOGML (Ours)                  | **0.928**   | **0.237** | **0.955** | **0.936** | **0.243** | **0.962** | **0.936** | **0.246** | **0.958** |

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 [1] identifies the best model by considering the models’ rankings observed on prior datasets. Instead of finding the globally best model, ISAC [20] and AS [28] select a model that performed well on similar datasets, where the dataset similarity is modeled in the meta-feature space by using clustering [20] or $k$-nearest neighbor search [28]. 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. For instance, Supervised Surrogates [45] learns a surrogate model that maps meta-features to model performance, and ALORS [27] models the performance as a dot product of latent factors of models and datasets. Notably, all of these methods, except the first simple approach, rely on meta-features, while focusing on non-graph datasets. Our proposed meta-graph features make them applicable to the graph model selection task.

**Model Selection in Graph Machine Learning (GML).** A majority of works on GML focus on developing new algorithms for certain graph tasks and applications [44, 48]. In comparison, there exist relatively few recent works [40, 13, 47, 5, 49] that address the GML model selection problem. They mainly focus on neural architecture search and hyperparameter optimization (HPO) for GML models, especially for graph neural networks. To achieve more efficient model selection than the naive exhaustive approach (Fig. 1b), they investigated techniques for efficient HPO, including subgraph sampling [40], graph coarsening [13], hierarchical evaluation [47], hypernets [49], and evolutionary algorithms [5]. However, for model selection, they still need to perform model training and/or evaluations on the new graph, which is much more costly than evaluation-free model selection. Also, they are mostly limited to finding the best HC of a specific model, and cannot select a model from a heterogeneous model set $\mathcal{M}$ with various GML models (which are often a combination of graph embedding methods, downstream task-specific methods, and their HPs). For the first time, AUTOGML enables evaluation-free model selection from among any heterogeneous set of GML models. Also, while earlier work on network similarity [4] is somewhat relevant to graph model selection, it focuses on extracting seven node-level features, without addressing model selection. In comparison, AUTOGML provides a much richer set of 300+ meta-graph features on node, edge, and graph level.

**6 Conclusion**

This work addressed the automatic graph model selection (AGMS) problem, i.e., selecting the best model for an unseen graph without any model training or evaluation on the new graph. As the first framework that tackles AGMS, our proposed AUTOGML capitalizes on the prior performances of various graph learning models on existing graph datasets, by designing specialized structural meta-graph features, and developing the graph meta-learner that estimates graph-to-model affinity.

As experiments demonstrate, this work democratizes graph machine learning to non-experts, while greatly reducing financial and environmental cost for training graph learning models. Future work to make AUTOGML even more useful includes making the model aware of potential bias and fairness issues in AGMS (e.g., how to recognize and handle unfair predictors), and exploiting structural relations between different HP configurations.
References

[1] Salisu Mamman Abdulrahman, Pavel Brazdil, Jan N. van Rijn, and Joaquin Vanschoren. 2018. Speeding up algorithm selection using average ranking and active testing by introducing runtime. Mach. Learn. 107, 1 (2018), 79–108.

[2] Nesreen K. Ahmed, Ryan A. Rossi, John Boaz Lee, Xiangnan Kong, Theodore L. Willke, Rong Zhou, and Hoda Eldardiry. 2018. Learning Role-based Graph Embeddings. CoRR abs/1802.02896 (2018).

[3] James Bergstra and Yoshua Bengio. 2012. Random Search for Hyper-Parameter Optimization. J. Mach. Learn. Res. 13 (2012), 281–305.

[4] Michele Berlingerio, Danai Koutra, Tina Eliassi-Rad, and Christos Faloutsos. 2012. NetSimile: A Scalable Approach to Size-Independent Network Similarity. CoRR abs/1209.2684 (2012).

[5] Chenyang Bu, Yi Lu, and Fei Liu. 2021. Automatic Graph Learning with Evolutionary Algorithms: An Experimental Study. In PRICAI (1) (Lecture Notes in Computer Science, Vol. 13031). Springer, 513–526.

[6] Lei Cai, Zhengzhang Chen, Chen Luo, Jiaping Gui, Jingchao Ni, Ding Li, and Haifeng Chen. 2021. Structural Temporal Graph Neural Networks for Anomaly Detection in Dynamic Graphs. In CIKM. ACM, 3747–3756.

[7] Shaosheng Cao, Wei Lu, and Qiongkai Xu. 2015. GraRep: Learning Graph Representations with Global Structural Information. In CIKM. ACM, 891–900.

[8] Zhe Cao, Tao Qin, Tie-Yan Liu, Ming-Feng Tsai, and Hang Li. 2007. Learning to rank: from pairwise approach to listwise approach. In ICML (ACM International Conference Proceeding Series, Vol. 227). ACM, 129–136.

[9] William L. Hamilton, Zhitao Ying, and Jure Leskovec. 2017. Inductive Representation Learning on Large Graphs. In NIPS. 1024–1034.

[10] Di Jin, Mark Heimann, Ryan A. Rossi, and Danai Koutra. 2019. node2bits: Compact Time- and Attribute-Aware Node Representations for User Stitching. In ECML/PKDD (1) (Lecture Notes in Computer Science, Vol. 11906). Springer, 483–506.
[20] Serdar Kadioglu, Yuri Malitsky, Meinolf Sellmann, and Kevin Tierney. 2010. ISAC - Instance-Specific Algorithm Configuration. In ECAI (Frontiers in Artificial Intelligence and Applications, Vol. 215). IOS Press, 751–756.

[21] Thomas N. Kipf and Max Welling. 2017. Semi-Supervised Classification with Graph Convolutional Networks. In ICLR (Poster). OpenReview.net.

[22] Junying Li, Deng Cai, and Xiaofei He. 2017. Learning Graph-Level Representation for Drug Discovery. CoRR abs/1709.03741 (2017).

[23] Lisha Li, Kevin G. Jamieson, Giulia DeSalvo, Afshin Rostamizadeh, and Ameet Talwalkar. 2017. Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization. J. Mach. Learn. Res. 18 (2017), 185:1–185:52.

[24] Petro Liashchynskyi and Pavlo Liashchynskyi. 2019. Grid Search, Random Search, Genetic Algorithm: A Big Comparison for NAS. CoRR abs/1912.06059 (2019).

[25] Bin Luo, Richard C. Wilson, and Edwin R. Hancock. 2003. Spectral embedding of graphs. Pattern Recognit. 36, 10 (2003), 2213–2230.

[26] Laurens van der Maaten and Geoffrey Hinton. 2008. Visualizing data using t-SNE. Journal of Machine Learning Research 9, 11 (2008), 2579–2605.

[27] Mustafa Misir and Michèle Sebag. 2017. Alors: An algorithm recommender system. Artif. Intell. 244 (2017), 291–314.

[28] Mladen Nikolić, Filip Marić, and Predrag Janičić. 2013. Simple algorithm portfolio for SAT. Artificial Intelligence Review 40, 4 (2013), 457–465.

[29] Namyong Park, Andrey Kan, Xin Luna Dong, Tong Zhao, and Christos Faloutsos. 2019. Estimating Node Importance in Knowledge Graphs Using Graph Neural Networks. In KDD. ACM, 596–606.

[30] Namyong Park, Andrey Kan, Xin Luna Dong, Tong Zhao, and Christos Faloutsos. 2020. MultiImport: Inferring Node Importance in a Knowledge Graph from Multiple Input Signals. In KDD. ACM, 503–512.

[31] Namyong Park, Andrey Kan, Christos Faloutsos, and Xin Luna Dong. 2020. J-Recs: Principled and Scalable Recommendation Justification. In ICDM. IEEE, 1208–1213.

[32] Namyong Park, Fuchen Liu, Purvanshi Mehta, Dana Cristofor, Christos Faloutsos, and Yuxiao Dong. 2022. EvoKG: Jointly Modeling Event Time and Network Structure for Reasoning over Temporal Knowledge Graphs. In WSDM. ACM, 794–803.

[33] Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. 2014. DeepWalk: online learning of social representations. In KDD. ACM, 701–710.

[34] Ryan A. Rossi and Nesreen K. Ahmed. 2015. The Network Data Repository with Interactive Graph Analytics and Visualization. In AAAI. http://networkrepository.com

[35] Ryan A. Rossi, Nesreen K. Ahmed, and Eunyee Koh. 2018. Higher-order Network Representation Learning. In WWW (Companion Volume). ACM, 3–4.

[36] Ryan A. Rossi, Rong Zhou, and Nesreen K. Ahmed. 2020. Deep Inductive Graph Representation Learning. IEEE Trans. Knowl. Data Eng. 32, 3 (2020), 438–452.

[37] Jasper Snoek, Hugo Larochelle, and Ryan P. Adams. 2012. Practical Bayesian Optimization of Machine Learning Algorithms. In NIPS. 2960–2968.

[38] Chang Su, Jie Tong, Yongjun Zhu, Peng Cui, and Fei Wang. 2020. Network embedding in biomedical data science. Briefings Bioinform. 21, 1 (2020), 182–197.

[39] Jian Tang, Meng Qu, Mingzhe Wang, Ming Zhang, Jun Yan, and Qiaozhu Mei. 2015. LINE: Large-scale Information Network Embedding. In WWW. ACM, 1067–1077.
[40] Ke Tu, Jianxin Ma, Peng Cui, Jian Pei, and Wenwu Zhu. 2019. AutoNE: Hyperparameter Optimization for Massive Network Embedding. In KDD. ACM, 216–225.

[41] David H. Wolpert and William G. Macready. 1997. No free lunch theorems for optimization. IEEE Trans. Evol. Comput. 1, 1 (1997), 67–82.

[42] Felix Wu, Amauri H. Souza Jr., Tianyi Zhang, Christopher Fifty, Tao Yu, and Kilian Q. Weinberger. 2019. Simplifying Graph Convolutional Networks. In ICML (Proceedings of Machine Learning Research, Vol. 97). PMLR, 6861–6871.

[43] Jia Wu, Xiu-Yun Chen, Hao Zhang, Li-Dong Xiong, Hang Lei, and Si-Hao Deng. 2019. Hyperparameter optimization for machine learning models based on Bayesian optimization. Journal of Electronic Science and Technology 17, 1 (2019), 26–40.

[44] Feng Xia, Ke Sun, Shuo Yu, Abdul Aziz, Liangtian Wan, Shirui Pan, and Huan Liu. 2021. Graph Learning: A Survey. IEEE Trans. Artif. Intell. 2, 2 (2021), 109–127.

[45] Lin Xu, Frank Hutter, Jonathan Shen, Holger H Hoos, and Kevin Leyton-Brown. 2012. SATzilla2012: Improved algorithm selection based on cost-sensitive classification models. Proceedings of SAT Challenge (2012), 57–58.

[46] Tong Yu and Hong Zhu. 2020. Hyper-Parameter Optimization: A Review of Algorithms and Applications. CoRR abs/2003.05689 (2020).

[47] Yingfang Yuan, Wenjun Wang, George M. Coghill, and Wei Pang. 2021. A Novel Genetic Algorithm with Hierarchical Evaluation Strategy for Hyperparameter Optimisation of Graph Neural Networks. CoRR abs/2101.09300 (2021).

[48] Ziwei Zhang, Peng Cui, and Wenwu Zhu. 2022. Deep Learning on Graphs: A Survey. IEEE Trans. Knowl. Data Eng. 34, 1 (2022), 249–270.

[49] Ronghang Zhu, Zhiqiang Tao, Yaliang Li, and Sheng Li. 2021. Automated Graph Learning via Population Based Self-Tuning GCN. In SIGIR. ACM, 2096–2100.
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 settings (Appendix F). We then provide additional details of AUTOGML (Appendix G), e.g., the meta-graph and the embedding function $f(\cdot)$ discussed in Section 3.4, as well as additional results (Appendix H), e.g., meta-graph feature visualization, and the model selection time of AUTOGML and baselines.

A Baselines

The baselines used in experiments can be organized into the following three categories.

(a) **No model selection** employs the same popular model for link prediction.

• **node2vec** [12] is a popular graph representation learning method.

• **GCN** [21] denotes graph convolutional network.

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

• **Global Best (GB)-Avg** selects the model with the largest mean performance across all meta-train graphs.

• **Global Best (GB)-Rank** selects the model that was the best performing most frequently for all meta-train graphs.

• **ISAC** [20] 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)** [28] 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.

Note that GB-Avg and GB-Rank do not rely on meta-features for model selection.

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

• **Supervised Surrogates (SS)** [45] learns a surrogate model (a regressor) that maps meta-graph features to model performances.

• **ALORS** [27] 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** [15] improves upon ALORS by replacing dot product with a more general neural architecture that estimates performance by combining the linearity of MF and non-linearity of DNNs.

In addition, we also include **Random Selection (RS)** as a baseline, which orders models randomly, to see how different meta-learners compared to random.

B Notations

Table 4 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 5 shows the complete list of 12 popular GRL methods and their specific hyperparameter settings, which compose 412 unique models in the model set $\mathcal{M}$. Note that the link predictor is omitted from Table 5 since we employ the same link predictor based on cosine similarity to all GRL methods.
Table 5: Graph representation learning (GRL) models and their hyperparameter settings, which collectively comprise the model set \( \mathcal{M} \) with 423 unique GRL models. For details of the hyperparameters, please refer to the cited paper.

| Methods          | Hyperparameter Settings                                                                 | Count |
|------------------|----------------------------------------------------------------------------------------|-------|
| SGC [42]         | # (number of) hops \( k \in \{1, 2, 3\} \)                                              | 3     |
| GCN [21]         | # layers \( L \in \{1, 2, 3\} \), # epochs \( N \in \{1, 10\} \)                      | 6     |
| GraphSAGE [14]   | # layers \( L \in \{1, 2, 3\} \), # epochs \( N \in \{1, 10\} \), aggregation functions \( f \in \{\text{mean}, \text{gen}, \text{ lstm}\} \) | 18    |
| node2vec [12]    | \( p, q \in \{1, 2, 4\} \)                                                             | 9     |
| role2vec [2]     | motif combinations \( \mathcal{H} \in \{\{H_1\}, \{H_2, H_3\}, \{H_2, H_3, H_4, H_5, H_6, H_7\}, \{H_1, H_2, \ldots, H_8\}\} \) | 180   |
| GraRep [7]       | \( k \in \{1, 2\} \)                                                                  | 2     |
| DeepWalk [33]    | \( p = 1, q = 1 \)                                                                     | 1     |
| HONE [35]        | \( k \in \{1, 2\} \), \( D_{\text{local}} \in \{4, 8, 16\} \), variant \( v \in \{1, 2, 3, 4, 5\} \) | 30    |
| node2bits [10]   | \begin{align*} \text{walk num } w_n & \in \{5, 10, 20\}, \text{walk len } w_l & \in \{5, 10, 20\}, \text{log base } b & \in \{2, 4, 8, 10\}, \text{feats } f & \in \{16\} \end{align*} | 36    |
| DeepGL [50]      | \( \alpha \in \{0, 0.3, 0.5, 0.7, 0.9\} \), 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 [39]        | \# hops/order \( k \in \{1, 2\} \)                                                      | 2     |
| Spectral Emb. [45] | tolerance \( t \in \{0.001\} \)                                                     | 1     |
| **Total Count**  |                                                                                | **423** |

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 \( A \) and \( AA^T \) where \( A \) 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 \( \Sigma \) of
global statistical functions (Table 6) 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 6: Summary of the global statistical functions $\Sigma$ 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        | $\text{card}(\mathbf{x})$                                                |
| Density                   | $\text{max}(\mathbf{x})/\text{|x|}$                                     |
| $Q_1, Q_3$                | median of the $\text{|x|}/2$ smallest (largest) values                   |
| IQR                       | $Q_3 - Q_1$                                                              |
| Outlier LB $\alpha \in \{1.5, 3\}$ | $\sum_i I(x_i < Q_1 - \alpha IQR)$                                       |
| Outlier UB $\alpha \in \{1.5, 3\}$ | $\sum_i I(x_i > Q_3 + \alpha IQR)$                                       |
| Total outliers $\alpha \in \{1.5, 3\}$ | $\sum_i I(x_i < Q_1 - \alpha IQR) + \sum_i I(x_i > Q_3 + \alpha IQR)$ |
| $(\alpha$-std) outliers $\alpha \in \{2, 3\}$ | $\mu_x \pm \alpha \sigma_x$                                          |
| Spearman ($\rho$, p-val)  | $\text{spearman}(\mathbf{x}, \pi(\mathbf{x}))$                        |
| Kendall ($\tau$, p-val)   | $\text{kendall}(\mathbf{x}, \pi(\mathbf{x}))$                        |
| Pearson ($r$, p-val)      | $\text{pearson}(\mathbf{x}, \pi(\mathbf{x}))$                        |
| Min, max                  | $\text{min}(\mathbf{x}), \text{max}(\mathbf{x})$                     |
| Range                     | $\text{max}(\mathbf{x}) - \text{min}(\mathbf{x})$                     |
| Median                    | $\text{med}(\mathbf{x})$                                               |
| Geometric Mean            | $|\mathbf{x}|^{-1} \prod_i x_i$                                        |
| Harmonic Mean             | $|\mathbf{x}| / \sum_i \frac{1}{x_i}$                                  |
| Mean, Stdev, Variance     | $\mu_x, \sigma_x, \sigma_x^2$                                         |
| Skewness                  | $\text{skewness}(\mathbf{x})$                                         |
| Kurtosis                  | $\text{kurtosis}(\mathbf{x})$                                         |
| Quartile Dispersion Coeff. | $\frac{Q_3-Q_1}{Q_3-Q_1}$                                     |
| Median Absolute Deviation | $\text{med}[|\mathbf{x} - \text{med}(\mathbf{x})|]$                   |
| Avg. Absolute Deviation   | $\frac{1}{|\mathbf{x}|} \text{e}^{|\mathbf{x} - \mu_x|}$             |
| Coeff. of Variation       | $\frac{\sigma_x}{\mu_x}$                                             |
| Efficiency ratio          | $\frac{\sigma_x^2}{\mu_x}$                                           |
| Variance-to-mean ratio    | $\frac{\sigma_x^2}{\mu_x}$                                           |
| Signal-to-noise ratio (SNR)| $\mu_x^2/\sigma_x^2$                                                |
| Entropy                   | $H(\mathbf{x}) = - \sum_i x_i \log x_i$                              |
| Norm. entropy             | $H(\mathbf{x})/\log_2|\mathbf{x}|$                                  |
| Gini coefficient          | $-$                                                                      |
| Quartile max gap          | $\text{max}(Q_{i+1} - Q_i)$                                           |
| Centroid max gap          | $\text{max}_{ij} |c_i - c_j|$                                          |
| Histogram prob. dist.     | $p_h = \frac{h}{k} e$ (with fixed # of bins)                          |

**Variants of Meta-Graph Features $\mathbf{m}$.** In Section 4.4, we use two meta-graph features different from $\mathbf{m}$, namely $\mathbf{m}_{\text{small}}$ and $\mathbf{m}_{\text{extended}}$. $\mathbf{m}$ is the default set with $\sim 300$ features, and $\mathbf{m}_{\text{small}}$ a subset of $\mathbf{m}$ with $\sim 60$ features. $\mathbf{m}_{\text{small}}$ comprises simple structural features such as degree and k-core. $\mathbf{m}_{\text{extended}}$ is a superset of $\mathbf{m}$ with $\sim 1000$ features, constructed by extending $\mathbf{m}$ with features related to edge-centric graphlet frequency. In particular, we count all 3 and 4 node graphlets (network motifs) for every edge in the graph. For each of the graphlet frequency distributions (3-stars, 4-cycles, 4-cliques, etc), we apply the functions in Table 6 over it, and obtain a vector representation for the edge graphlet frequency distribution. Then we obtain $\mathbf{m}_{\text{extended}}$ by concatenating these meta-graph features with $\mathbf{M}$. 


E Graph Datasets

The testbed used in this work contains 301 graphs taken from 21 domains, which have widely different structural properties. Table 7 shows the distribution of testbed graphs across graph domains. All graph data are from [34]; they are publicly available under the Creative Commons Attribution-ShareAlike License. Also, the data that we use in this work do not contain personally identifiable information or offensive content.

Table 7: Domains of the graph datasets in the testbed, and the number of graphs for each domain. In sum, our testbed contains 301 graphs drawn from 21 domains, which have fundamentally different structural characteristics.

| Graph Data Domain          | Number of Graphs |
|----------------------------|------------------|
| Protein Networks           | 50               |
| Cheminformatics Network    | 50               |
| Retweet Network            | 27               |
| Synthetic-KPGM             | 25               |
| Biological Network         | 23               |
| Synthetic-BA               | 18               |
| Facebook Network           | 17               |
| Synthetic-CL               | 15               |
| Web Graph                  | 10               |
| Collaboration Network      | 10               |
| Social Network             | 10               |
| Brain Network              | 9                |
| Synthetic-ER               | 6                |
| Ecology Network            | 6                |
| Road Network               | 6                |
| Email Network              | 6                |
| Power Networks             | 6                |
| Recommendation Network     | 2                |
| Technological Network      | 2                |
| Infrastructure Network     | 2                |
| Scientific Computing Network| 1               |

Total Count 301

F Experimental Settings

Hyperparameters. We set the embedding size $k$ to 32 for AutoGML and other meta-learners that learn embeddings of models and graphs. For AutoGML, we created the meta-graph by connecting nodes to their top-10 similar nodes. As an embedding function $f(\cdot)$ in AutoGML, we used HGT [17] 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.

Software. We used PyTorch[17] for implementing the training and inference pipeline, and used the DGL’s implementation of HGT[17]. We used open source libraries, such as NetworkX[18] and NumPy[19] for implementing meta-graph feature extractors.

Compute Resources. We used a Linux machine with 8 cores of Intel(R) Xeon(R) CPU E5-2686 v4 @ 2.30GHz, 60GB RAM, and an NVIDIA Tesla V100 SXM2 16GB GPU.

[17] https://pytorch.org/
[18] https://www.dgl.ai/
[19] https://networkx.org/
[20] https://numpy.org/
Algorithm 1: AUTOGML: Offline Meta-Training (Top) and Online Model Selection (Bottom)

**Input:** Meta-train graph database \( \mathcal{G} \), model set \( \mathcal{M} \), embedding dimension \( k \)
**Output:** Meta-learner for model selection

\( /* \) (Offline) Meta-Learner Training \( */ \)
1. Train & evaluate models in \( \mathcal{M} \) on graphs in \( \mathcal{G} \) to get performance matrix \( P \)
2. Extract meta-graph features \( M \) for each graph \( G_i \) in \( \mathcal{G} \) (Sec. 3.3)
3. Factorize \( P \) to obtain latent graph factors \( U \) and model factors \( V \), i.e., \( P \approx UV^\top \)
4. Learn an estimator \( \phi(\cdot) \) such that \( \phi(m) = \hat{U}_i \approx U_i \)
5. Create meta-train graph \( G_{\text{train}} \) (Sec. 3.4)

while not converged

for \( i = 1, \ldots, n \) do

Get embeddings \( f(W[m; \phi(m)]) \) of train graph \( G_i \) on \( G_{\text{train}} \)

for \( j = 1, \ldots, m \) do

Get embeddings \( f(V_j) \) of each model \( M_j \) on \( G_{\text{train}} \)

Estimate \( \hat{p}_{ij} = \langle f(W[m; \phi(m)]), f(V_j) \rangle \) (Eqn. 2)
end
end

Compute meta-training loss \( L(P, \hat{P}) \) (Eqn. 4) and optimize parameters

end

\( /* \) (Online) Model Selection (Section 3.2) \( */ \)

**Input:** new graph \( G_{\text{test}} \)
**Output:** selected model \( M^* \) for \( G_{\text{test}} \)

16. Extract graph meta-features \( m_{\text{test}} = \psi(G_{\text{test}}) \)
17. Estimate latent factor \( \hat{U}_{\text{test}} = \phi(m_{\text{test}}) \) for test graph \( G_{\text{test}} \)
18. Create meta-test graph \( G_{\text{test}} \) by extending \( G_{\text{train}} \) with new edges between test graph node and existing nodes in \( G_{\text{train}} \) (Sec. 3.4)
19. Get embeddings \( f(W[m_{\text{test}}; \hat{U}_{\text{test}}]) \) of test graph on \( G_{\text{test}} \)
20. Get embeddings \( f(V_j) \) of each model \( M_j \) on \( G_{\text{test}} \)
21. Return the best model \( M^* \leftarrow \arg \max_{M_j \in \mathcal{M}} \langle f(W[m_{\text{test}}; \hat{U}_{\text{test}}]), f(V_j) \rangle \)

G Additional Details of AUTOGML

G.1 AUTOGML Algorithm

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

G.2 Attentive Graph Neural Networks and Heterogeneous Graph Transformer

The embedding function \( f(\cdot) \) in AUTOGML (Section 3.4) produces embeddings of models and graphs via weighted neighborhood aggregation over the multi-relational meta-graph. Specifically, we define \( f(\cdot) \) using Heterogeneous Graph Transformer (HGT) [17], which is a relation-aware graph neural network (GNN) that performs attentive neighborhood aggregation over the meta-graph. Let \( z_t^\ell \) denote the node \( t \)'s embedding produced by the \( \ell \)-th HGT layer, which becomes the input of the \( (\ell + 1) \)-th layer. Given \( L \) total layers, the embedding of node \( t \) is obtained to be the output from the last layer, i.e., \( z_t^L \). In general, node embeddings \( z_t^\ell \) produced by the \( \ell \)-th layer in an attention-based GNN, such as HGT, can be expressed as:

\[
    z_t^\ell = \underset{\forall s \in N(t), \forall e \in E(s,t)}{\text{Aggregate}} \left( \text{Attention}(s, t) \cdot \text{Message}(s) \right)
\]

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 meta-graph, 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 [17] for the details of how HGT defines the above three operators. In summary, AUTOGLM computes the embedding function \( f(h_t) \) by providing node \( t \)'s input features \( h_t \) as the initial embedding (i.e., \( z_0^t \)) to HGT, and returning \( z_L^t \), the output from the last layer, which is computed over the meta-graph via relation-aware attentive neighborhood aggregation.

G.3 Meta-Graph

Figure 5 illustrates the meta-graph (Section 3.4), which is a multi-relational bipartite graph between model nodes and graph nodes. In the meta-graph, 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 5 shows only one edge per edge type, in the meta-graph, each node is connected to its top-\( k \) similar nodes.

H Additional Results

H.1 Model Selection Time

Table 8 shows results comparing the runtime (in seconds) for naive model selection to the runtime of AUTOGLM. Note that naive model selection requires training and evaluating each method in the model set, while in AUTOGLM, the runtime involves only the time to generate meta-graph feature (penultimate row) and select the model via a forward pass (last row). Results show that AUTOGLM is fast, and incurs negligible computational overhead.

| Method          | bio-grid-plant | web-pollslogs | soc-wiki-Vote | eco-mangwet | ia-reality | tech-routers-rf | web-EPA | socfb-Caltech |
|-----------------|---------------|---------------|---------------|-------------|------------|----------------|---------|---------------|
| line            | 6.22          | 6.40          | 5.45          | 6.37        | 5.85       | 5.40           | 7.28    | 8.19          |
| node2vec        | 36.48         | 52.34         | 65.28         | 18.40       | 504.38     | 154.54         | 317.55  | 184.09        |
| deepwalk        | 3.84          | 5.44          | 7.03          | 1.84        | 55.01      | 16.89          | 33.09   | 18.24         |
| HONE            | 19.24         | 169.22        | 203.71        | 11.20       | 53.15      | 552.31         | 882.35  | 737.49        |
| node2bits      | 44.33         | 55.12         | 64.85         | 43.35       | 113.06     | 92.22          | 117.55  | 106.66        |
| deepGL          | 72.81         | 106.95        | 145.93        | 71.08       | 633.44     | 331.87         | 880.03  | 445.89        |
| GraphSage       | 108.20        | 301.22        | 272.97        | 339.73      | 1451.87    | 513.18         | 1020.30 | 2586.93       |
| GCN             | 15.04         | 22.00         | 26.30         | 17.12       | 57.10      | 45.64          | 66.12   | 94.65         |
| AUTOGLM         | 0.10          | 0.14          | 0.16          | 0.06        | 0.97       | 0.36           | 0.78    | 0.61          |

Table 8: Results comparing the runtime (in seconds) for naive model selection (i.e., training and evaluating each method using every hyperparameter configuration in the model set \( \mathcal{M} \)) to the runtime of AUTOGLM (the penultimate row refers to the time to generate meta-graph features, and the last row is the average time taken for model prediction). The datasets are taken from [34].
H.2 Visualizing Meta-Graph Features

Figure 6 shows the distribution of the 301 graphs in the testbed, in the two-dimensional embedding space obtained by applying t-SNE [26] to the meta-graph features $\mathbf{m}$ (Section 3.3). Each dot in the figure corresponds to a graph and the color of a dot denotes the domain of the graph. In Figure 6, graphs from the same domain are often closer to each other than to those belonging to different domains. For instance, retweet networks (brown dots) are near the bottom right corner, Facebook networks (light brown dots) are clustered near the origin, while cheminformatics networks (pink dots) are rather widely distributed in the top left corner. The result shows that the proposed meta-graph features $\mathbf{m}$ effectively capture different structural characteristics of real-world networks drawn from different domains. In experiments, simple meta-learners, such as ISAC, perform reasonably well in different evaluation settings, which also demonstrates the quality of meta-graph features, since the performance of model selection by these simple meta-learners directly depend on the quality of meta-graph features.

Figure 6: The proposed meta-graph features effectively capture the characteristics of real-world networks. Distribution of the 301 graphs in the testbed in the two-dimensional embedding space obtained by applying t-SNE [26] to the meta-graph features $\mathbf{m}$. Each dot corresponds to a graph and the color of a dot denotes the domain of the graph.