Open Graph Benchmark: Datasets for Machine Learning on Graphs

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Abstract

We present the OPEN GRAPH BENCHMARK (OGB), a diverse set of challenging and realistic benchmark datasets to facilitate scalable, robust, and reproducible graph machine learning (ML) research. OGB datasets are large-scale, encompass multiple important graph ML tasks and cover a diverse range of domains, ranging from social and information networks to biological networks, molecular graphs, and knowledge graphs. For each dataset, we provide a unified evaluation protocol using application-specific data splits and evaluation metrics. Our empirical investigation reveals the challenges of existing graph methods in handling large-scale graphs and predicting out-of-distribution data. OGB presents an automated end-to-end graph ML pipeline that simplifies and standardizes the process of graph data loading, experimental setup, and model evaluation. OGB will be regularly updated and welcomes inputs from the community. OGB datasets as well as data loaders and evaluation scripts are available at https://ogb.stanford.edu

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Introduction

Graphs are widely used for abstracting complex systems of interacting objects, such as social networks (Easley et al., 2010), knowledge graphs (Nickel et al., 2015), molecular graphs (Wu et al., 2018), and biological networks (Barabasi & Oltvai, 2004), as well as for modeling 3D objects (Simonovsky & Komodakis, 2017), manifolds (Bronstein et al., 2017), and source code (Allamanis et al., 2017). Machine learning (ML), especially deep learning, on graphs is an emerging field (Hamilton et al., 2017b; Bronstein et al., 2017). Recently, significant methodological advances (Kipf & Welling, 2017; Ying et al., 2018; Veličković et al., 2019; Xu et al., 2019) have been made in graph ML, which have produced promising results in applications from diverse domains.

How can we further advance research in graph ML? Historically, high-quality and large-scale datasets have played significant roles in advancing research, as exemplified by IMAGENET (Deng et al., 2009) and MS COCO (Lin et al., 2014) in computer vision, GLUE BENCHMARK (Wang et al., 2018) and SQUAD (Rajpurkar et al., 2016) in natural language processing, and LIBRISPEECH (Panayotov et al., 2015) and CHiME (Barker et al., 2015) in speech processing. However, in graph ML research, commonly-used datasets and evaluation procedures present issues that may negatively impact future progress.

Issues with current benchmarks. Most of the frequently-used graph datasets, such as Cora, CiteSeer (Yang et al., 2016), and the TU datasets (Yanardag & Vishwanathan, 2015; Kersting et al., 2016), are far too small to fully leverage the power of data-hungry ML models, such as graph neural networks (GNNs). Additionally, data duplication and leakage issues have been identified in some widely-used graph datasets (Zou et al., 2020). These hinder the reliable evaluation and rigorous comparison for furthering graph ML.

Furthermore, there is no unified and commonly-followed experimental protocol (Errica et al., 2019; Dwivedi et al., 2020). Different studies adopt their own dataset splits, evaluation metrics, and cross-validation protocol, making it challenging to compare performance reported across various studies (Shchur et al., 2018). In addition, many studies follow the convention of using random splits to generate training/test sets (Kipf & Welling, 2017; Xu et al., 2019; Bordes et al., 2013), which is not realistic or useful for real-world applications of graphs and generally leads to overly optimistic performance results (Lohr, 2009).

Thus, there is a need for a comprehensive suite of real-world benchmarks that combine a diverse set of datasets of various sizes coming from different domains. Data splits as well as evaluation metrics are important so that progress can be measured in a consistent and reproducible way. Last but not least, benchmarks also need to provide different types of tasks, such as node classification, link prediction, and graph classification.

Present work: OGB. Here, we present the OPEN GRAPH BENCHMARK (OGB) with the goal of facilitating scalable, robust, and reproducible graph ML research. The premise of OGB is to develop a diverse set of challenging and realistic benchmark datasets that can empower the rigorous
Figure 2: **Overview of OGB:** (a) OGB provides realistic graph benchmark datasets that cover different prediction tasks (node, link, graph), are from diverse application domains, and are at different scales. (b) OGB fully automates dataset processing and splitting. That is, the OGB data loaders automatically download and process graphs, provide graph objects (compatible with PyTorch\(^1\) [Paszke et al., 2019] and its associated graph libraries, PyTorch Geometric\(^2\) [Fey & Lenssen, 2019] and Deep Graph Library\(^3\) [Wang et al., 2019a]), and further split the datasets in a standardized manner. (c) After an ML model is developed, (d) OGB evaluates the model in a dataset-dependent manner, and outputs the model performance appropriate for the task at hand. Finally, (e) OGB provides leaderboards to help to keep track of recent advances.

advancements in graph ML. As illustrated in Figure 1, the OGB datasets are designed to have the following three characteristics.

1. **Large scale.** OGB datasets are orders-of-magnitude larger than existing benchmarks and can be categorized into three different scales (small, medium, and large). Even the “small” OGB graphs have more than 100,000 nodes, but are small enough to fit into the memory of a single GPU, making them suitable for testing computationally intensive algorithms. Additionally, OGB introduces “medium” (1–10 million nodes) and “large” (beyond 10 million nodes) datasets, which can facilitate the development of methods for addressing problems of sampling and partitioning, distributed training, and scalability.

2. **Diverse domains.** The OGB datasets aim to include graphs that are representative of a wide range of domains, as shown in Table 1. The broad coverage of domains in OGB empowers the development and demonstration of general-purpose models and can be used to distinguish them from domain-specific techniques. Furthermore, for each dataset, OGB adopts domain-specific data splits (e.g., based on time, species, molecular structure, etc.) that are more realistic and meaningful than conventional random split. Such data splits are often much more challenging than the random split, and present a research opportunity to improve out-of-distribution generalization of graph ML models.

3. **Multiple task categories.** In addition to data diversity, OGB supports three categories of fundamental graph ML tasks, i.e., node, link, and graph property predictions, each of which requires the models to make predictions at different levels of graphs, i.e., at the level of a node, link, and entire graph, respectively. Currently, OGB includes at least 3 graph datasets for each task category.

The currently-available OGB datasets are listed in Table 1. We will update the table as new datasets are released.

In addition to building graph datasets, OGB also presents an automated end-to-end graph ML pipeline that simplifies and standardizes the process of graph data loading, experimental setup, and model evaluation, as illustrated in Figure 2. Given the OGB datasets (a), the end-users can focus on developing their graph ML models (c) by using the OGB data loaders (b) and evaluators (d), both of which are provided by our OGB Python package\(^4\). OGB also hosts a public leaderboard\(^5\) for publicizing state-of-the-art, reproducible graph ML research. As a starting point, for each dataset, we include results from a suite of well-known baselines, particularly GNN-based methods, together with code to reproduce our results.

OGB is an on-going open-source and community-driven initiative. Over time we plan to release new versions of the datasets and methods, and provide updates to the leaderboard. Our immediate future plan is to add more graph datasets to increase the coverage in Table 1. The OGB website (https://ogb.stanford.edu/docs/leader_overview)

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\(^1\) https://pytorch.org
\(^2\) https://pytorch-geometric.readthedocs.io
\(^3\) https://www.dgl.ai
\(^4\) https://github.com/snap-stanford/ogb
\(^5\) https://ogb.stanford.edu/docs/leader_overview
Table 1: Overview of currently-available OGB datasets (denoted in green). Nature domain includes biological networks and molecular graphs, Society domain includes academic graphs and e-commerce networks, and Information domain includes knowledge graphs.

| Task                  | Nature | Society | Information |
|-----------------------|--------|---------|-------------|
| **Node property prediction** |        |         |             |
| Domain | Small | Medium | Large |
| Small | arxiv | proteins | products |
| Medium | | | |
| Large | | | |
| **Link property prediction** |        |         |             |
| Domain | Small | Medium | Large |
| Small | collab | ppa | citation, wikikg |
| Medium | | | |
| Large | | | |
| **Graph property prediction** |        |         |             |
| Domain | Small | Medium | Large |
| Small | molhiv | | |
| Medium | molpcba, ppa | | |
| Large | | | |

//ogb.stanford.edu) provides the documentation, example scripts, and public leaderboard. We also welcome inputs from the community at ogb@cs.stanford.edu.

2 Shortcomings of Current Benchmarks

We first review commonly-used graph benchmarks and discuss the current state of the field. We organize the discussion around three categories of graph ML tasks: predictions at the level of nodes, links, and graphs.

**Node property prediction.** Currently, the three graphs (Cora, CiteSeer and PubMed) proposed in Yang et al. (2016) have been widely used as semi-supervised node classification datasets, particularly for evaluating GNNs. The sizes of these graphs are rather small, ranging from 2,700 to 20,000 nodes. Recent studies suggest that datasets at this small scale can limit the capacity of advanced neural architectures (Shchur et al., 2018), as most recent performance improvements on these datasets are nearly statistically identical (Dwivedi et al., 2020). Furthermore, there is no consensus on the splitting procedures for these datasets, which results in reported performance metrics that are incomparable with each other for gauging model designs (Shchur et al., 2018). Finally, a recent study (Zou et al., 2020) shows that these datasets are hindered by some fundamental data quality issues. For example, in Cora, 42% of the nodes leak information between their features and labels, and 1% of the nodes are duplicated. The situation for CiteSeer is even worse, with leakage rates of 62% and duplication rates of 5%.

Some recent works in graph ML have proposed relatively large datasets, such as PPI (56,944 nodes), Reddit (334,863 nodes) (Hamilton et al., 2017b) and Amazon2M (2,449,029 nodes) (Chiang et al., 2019). However, there exist some inherent issues with the proposed data splits. Specifically, 83%, 65% and 90% of the nodes are used for training in the PPI, Reddit and Amazon2M datasets, respectively, which results in an artificially small distribution shift across the training/validation/test sets. Consequently, as may be expected, the performance improvements on these benchmarks have
quickly saturated. For example, recent GNN models (Chiang et al., 2019; Zeng et al., 2020) can already yield F1 scores of 99.5 for PPI and 97.0 for Reddit, and 90.4% accuracy for Amazon2M. To sum up, several factors (e.g., size, leakage, splits) associated with the current use of these datasets lead to very small generalization gaps, making them unsuitable as benchmark datasets for graph ML.

Link property prediction. Broadly, there are two lines of efforts for the link-level task: link prediction in homogeneous networks (Liben-Nowell & Kleinberg, 2007; Zhang & Chen, 2018) and relation completion in (heterogeneous) knowledge graphs (Bordes et al., 2013; Hu et al., 2020b). There are several problems with the current benchmark datasets in this area. First, representative datasets for both types of tasks either do not come with input node features or are at a scale of only 1-100 thousand nodes. For example, while the well-known recommender system datasets used in (Berg et al., 2017) include node features, their sizes are very small, with the largest having only 6,000 nodes. On the other hand, though the Open Academic Graph (OAG) used in (Qiu et al., 2019) comprises tens of millions of nodes, there are no associated node features. Second, similar to the node-level task, random splits are also predominantly used in link-level prediction (Bordes et al., 2013; Grover & Leskovec, 2016). Finally, the existing datasets for this task are mostly oriented to applications in recommender systems, social media and knowledge graphs, in which the graphs are typically very sparse. This may result in techniques specialised for sparse link inference that are not generalizable to domains with dense graphs, such as the protein-protein interaction (PPI) graphs typically found in biology (Szklarczyk et al., 2019).

Graph property prediction. Graph-level prediction tasks are found in important applications in natural sciences, such as predicting molecular properties in chemistry (Duvenaud et al., 2015; Gilmer et al., 2017; Hu et al., 2020a), where molecules are naturally represented as molecular graphs. Here, the most widely-used graph-level datasets from the TU collection (Kersting et al., 2016) are known to have many issues, such as small sizes (i.e., less than 1,000 graphs), unrealistic settings (e.g., no bond features for molecules), random data splits, inconsistent evaluation protocols, and isomorphism bias (Ivanov et al., 2019). A very recent attempt (Duvedi et al., 2020) to address these issues mainly focuses on benchmarking ML models, specifically the building blocks of GNNs, rather than developing application-oriented realistic datasets. In fact, five out of six datasets considered are synthetic. Nevertheless, this effort is complementary to OGB. Recent work in graph ML (Hu et al., 2020a; Ishiguro et al., 2019) has started to adopt MÔLECULENET (Wu et al., 2018) that contains a set of realistic and large-scale molecular property prediction datasets. However, there is limited consensus in the dataset splitting as well as choices in molecular graph features, making it hard to compare different models in a fair manner. OGB adopts the MÔLECULENET datasets, while providing unified dataset splits as well as the molecular graph features that we found to provide favorable performance over naive features. Beyond molecular graphs, OGB also provides graphs from other domains, such as biological networks and ASTs of source code (to be included in the next release). Both of them exhibit distinct characteristics from molecular graphs, which enables evaluating the versatility of graph ML models.

3 OGB: Overview

The goal of OGB is to support and catalyze research in the area of machine learning with graphs, which is a fast-growing and increasingly important area. OGB datasets cover a variety of real-world applications and span several important domains. Furthermore, OGB provides a common codebase using popular deep learning frameworks for loading, constructing, and representing graphs as well as code implementation of established performance metrics for fast model evaluation and comparison.

In the subsequent sections (Sections 4, 5, and 6), we describe in detail each of the datasets in OGB, focusing on the properties of the graph(s), the prediction task, and the dataset splitting scheme. The currently-available datasets are summarized in Table 2. We also compare datasets from diverse application domains by inspecting their basic graph statistics, e.g., node degree, clustering coefficient, and diameter. We show that they exhibit diverse graph characteristics, which is crucial to evaluate the versatility of graph ML models. The dataset statistics are summarized in Table 3.

In the same sections, we additionally show our first individual benchmark analyses of the datasets, discuss our initial findings, and highlight research challenges and opportunities of scaling models to large graphs and improving generalization performance under the realistic data split scenarios. We repeat each experiment 10 times using different random seeds and report the mean and unbiased standard deviation of all training and test results corresponding to the best validation results. All code to reproduce our baseline experiments is publicly available at [https://](https://)
Table 2: Summary of currently-available OGB datasets. An OGB dataset, e.g., ogbg-molhiv, is identified by its prefix (ogbg-) and its name (molhiv). The prefix specifies the category of the graph ML task, i.e., node (ogbn-), link (ogbl-), or graph (ogbg-) property prediction. A realistic split scheme is adopted for each dataset, whose detail can be found in Sections 4, 5, and 6 for each dataset.

| Category | Name  | Features | Edge Features | Directed | #Tasks | Split Scheme | Split Ratio | Task Type | Metric |
|----------|-------|----------|---------------|----------|--------|-------------|------------|----------|--------|
| Node     | ogbn- | products | ✔️            | ❌        | ❌      | 1 Sales rank | 10/02/88   | Multi-class. | Accuracy |
|          |       | arxiv    | ✔️            | ❌        | ✔️      | 1 Time       | 54/18/28   | Multi-class. | Accuracy |
|          |       | proteins | ❌            | ✔️        | ✔️      | 112 Species  | 65/16/19   | Binary class. |        |
| Link     | ogbl- | ppa      | ✔️            | ❌        | ❌      | 1 Throughput | 70/20/10   | Link prediction | Hits@100 |
|          |       | collab   | ✔️            | ❌        | ✔️      | 1 Time       | 92/4/4     | Link prediction | Hits@10  |
|          |       | citation | ✔️            | ❌        | ✔️      | 1 Time       | 99/1/1     | Link prediction | MRR     |
|          |       | wikig    | ❌            | ✔️        | ✔️      | 1 Time       | 94/3/3     | KG completion |        |
| Graph    | ogbg- | molhiv   | ✔️            | ✔️        | ❌      | 1 Scaffold   | 80/10/10   | Binary class. | ROC-AUC  |
|          |       | molpcba  | ✔️            | ✔️        | ❌      | 128 Scaffold | 80/10/10   | Binary class. | PRC-AUC  |
|          |       | ppa      | ❌            | ✔️        | ✔️      | 1 Species    | 49/29/22   | Multi-class. | Accuracy |

Table 3: Statistics of currently-available OGB datasets. All the directed graphs are first converted into undirected ones before the last three graph statistics are calculated using the SNAP library (Leskovec & Sosić, 2016). The diameter is approximated by performing BFS from 1,000 randomly-sampled nodes.

| Category | Name  | #Graphs | Average #Nodes | Average #Edges | Average Node Deg. | Average Node Clust. | Average Degree Coeff. | Average Diameter |
|----------|-------|---------|----------------|----------------|-------------------|---------------------|-----------------------|------------------|
| Node     | ogbn- | products | 1 2,449,029 | 61,859,140 | 50.5 | 0.411 | 29 |
|          |       | arxiv    | 1 169,343 | 1,166,243 | 13.8 | 0.226 | 22 |
|          |       | proteins | 1 132,534 | 39,561,252 | 597.0 | 0.280 | 8 |
| Link     | ogbl- | ppa      | 1 576,289 | 30,326,273 | 73.7 | 0.223 | 14 |
|          |       | collab   | 1 235,868 | 1,285,465 | 10.0 | 0.729 | 21 |
|          |       | citation | 1 2,927,963 | 30,561,187 | 20.8 | 0.178 | 21 |
|          |       | wikig    | 1 2,500,604 | 17,137,181 | 12.9 | 0.168 | 26 |
| Graph    | ogbg- | molhiv   | 41,127 | 25.5 | 27.5 | 2.2 | 0.002 | 12.0 |
|          |       | molpcba  | 437,929 | 26.0 | 28.1 | 2.2 | 0.002 | 13.6 |
|          |       | ppa      | 158,100 | 243.4 | 2,266.1 | 18.3 | 0.513 | 4.8 |

//github.com/snap-stanford/ogb/tree/master/examples and is meant as a starting point to accelerate further research on our proposed datasets. We refer the interested reader to our code base for a detailed overview of model architectures and hyperparameter settings.

Finally, in Section 7, we briefly explain the usage of our OGB Python package that can be readily installed via pip. We demonstrate how the OGB package makes it easy to develop the pipeline of Figure 2 by providing the automatic data loaders and evaluators. The package is publicly available at https://github.com/snap-stanford/ogb and its documentation can be found at https://ogb.stanford.edu.

4 OGB Node Property Prediction

We currently provide three datasets, adopted from different application domains, for predicting the properties of individual nodes. Specifically, ogbn-products is an Amazon products co-purchasing network (Kush Bhatia, 2016) (cf. Section 4.1), ogbn-arxiv is an ARXIV paper citation network extracted from the Microsoft Academic Graph (MAG) (Wang et al., 2020) (cf. Section 4.2), and ogbn-proteins is a protein-protein association network (Szklarczyk et al., 2019) (cf. Section 4.3).

The three datasets show highly different graph statistics, as shown in Table 3. For example, the biological network—ogbn-proteins—is much denser than the social/information networks (ogbn-arxiv and ogbn-products) as can be observed from its large average node degree and
small graph diameter. On the other hand, the co-purchasing network—*ogbn-products*—has more clustered graph structure than the other datasets, as can be seen from its large average clustering coefficient.

**Baselines.** We consider the following representative models as our baselines unless otherwise specified.

- **MLP:** An MLP predictor that uses the given raw node features directly as input. Graph structure information is not included.
- **NODE2VEC:** An MLP predictor that uses as input the concatenation of the raw node features and NODE2VEC embeddings [Grover & Leskovec, 2016; Perozzi et al., 2014].
- **GCN:** Full-batch Graph Convolutional Network [Kipf & Welling, 2017].
- **GRAPHSAGE:** Full-batch GraphSAGE [Hamilton et al., 2017a], where we adopt its mean pooling variant and a simple skip connection to preserve central node features.
- **CLUSTERGCN (optional):** A scalable training technique of GNNs [Chiang et al., 2019] that partitions the graphs into a fixed number of subgraphs and draws mini-batches from them.
- **GRAPHSAINT (optional):** A scalable training technique of GNNs [Zeng et al., 2020] that samples subgraphs via a random walk sampler.

The two scalable GNN variants, CLUSTERGCN and GRAPHSAINT, are experimented only for graph datasets where full-batch GCN/GRAPHSAGE did not fit into the common GPU memory size of 11GB. The scalable GNNs are more GPU memory-efficient than the full-batch GNNs because they first partition/sample the graph into subgraphs. Hence, in order to train the network, they require only a small amount of nodes to be put onto the GPU memory at each mini-batch. Inference is then performed on the whole graph without GPU usage. To choose the architecture for the scalable GNNs, we first run full-batch GCN and GRAPHSAGE on an NVIDIA Quadro RTX 8000 with 48GB of memory, and then adopt the best performing full-batch GNN architecture for the scalable GNNs. All models are trained with a fixed hidden dimensionality of 256, a fixed number of three layers, and a tuned dropout ratio \( \in \{0.0, 0.5\} \).

### 4.1 ogbn-products: Amazon Products Co-purchasing Network

The dataset *ogbn-products* is an undirected and unweighted graph, representing an Amazon product co-purchasing network [Kush Bhatia, 2016]. Nodes represent products sold in Amazon, and edges between two products indicate that the products are purchased together. We follow Chiang et al. (2019) to process node features and target categories. Specifically, node features are generated by extracting bag-of-words features from the product descriptions followed by a Principal Component Analysis to reduce the dimension to 100.

**Prediction task.** The task is to predict the category of a product in a multi-class classification setup, where the 47 top-level categories are used for target labels.

**Dataset splitting.** We consider a more challenging and realistic dataset splitting that differs from the one used in Chiang et al. (2019). Instead of randomly assigning 90% of the nodes for training and 10% of the nodes for testing (without use of a validation set), we use the sales ranking (popularity) to split nodes into training/validation/test sets. Specifically, we sort the products according to their sales ranking and use the top 10% for training, next top 2% for validation, and the rest for testing. This is a more challenging splitting procedure that closely matches the real-world application where labels are first assigned to important nodes in the network and ML models are subsequently used to make predictions on less important ones.

**Discussion.** Overall, our initial benchmarking results in Table 4 show that the highest test performances are attained by GNN architectures, while the MLP baseline that solely relies on a product’s description is not sufficient for accurately predicting the category of a product. We also perform additional experiments on the conventional random split with the same split ratio as our sales rank split. We find that the generalization gap of GNNs is much larger on the sales rank split (≈ 14-23 percentage points) than the random split (≈ 2-3 percentage points, with, e.g., 87.74 ± 0.06% test accuracy for GRAPHSAGE). Figure 3 illustrates that the sales rank splitting creates a significant distribution shift from training to test nodes, which explains the huge generalization gap. Furthermore, our scalable GNN experiments CLUSTERGCN and GRAPHSAINT perform slightly worse than

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*Defined by the difference between training and test accuracy.*
Table 4: Results for ogbn-products.
†Requires a GPU with 48GB of memory.

| Method          | Accuracy (%) | Training | Validation | Test   |
|-----------------|--------------|----------|------------|--------|
| MLP             | 84.24 ± 0.54 | 75.60 ± 0.13 | 61.12 ± 0.10 |
| NODE2Vec        | 94.24 ± 0.52 | 89.85 ± 0.12 | 72.12 ± 0.24 |
| GCN†            | 92.86 ± 0.11 | 91.66 ± 0.06 | 75.65 ± 0.20 |
| GRAPH SAGE†     | 92.98 ± 0.16 | 91.59 ± 0.12 | 78.03 ± 0.22 |
| CLUSTER GCN     | 92.79 ± 0.41 | 90.42 ± 0.33 | 75.18 ± 0.41 |
| GRAPH SAINT     | 93.30 ± 0.05 | 91.75 ± 0.06 | 77.29 ± 0.19 |

Figure 3: t-SNE visualization of training/validation/test nodes in ogbn-products.

their full-batch counterpart, which raises a research opportunity to improve the existing mini-batch training techniques of GNNs. Overall, ogbn-products provides exciting opportunities for the development of scalable GNN models that robustly make predictions on out-of-distribution nodes.

4.2 ogbn-arxiv: Paper Citation Network

The dataset ogbn-arxiv is a directed graph, representing the citation network between all Computer Science (CS) ARXIV papers indexed by MAG (Wang et al., 2020). Each node is an ARXIV paper and each directed edge indicates that one paper cites another one. Each paper comes with a 128-dimensional feature vector obtained by averaging the embeddings of words in its title and abstract. The embeddings of individual words are computed by running the skip-gram model (Mikolov et al., 2013) over the MAG corpus. In addition, all papers are also associated with the year that the corresponding paper was published.

Prediction task. The task is to predict the 40 subject areas of ARXIV CS papers, e.g., cs.AI, cs.LG, and cs.OS, which are manually determined (i.e., labeled) by the paper’s authors and ARXIV moderators. With the volume of scientific publications doubling every 12 years over the past century (Dong et al., 2017), it is practically critical to automatically classify each publication’s areas and topics. Formally, this prediction task is formulated as a 40-class classification problem.

Dataset splitting. The previously-used Cora, CiteSeer, and PubMed citation networks are split randomly (Yang et al., 2016). In contrast, we consider a realistic data split based on the publication dates of the papers. The general setting is that the ML models are trained on existing papers and then used to predict the subject areas of newly-published papers, which supports the direct application of them into real-world scenarios, such as replacing the ARXIV moderators. Specifically, we propose to train on papers published until 2017, validate on those published in 2018, and test on those published in 2019.

Discussion. Our initial benchmarking results are shown in Table 5, where the directed graph is converted to an undirected one for simplicity. First, we observe that the naïve MLP baseline that does not utilize any graph information is significantly outperformed by the other three models that utilize

https://arxiv.org/corr/subjectclasses
Table 5: Results for ogbn-arxiv.

| Method    | Accuracy (%) |          |          |          |
|-----------|--------------|----------|----------|----------|
|           | Training     | Validation | Test     |          |
| MLP       | 63.58±0.81   | 57.65±0.12 | 55.50±0.23 |
| NODE2VEC  | 76.43±0.81   | 71.29±0.13 | 70.07±0.13 |
| GCN       | 78.87±0.66   | 73.00±0.17 | 71.74±0.29 |
| GRAPHSAGE | 82.35±1.51   | 72.77±0.16 | 71.49±0.27 |

Table 6: Results for ogbn-proteins.

| Method    | ROC-AUC (%) |          |          |
|-----------|-------------|----------|----------|
|           | Training    | Validation | Test     |
| MLP       | 81.78±0.48  | 77.06±0.14 | 72.04±0.48 |
| NODE2VEC  | 79.76±1.88  | 70.07±0.53 | 68.81±0.65 |
| GCN       | 75.64±0.36  | 72.60±0.44 | 65.11±1.52 |
| GRAPHSAGE | 87.86±0.13  | 83.34±0.13 | 77.68±0.20 |

Graph information. This suggests that graph information can dramatically improve the performance of predicting a paper’s category. Comparing models that do utilize graph information, we find GNN models, i.e., GCN and GRAPHSAGE, slightly outperform the NODE2VEC model. We also conduct experiments on random split with the same split ratio. We find that GCN achieves 73.54±0.13% test accuracy on the random split, suggesting that the realistic time split is indeed more challenging than the random split, providing an opportunity to improve the out-of-distribution generalization performance. Furthermore, it is a fruitful direction to explore how the direction of edges as well as temporal information on nodes (e.g., year in which papers are published) can be taken into account to improve the model performance.

4.3 ogbn-proteins: Protein-Protein Association Network

The dataset ogbn-proteins is an undirected, weighted, and typed (according to species) graph. Nodes represent proteins, and edges indicate different types of biologically meaningful associations between proteins, e.g., physical interactions, co-expression or homology (Szklarczyk et al., 2019; Consortium, 2018). All edges come with 8-dimensional features, where each dimension represents the strength of a single association type and takes values between 0 and 1 (the larger the value is, the stronger the association is). The proteins come from 8 species.

Prediction task. The task is to predict the presence of protein functions in a multi-label binary classification setup, where there are 112 kinds of labels to predict in total. The performance is measured by the average of ROC-AUC scores across the 112 tasks.

Dataset splitting. We split the protein nodes into training/validation/test sets according to the species which the proteins come from. This enables the evaluation of the generalization performance of the model across different species.

Discussion. The dataset ogbn-proteins does not have input node features but has edge features on more than 30 million edges. In our baseline experiments, we opt for simplicity and use the average edge features of incoming edges as node features.

Benchmarking results are shown in Table 6. Surprisingly, simple MLPs perform better than more sophisticated approaches like NODE2VEC and GCN. Only GRAPHSAGE is able to outperform the naïve MLP approach which indicates that central node information (which is not explicitly modeled in GCN in its message-passing) already contains a lot of crucial information for making correct predictions.

We further evaluate the best performing GRAPHSAGE on conventional random split with the same split ratio as the species split. On the random split, the generalization gap is extremely low, with

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*In our preliminary experiments, we used one-hot encodings of species ID as node features, but that did not work well empirically, which can be explained by the fact that the species ID is used for dataset splitting.*
87.83±0.03% test ROC-AUC that is only 0.27 percentage points lower than the training ROC-AUC (88.10±0.01%). This is in contrast to 10.18 percentage points of generalization gap (training AUC minus test AUC) in the species split, as calculated from the GRAPHSAGE experiment in Table 6. The result suggests the unique challenge of across-species generalization that needs to be tackled in future research.

Since the number of nodes in ogbn-proteins is fairly small and easily fit onto common GPUs, we did not run the CLUSTERGCN and GRAPHSaint experiments. Nonetheless, this dataset presents an interesting research question of how to utilize edge features in a more sophisticated way than just naïve averaging, e.g., by the usage of attention or by treating the graph as a multi-relational graph (as there are 8 different association types between proteins). The challenge is to scalably handle the huge number of edge features efficiently on GPU, which might require clever graph partitioning based on the edge weights.

5 OGB Link Property Prediction

We currently provide four datasets, adopted from diverse application domains, for predicting the properties of links (pairs of nodes). Specifically, ogbl-ppa is a protein-protein association network (Szklarczyk et al., 2019) (cf. Section 5.1), ogbl-collab is an author collaboration network (Wang et al., 2020) (cf. Section 5.2), ogbl-citation is a paper citation network (Wang et al., 2020) (cf. Section 5.3), and ogbl-wikikg is a Wikidata knowledge graph (Vrandečić & Krötzsch, 2014) (cf. Section 5.4).

The different datasets are highly diverse in their graph structure, as shown in Table 3. For example, the biological network, ogbl-ppa, is much denser than the academic networks (ogbl-collab and ogbl-citation) as well as the knowledge graph (ogbl-wikikg), as can be seen from the large average node degree, small number of nodes, and the small graph diameter. On the other hand, the collaboration network, ogbl-collab, has more clustered graph structure than the other datasets, as can be seen from its high average clustering coefficient.

Baselines. We implement different sets of baselines for link prediction datasets that only have a single edge type and KG completion datasets that have multiple edge/relation types.

Baselines for link prediction datasets. We consider the following representative models as our baselines unless otherwise specified. For all models, edge features are obtained by using the Hadamard operator ∙ between pair-wise node embeddings, and are finally inputted to an MLP for the final prediction. During training, we randomly sample edges and use them as negative examples. We use the same number of negative edges as there are positive edges. Below, we describe how each model obtains node embeddings:

- **MLP**: Input node features are directly used as node embeddings.
- **Node2Vec**: The node embeddings are obtained by concatenating input features and Node2Vec embeddings (Grover & Leskovec, 2016; Perozzi et al., 2014).
- **GCN**: The node embeddings are obtained by full-batch Graph Convolutional Networks (GCN) (Kipf & Welling, 2017).
- **GRAPHSAGE**: The node embeddings are obtained by full-batch GraphSAGE (Hamilton et al., 2017a), where we adopt its mean pooling variant and a simple skip connection to preserve central node features.
- **MatrixFactorization**: The distinct embeddings are assigned to different nodes and are learned in an end-to-end manner together with the MLP predictor.
- **CLUSTERGCN** (optional): A scalable training technique of GNNs (Chiang et al., 2019) that partitions the graphs into a fixed number of subgraphs and draws mini-batches from them.
- **GRAPHSaint** (optional): A scalable training technique of GNNs (Zeng et al., 2020) that samples subgraphs via a random walk sampler.

Similar to the node property prediction baselines, the scalable GNN variants, CLUSTERGCN and GRAPHSaint, are experimented only for graph datasets where full-batch GCN and GRAPHSAGE did not fit into the common GPU memory size of 11GB. To choose the GNN architecture for the scalable GNNs, we first run full-batch GCN and GRAPHSAGE on a NVIDIA Quadro RTX 8000 with 48GB of memory, and then adopt the best performing full-batch GNN architecture for the scalable GNNs. All models are trained with a fixed hidden dimensionality of 256, a fixed number of three layers, and a tuned dropout ratio ∈ {0.0, 0.5}.
Table 7: Results for ogbl-ppa.

| Method          | Hits@100 (%) |       |       |
|-----------------|--------------|-------|-------|
|                 | Training     | Validation | Test  |
| MLP             | 0.46±0.00    | 0.46±0.00 | 0.46±0.00 |
| NODE2VEC        | 24.43±0.92   | 22.53±0.88 | 22.26±0.83 |
| GCN             | 12.41±1.55   | 12.13±1.49 | 11.55±1.53 |
| GRAPH SAGE      | 11.44±2.68   | 10.86±2.51 | 10.63±2.44 |
| MATRIX FACTORIZATION | 81.65±9.15 | 32.28±4.28 | 32.29±0.94 |

Baselines for KG completion datasets. We consider the following representative KG embedding models as our baselines unless otherwise specified.

- **TRANSE**: Translation-based KG embedding model by Bordes et al. (2013).
- **DISTMULT**: Multiplication-based KG embedding model by Yang et al. (2015).
- **COMPLEX**: Complex-valued multiplication-based KG embedding model by Trouillon et al. (2016).
- **ROTATE**: Rotation-based KG embedding model by Sun et al. (2019).

For KG with many entities and relations, the embedding dimensionality can be limited by the available GPU memory, as all the embeddings need to be put on GPU at once. We therefore choose the dimensionality such that training can be performed on a fixed-budget of GPU memory. Our training procedure follows Sun et al. (2019), where we perform negative sampling and use margin-based logistic loss for the loss function.

5.1 ogbl-ppa: Protein-Protein Association Network

The dataset ogbl-ppa is an undirected, unweighted graph. Nodes represent proteins from 58 different species, and edges indicate biologically meaningful associations between proteins, e.g., physical interactions, co-expression, homology or genomic neighborhood (Szklarczyk et al., 2019). We provide a graph object constructed from training edges (no validation and test edges are contained). Each node contains a 58-dimensional one-hot feature vector that indicates the species that the corresponding protein comes from.

**Prediction task.** The task is to predict new association edges given the training edges. The evaluation is based on how well a model ranks positive test edges over negative test edges. Specifically, we rank each positive edge in the validation/test set against 3,000,000 randomly-sampled negative edges, and count the ratio of positive edges that are ranked at $K$-th place or above (Hits@$K$). We found $K = 100$ to be a good threshold to rate a model’s performance in our initial experiments. Overall, this metric is way more challenging than ROC-AUC because the model needs to consistently rank the positive edges higher than nearly all the negative edges.

**Dataset splitting.** We provide a biological throughput split of the edges into training/validation/test edges. Training edges are protein associations that are measured experimentally by a high-throughput technology (e.g., cost-effective, automated experiments that make large scale repetition feasible (Macarron et al., 2011; Bajorath, 2002; Younger et al., 2017)) or are obtained computationally (e.g., via text-mining). In contrast, validation and test edges contain protein associations that can only be measured by low-throughput, resource-intensive experiments performed in laboratories. In particular, the goal is to predict a particular type of protein association, e.g., physical protein-protein interaction, from other types of protein associations (e.g., co-expression, homology, or genomic neighborhood) that can be more easily measured and are known to correlate with associations that we are interested in.

**Discussion.** Our initial benchmarking results are shown in Table 7. First, the MLP baseline performs extremely poorly, which is to be expected since the node features are not rich in this dataset. Surprisingly, both GNN baselines (GCN, GRAPH SAGE) and NODE2VEC fail to overfit on the training data and show similar performances across training/validation/test splits. The poor training performance of GNNs suggests that positional information, which cannot be captured by GNNs alone (You et al., 2019), might be crucial to fit training edges and obtain meaningful node embeddings.

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9Here we obtain node embeddings by applying a linear layer to the raw one-hot node features.
Table 8: Results for ogbl-collab.

| Method          | Hits@10 (%)       |
|-----------------|-------------------|
|                 | Training | Validation | Test    |
| MLP             | 30.04±3.07 | 12.08±1.84 | 9.20±1.61 |
| NODE2VEC        | 90.13±1.13 | 51.56±1.44 | 42.81±1.40 |
| GCN             | 59.95±4.52 | 36.89±2.27 | 33.29±1.90 |
| GRAPH SAGE      | 69.21±9.70 | 38.04±6.26 | 31.21±6.20 |
| MATRIX FACTORIZATION | 99.99±0.02 | 48.05±0.20 | 38.05±0.18 |

On the other hand, we see that MATRIX FACTORIZATION, which learns a distinct embedding for each node (thus, it can express any positional information of nodes), is indeed able to overfit on the training data, while also reaching better validation and test performance. However, the poor generalization performance still encourages the development of new research ideas to close this gap, e.g., by injecting positional information into GNNs or by developing more sophisticated negative sampling techniques.

5.2 ogbl-collab: Author Collaboration Network

The dataset ogbl-collab is an undirected graph, representing a subset of the collaboration network between authors indexed by MAG (Wang et al., 2020). Each node represents an author and edges indicate the collaboration between authors. All nodes come with 128-dimensional features, obtained by averaging the word embeddings of papers that are published by the authors. All edges are associated with two meta-information: the year and the edge weight, representing the number of co-authored papers published in that year. The graph can be viewed as a dynamic multi-graph since there can be multiple edges between two nodes if they collaborate in more than one year.

**Prediction task.** The task is to predict the future author collaboration relationships given the past collaborations. The evaluation metric is similar to ogbl-ppa in Section 5.1, where we would like the model to rank true collaborations higher than false collaborations. Specifically, we rank each true collaboration among a set of 100,000 randomly-sampled negative collaborations, and count the ratio of positive edges that are ranked at $K$-place or above (Hits@$K$). We found $K = 10$ to be a good threshold in our preliminary experiments.

**Dataset splitting.** We split the data according to time, in order to simulate a realistic application in collaboration recommendation. Specifically, we use the collaborations until 2017 as training edges, those in 2018 as validation edges, and those in 2019 as test edges.

**Discussion.** Our initial benchmarking results are shown in Table 8. Here, NODE2VEC achieves the best results, followed by MATRIX FACTORIZATION and the two GNN models. This can be explained by the fact that positional information, i.e., past collaborations, is a much more indicative feature for predicting future collaboration than solely relying on the average paper representations of authors, i.e., the same research interest. Notably, MATRIX FACTORIZATION achieves nearly perfect training results, but cannot transfer the good results to the validation and test splits, even when heavy regularization is applied. Overall, it is fruitful to explore injecting positional information into GNNs, and develop better regularization methods. This dataset further provides a unique research opportunity for dynamic multi-graphs. One promising direction to explore is to treat edges at different timestamps differently, as recent collaborations may be more indicative about the future collaborations than the past ones.

5.3 ogbl-citation: Paper Citation Network

The dataset ogbl-citation is a directed graph, representing the citation network between a subset of papers extracted from MAG (Wang et al., 2020). Similar to ogbn-arxiv in Section 4.2, each node is a paper with 128-dimensional WORD2VEC features that summarizes its title and abstract, and each directed edge indicates that one paper cites another. All nodes also come with meta-information indicating the year the corresponding paper was published.

**Prediction task.** The task is to predict missing citations given existing citations. Specifically, for each source paper, two of its references are randomly dropped, and we would like the model to rank
Table 9: Results for ogbl-citation.
†Requires a GPU with 48GB of memory. Repeated only for 5 times due to resource constraints.

| Method               | MRR          | Training | Validation | Test      |
|----------------------|--------------|----------|------------|-----------|
| MLP                  | 0.2885±0.0011| 0.2891±0.0014| 0.2897±0.0011|
| NODE2Vec             | 0.6918±0.0007| 0.5933±0.0011| 0.5960±0.0013|
| GCN†                 | 0.9083±0.0036| 0.8474±0.0040| 0.8480±0.0040|
| GRAPH SAGE†          | 0.8840±0.0100| 0.8129±0.0079| 0.8167±0.0110|
| MATRIX FACTORIZATION | 0.9659±0.0047| 0.6143±0.0117| 0.6162±0.0112|
| CLUSTER GCN          | 0.8726±0.0053| 0.7980±0.0040| 0.7997±0.0037|
| GRAPH SAINT          | 0.8423±0.0121| 0.7855±0.0058| 0.7875±0.0060|

the missing two references higher than 1,000 negative reference candidates. The negative references are randomly-sampled from all the previous papers that are not referenced by the source paper. The evaluation metric is Mean Reciprocal Rank (MRR), where the reciprocal rank of the true reference among the negative candidates is calculated for each source paper, and then the average is taken over all source papers.

Dataset splitting. We split the edges according to time, in order to simulate a realistic application in citation recommendation (e.g., a user is writing a new paper and has already cited several existing papers, but wants to be recommended additional references). To this end, we use the most recent papers (those published in 2019) as the source papers for which we want to recommend the references. For each source paper, we drop two papers from its references—the resulting two dropped edges (pointing from the source paper to the dropped papers) are used respectively for validation and testing. All the rest of the edges are used for training.

Discussion. Our initial benchmarking results are shown in Table 9, where the directed graph is converted to an undirected one for simplicity. Here, the GNN models achieve the best results, followed by MATRIX FACTORIZATION and NODE2VEC. Among the GNNs, GCN performs better than GRAPH SAGE. However, these GNNs use full-batch training; thus, they are not scalable and require more than 40GB of GPU memory to train, which is intractable on most of today’s GPU machines. Hence, we also experiment with the scalable mini-batch training techniques of GNNs, CLUSTER GCN and GRAPH SAINT, on top of the GCN architecture. We see from Table 9 that these techniques give significantly worse performance than the full-batch counterpart, suggesting a research opportunity to further improve the scalable mini-batch training techniques for the link prediction dataset. The significant performance degradation of the mini-batch methods might be explained by the biased sampling, i.e., intra-links within the same cluster partition are sampled more often than inter-links between different clusters. This limitation presents a unique set of challenges for applying the mini-batch techniques to link prediction tasks, differently from those pertaining to node prediction tasks.

5.4  ogbl-wikikg: Wikidata Knowledge Graph

The dataset ogbl-wikikg is a Knowledge Graph (KG) extracted from the Wikidata knowledge base (Vrandečić & Krötzsch, 2014). It contains a set of triplet edges (head, relation, tail), capturing the different types of relations between entities in the world, e.g., Canada citizen Hinton. We retrieve all the relational statements in Wikidata and filter out rare entities. Our KG contains 2,500,604 entities and 534 relation types.

Prediction task. The task is to predict new triplet edges given the training edges. The evaluation metric follows the standard filtered metric widely used in KG (Bordes et al., 2013; Yang et al., 2015; Trouillon et al., 2016; Sun et al., 2019). Specifically, we corrupt each test triplet edges by replacing its head or tail with randomly-sampled 1,000 negative entities (500 for head and 500 for tail), while ensuring the resulting triplets do not appear in KG. The goal is to rank the true head (or tail) entities higher than the negative entities, which is measured by Mean Reciprocal Rank (MRR).

Dataset splitting. We split the triplets according to time, simulating a realistic KG completion scenario that aims to fill in missing triplets that are not present at a certain timestamp. Specifically,
we downloaded Wikidata at three different time stamps\(^\text{10}\) (May, August, and November of 2015), and construct three KGs, where we only retain entities and relation types that appear in the earliest May KG. We use the triplets in the May KG for training, and use the additional triplets in the August and November KGs for validation and test, respectively. Note that our dataset split is different from the existing Wikidata KG dataset that adopts conventional random split (Wang et al., 2019b), which does not reflect the practical usage.

**Discussion.** Our benchmark results are provided in Table 10, where the upper-half baselines are implemented on a single commodity GPU with 11GB memory, while the bottom-half baselines are implemented on a high-end GPU with 48GB memory\(^{\dagger}\).

First, we see from the upper-half of Table 10 that when the limited embedding dimensionality is used, COMPLEX performs the best among the four baselines. With the increased dimensionality, all four models are able to achieve higher MRR on training\(^{12}\), validation and test sets, as seen from the bottom-half of Table 10. This suggests the importance of using sufficient embedding dimensionality to achieve good performance in this dataset. Interestingly, although TRANSE performs the worst with the limited dimensionality, it obtains the best performance with the increased dimensionality. Nevertheless, the extremely low test MRR\(^{13}\) suggests that our realistic KG completion dataset is highly non-trivial. It presents a realistic generalization challenge of discovering new triplets based on existing ones, which necessitates the development of KG models with more robust and generalizable reasoning capability. Furthermore, this dataset presents an important challenge of effectively scaling embedding models to large KGs – naïvely training KG embedding models with reasonable dimensionality would require a high-end GPU, which is extremely costly and not scalable to even larger KGs. A promising approach to improve scalability is to distribute training across multiple commodity GPUs (Zheng et al., 2020; Zhu et al., 2019; Lerer et al., 2019). A different approach is to share parameters across entities and relations, so that a smaller number of embedding parameters need to be put onto the GPU memory at once.

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\(^{10}\)Available at [https://archive.org/search.php?query=creator%3A%22Wikidata+editors%22](https://archive.org/search.php?query=creator%3A%22Wikidata+editors%22)

\(^{11}\)Given a fixed 11GB GPU memory budget, we adopt 100-dimension embeddings for DISTMULT and TRANSE. Since ROTATE and COMPLEX require doubling the entity embedding dimensionality, we train these two models with dimensionality of 50. On the other hand, on the high-end GPU with 48GB memory, we are able to train models with sextupled embedding dimensionality.

\(^{12}\)The training MRR here is computed based on 500 randomly-sampled entities without filtering, as filtering is computationally costly. The unfiltered MRR has the systematic bias of being smaller than the filtered counterpart (Bordes et al., 2013).

\(^{13}\)Note that our test MRR on ogbl-wikikg is computed using only 500 negative entities per triplet, which is much less than the number of negative entities used to compute MRR in the existing KG datasets, such as FB15k and FB15k-237 (around 15,000 negative entities). Nevertheless, ROTATE gives either lower or comparable test MRR on ogbl-wikikg compared to FB15k and FB15k-237 (Sun et al., 2019).
6 OGB Graph Property Prediction

We currently provide three datasets, adopted from two distinct application domains, for predicting the properties of entire graphs or subgraphs. Specifically, ogbg-molhiv and ogbg-molpcba are molecular graphs [Wu et al., 2018] (cf. Section 6.1), and ogbg-ppa is a set of protein-protein association subgraphs [Zitnik et al., 2019] (cf. Section 6.2).

The different datasets are highly diverse in their graph structure, as shown in Table 3. For example, the molecular graphs (ogbg-molhiv and ogbg-molpcba) are tree-like graphs with small number of nodes per graph, small average node degrees, small average clustering coefficient, and large average graph diameter. This is in stark contrast to the biological subgraphs, ogbg-ppa, which has much larger number of nodes per graph, as well as much denser and clustered graph structure, as seen by the large average node degree, large average clustering coefficient, and large graph diameter.

Baselines. We consider the following representative GNNs as our baselines unless otherwise specified. GNNs are used to obtain node embeddings, which are then pooled to give the embedding of the entire graph. Finally, a linear model is applied to the graph embedding to make predictions.

- GCN: Graph Convolutional Networks [Kipf & Welling, 2016].
- GCN+VIRTUAL NODE: GCN that performs message passing over augmented graphs with virtual nodes, i.e., additional nodes that are connected to all nodes in the original graphs (Gilmer et al., 2017; Li et al., 2017; Ishiguro et al., 2019).
- GIN: Graph Isomorphism Network [Xu et al., 2019].
- GIN+VIRTUAL NODE: GIN that performs message passing over augmented graphs with virtual nodes.

To include edge features, we follow [Hu et al., 2020a] and simply add edge features into the incoming node features. For all the experiments, we use 5-layer GNNs, average graph pooling, a hidden dimensionality of 300, and the dropout ratio of 0.5.

6.1 ogbg-mol*: Molecular Graphs

The datasets ogbg-molhiv and ogbg-molpcba are two molecular property prediction datasets of different sizes: ogbg-molhiv (small) and ogbg-molpcba (medium). They are adopted from the MOLECULENET [Wu et al., 2018], and are among the largest of the MOLECULENET datasets. All the molecules are pre-processed using RDKIT [Landrum et al., 2006]. Each graph represents a molecule, where nodes are atoms, and edges are chemical bonds. Input node features are 9-dimensional, containing atomic number and chirality, as well as other additional atom features such as formal charge and whether the atom is in the ring or not. Input edge features are 3-dimensional, containing bond type, bond stereochemistry as well as an additional bond feature indicating whether the bond is conjugated. Note that the above additional features are not needed to uniquely identify molecules. In the experiments, we perform ablation study on the molecule features and find that including the additional features improves performance.

Prediction task. The task is to predict the target molecular properties as accurately as possible, where the molecular properties are cast as binary labels, e.g., whether a molecule inhibits HIV virus replication or not. For evaluation metric, we closely follow [Wu et al., 2018]. Specifically, for ogbg-molhiv, we use ROC-AUC for evaluation. For ogbg-molpcba, as the class balance is extremely skewed (only 1.4% of data is positive) and the dataset contains multiple classification tasks, we use the PRC-AUC averaged over the tasks as the evaluation metric.

Dataset splitting. We adopt the scaffold splitting procedure that splits the molecules based on their two-dimensional structural frameworks. The scaffold splitting attempts to separate structurally different molecules into different subsets, which provides a more realistic estimate of model performance in prospective experimental settings [Wu et al., 2018].

Discussion. Benchmarking results are given in Tables 11 and 12. We see that GIN with additional features and virtual nodes provides the best performance in the two datasets. In our preliminary experiments, we find this to be the case even for the other smaller MOLECULENET datasets. In OGB, we therefore include the additional node/edge features in our molecular graphs. Beside the two main molecule datasets, we also provide the ten other MOLECULENET datasets, together with their data loaders and splits. These datasets can be used to stress-test molecule-specific methods [Yang et al., 2019; Jin et al., 2020] and transfer learning [Hu et al., 2020a].
Table 11: Results for ogbg-molhiv.

| Method | Additional Features | Virtual Node | ROC-AUC (%) |
|--------|---------------------|--------------|-------------|
|        |                     | Training     | Validation  | Test        |
| GCN    | ×                   | 88.65±1.01   | 83.73±0.78  | 74.18±1.22  |
|        | ✓                   | 88.65±2.19   | 82.04±1.41  | 76.06±0.97  |
|        | ✓                   | 90.07±4.69   | 83.84±0.91  | 75.99±1.19  |
| GIN    | ×                   | 93.89±2.96   | 84.1±1.05   | 75.2±1.30   |
|        | ✓                   | 88.64±2.54   | 82.32±0.90  | 75.58±1.40  |
|        | ✓                   | 92.73±3.80   | 84.79±0.68  | 77.07±1.49  |

Table 12: Results for ogbg-molpcba.

| Method | Additional Features | Virtual Node | PRC-AUC (%) |
|--------|---------------------|--------------|-------------|
|        |                     | Training     | Validation  | Test        |
| GCN    | ×                   | 36.05±0.67   | 23.45±0.13  | 22.58±0.32  |
|        | ✓                   | 27.93±0.12   | 20.39±0.30  | 19.83±0.16  |
|        | ✓                   | 38.37±0.44   | 24.72±0.23  | 23.97±0.23  |
| GIN    | ×                   | 45.17±0.81   | 26.92±0.24  | 26.0±0.43   |
|        | ✓                   | 36.89±0.35   | 22.32±0.23  | 22.17±0.23  |
|        | ✓                   | 46.82±0.58   | 27.54±0.27  | 26.55±0.27  |

We further report the performance on the random splitting, keeping the split ratio the same as the scaffold splitting. We find the random split to be much easier than scaffold split. On random split of ogbg-molhiv and ogbg-molpcba, the best GIN achieves the ROC-AUC of 82.73±2.02% (5.66 percentage points higher than scaffold) and PRC-AUC of 34.14±0.49% (7.49 percentage points higher than scaffold), respectively. The same trend holds true for the other MOLECULENET datasets, e.g., the best GIN performance on the random split of ogbg-moltox21 is 86.03±1.37%, which is 8.46 percentage points higher than that of the best GIN for the scaffold split (77.57±0.62% ROC-AUC). These results highlight the challenges of the scaffold split compared to the random split, and opens up a fruitful research opportunity to increase the out-of-distribution generalization capability of GNNs.

6.2 ogbg-ppa: Protein-Protein Association Network

The dataset ogbg-ppa is a set of undirected protein association neighborhoods extracted from the protein-protein association networks of 1,581 different species (Szklarczyk et al., 2019) that cover 37 broad taxonomic groups (e.g., mammals, bacterial families, archaeans) and span the tree of life (Hug et al., 2016). To construct the neighborhoods, we randomly selected 100 proteins from each species and constructed 2-hop protein association neighborhoods centered on each of the selected proteins (Zitnik et al., 2019). We then removed the center node from each neighborhood and subsampled the neighborhood to ensure the final protein association graph is small enough (less than 300 nodes). Nodes in each protein association graph represent proteins, and edges indicate biologically meaningful associations between proteins. The edges are associated with 7-dimensional features, where each element takes a value between 0 and 1 and represents the strength of a particular type of protein protein association such as gene co-occurrence, gene fusion events, and co-expression.

Prediction task. Given a protein association neighborhood graph, the task is a 37-way multi-class classification to predict what taxonomic group the graph originates from. The ability to successfully tackle this problem has implications for understanding the evolution of protein complexes across species (De Juan et al., 2013), the rewiring of protein interactions over time (Sharan et al., 2005; Zitnik et al., 2019), the discovery of functional associations between genes even for otherwise rarely-studied organisms (Cowen et al., 2017), and would give us insights into key bioinformatics tasks, such as biological network alignment (Malod-Dognin et al., 2017).
Table 13: Results for ogbg-ppa.

| Method | Virtual Node | TrainingAccuracy (%) | ValidationAccuracy (%) | TestAccuracy (%) |
|--------|--------------|-----------------------|------------------------|-----------------|
| GCN    |              | 97.68 ± 0.22          | 64.97 ± 0.34           | 68.39 ± 0.84    |
|        | ✓            | 97.00 ± 1.00          | 65.11 ± 0.48           | 68.57 ± 0.61    |
| GIN    |              | 97.55 ± 0.52          | 65.62 ± 1.07           | 68.92 ± 1.00    |
|        | ✓            | 98.28 ± 0.46          | **66.78 ± 1.05**       | **70.37 ± 1.07**|

Dataset splitting. Similar to ogbn-proteins in Section 4.3, we adopt the *species split*, where the neighborhood graphs in validation and test sets are extracted from protein association networks of species that are not seen during training but belong to one of the 37 taxonomic groups. This split stress-tests the model’s capability to extract graph features that are essential to the prediction of the taxonomic groups, which is important for biological understanding of protein associations.

Discussion. Benchmarking results are given in Table 13. Interestingly, similar to the ogbg-mol* datasets, GIN with virtual nodes provides the best performance. Nevertheless, the generalization gap is huge (almost 30 percentage points). For reference, we also experiment with the random splitting scenario, where we use the same model (GIN + Virtual node) on the same split ratio. On the random split, the test accuracy is 92.91 ± 0.27%, which is more than 20 percentage points higher than the species split. This again encourages future research to improve the out-of-distribution generalization with more challenging and meaningful split procedures.

7 OGB Package

The OGB package is designed to make the pipeline of Figure 2 easily accessible to researchers, by automating the data loading and the evaluation parts. OGB is fully compatible with PyTorch and its associated graph libraries: PyTorch Geometric and Deep Graph Library. OGB additionally provides library-agnostic dataset objects that can be used by any other PyTorch deep learning frameworks such as Tensorflow (Abadi et al., 2016) and MXNet (Chen et al., 2015). Below, we explain the data loading (cf. Section 7.1) and evaluation (cf. Section 7.2). For simplicity, we focus on the task of the graph property prediction (cf. Section 6) using PyTorch Geometric. For the other tasks, libraries, and more details, refer to https://ogb.stanford.edu/.

7.1 OGB Data Loaders

The OGB package makes it easy to obtain a dataset object that is fully compatible with PyTorch Geometric. As shown in Code Snippet 1, it can be done with only a single line of code, with the end-users only needing to specify the name of the dataset. The OGB package will then download, process, store, and return the requested dataset object. Furthermore, the standardized dataset splitting can be readily obtained from the dataset object.

```python
>>> from ogb.graphproppred import PygGraphPropPredDataset
>>> dataset = PygGraphPropPredDataset(name="ogbg-molhiv")
# Pytorch Geometric dataset object
>>> split_idx = dataset.get_idx_split()
# Dictionary containing train/valid/test indices.
>>> train_idx = split_idx["train"]
# torch.tensor storing a list of training indices.
```

Code Snippet 1: OGB Data Loader

7.2 OGB Evaluators

OGB also enables standardized and reliable evaluation with the `ogb.*.Evaluator` class. As shown in Code Snippet 2, the end-users first specify the dataset they want to evaluate their models on,
after which the users can learn the format of the input they need to pass to the Evaluator object. The input format is dataset-dependent. For example, for ogbg-molpcba, the Evaluator object requires as input a dictionary with `y_true` (a matrix storing the ground-truth binary labels), and `y_pred` (a matrix storing the scores output by the model). Once the end-users pass the specified dictionary as input, the Evaluator object returns the model performance that is appropriate for the dataset at hand, e.g., PRC-AUC for ogbg-molpcba.

```python
>>> from ogb.graphproppred import Evaluator
# Get Evaluator for ogbg-molhiv
>>> evaluator = Evaluator(name = "ogbg-molhiv")
# Learn about the specification of input to the Evaluator.
>>> print(evaluator.expected_input_format)
# Prepare input that follows input spec.
>>> input_dict = {
    "y_true": y_true,
    "y_pred": y_pred
}
# Get the model performance.
result_dict = evaluator.eval(input_dict)
```

Code Snippet 2: OGB Evaluator

8 Conclusion and Future Plans

To enable scalable, robust, and reproducible graph ML research, we introduce the Open Graph Benchmark (OGB)—a diverse set of realistic graph datasets in terms of scales, domains, and task categories. We employ realistic splitting schemes for the given datasets, driven by application-specific use cases. Through extensive benchmark analysis, we highlight the challenges of scaling up ML models to large-scale graphs and making accurate prediction under the realistic data splitting scenarios. Altogether, our aim is for OGB to push the frontier of graph ML research.

Our immediate future plan is to increase the coverage in Table 1 by adding large graph datasets with over 10 million nodes, as well as heterogeneous knowledge graphs. The paper will be updated as more datasets are included in OGB.

Finally, OGB is an open-source initiative implemented in Python based on popular deep learning packages—PYTORCH, PYTORCH GEOMETRIC, and DEEP GRAPH LIBRARY—we hereby invite the community to develop and benchmark state-of-the-art graph ML models at https://ogb.stanford.edu.

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[14] The shape of the matrix is the number of data points times the number of tasks. The matrix can be either a PYTORCH tensor or NUMPY array.
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