FedGraphNN: A Federated Learning System and Benchmark for Graph Neural Networks

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Abstract

Graph Neural Network (GNN) research is rapidly growing thanks to the capacity of GNNs to learn representations from graph-structured data. However, centralizing a massive amount of real-world graph data for GNN training is prohibitive due to user-side privacy concerns, regulation restrictions, and commercial competition. Federated learning (FL), a trending distributed learning paradigm, aims to solve this challenge while preserving privacy. Despite recent advances in vision and language domains, there is no suitable platform for the federated training of GNNs. To this end, we introduce FedGraphNN, an open research federated learning system and the benchmark to facilitate GNN-based FL research. FedGraphNN is built on a unified formulation of federated GNNs and supports commonly used datasets, GNN models, FL algorithms, and flexible APIs. We also include a new molecular dataset, hERG, to promote research exploration. Our experimental results present significant challenges from federated GNN training: federated GNNs perform worse in most datasets with a non-I.I.D split than centralized GNNs; the GNN model that performs the best in centralized training may not hold its advantage in the federated setting. These results imply that more research effort is needed to unravel the mystery of federated GNN training. Moreover, our system performance analysis demonstrates that the FedGraphNN system is affordable to most research labs with a few GPUs. We maintain the source code at https://github.com/FedML-AI/FedGraphNN.

1 Introduction

Graph Neural Networks (GNN) are state-of-the-art models that learn representations from complex graph-structured data in various domains such as drug discovery (Rong et al., 2020b), social network recommendation (Wu et al., 2018a; Sun et al., 2019; He et al., 2019b), and traffic flow modeling (Wang et al., 2020b; Cui et al., 2019). However, for reasons such as user-side privacy, regulation restriction, and commercial competition, there are surging real-world cases in which graph data is decentralized, limiting the data size of a single party (client). For example, in the AI-based drug discovery industry, pharmaceutical research institutions would significantly benefit from the private data of another institution, but neither cannot afford to disclose their private data for commercial reasons. Federated Learning (FL) is a distributed learning paradigm with provable privacy guarantees (McMahan et al., 2017; Kairouz et al., 2019; He et al., 2019a).

Despite FL being successfully applied in domains like computer vision (Liu et al., 2020; Hsu et al., 2020) and natural language processing (Hard et al., 2018; Ge et al., 2020), FL has yet to be widely

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adopted in the domain of graph machine learning. There are multiple reasons for this: 1. Most existing FL libraries, as summarized by (He et al., 2020b) do not support GNNs. Given the complexity of graph data, the dynamics of training GNNs in a federated setting may be different from training vision or language models. A fair and easy-to-use benchmark is essential to distinguish the advantages of different GNN models and FL algorithms; 2. The definition of federated GNNs is vague in current literature. This makes it difficult for researchers who focus on SGD-based federated optimization algorithms to understand challenges in federated GNNs; 3. Applying existing FL algorithms to GNNs is nontrivial and requires significant engineering effort to transplant and reproduce existing algorithms to GNN models and graph datasets. Recent works (Wang et al., 2020a; Meng et al., 2021; Wu et al., 2021), only use the naive FedAvg algorithm (McMahan et al., 2017), which we demonstrate is sub-optimal in many cases.

To address these issues, we present an open-source federated learning system for GNNs, namely FedGraphNN, that enables the training of a variety of GNN models effectively and efficiently in a federated setting as well as benchmarks in non-I.I.D. graph datasets (e.g., molecular graphs). We first formulate federated graph neural networks (Section 2). Under this formulation, we design a federated learning system to support federated GNNs with a curated list of FL algorithms and provide low-level APIs for algorithmic research customization and deployment (Section 3). We then provide a benchmark on commonly used molecular datasets and GNNs. We also contribute a large-scale federated molecular dataset named hERG for further research exploration (Section C). Our experiments show that the straightforward deployment of FL algorithms for GNNs is sub-optimal (Section 4). Finally, we highlight future directions for federated GNNs (Section 5).

2 FORMULATION: FEDERATED GRAPH NEURAL NETWORKS

We consider a graph level GNN-based federated learning setting, depicted in Figure 1, where graph datasets are dispersed over multiple edge servers that cannot be centralized for training due to privacy or regulation restrictions. For instance, compounds in molecular trials (Rong et al., 2020b) or knowledge graphs for recommendation systems (Chen et al., 2020) may not be shared across entities because of intellectual property concerns. Under this setting, we assume that there are $K$ clients in the FL network, and the $k^{th}$ client has its own dataset $D^{(k)} := \{ (G^{(k)}_i, y^{(k)}_i) \}_{i=1}^{N^{(k)}}$, where $G^{(k)}_i = (V^{(k)}_i, E^{(k)}_i)$ is the $i^{th}$ graph sample in $D^{(k)}$ with node & edge feature sets $X^{(k)} = \{ x^{(k)}_m \}_{m \in V^{(k)}}$ & $Z^{(k)} = \{ e^{(k)}_{m,n} \}_{m,n \in V^{(k)}}$, $y^{(k)}_i$ is the corresponding multiclass label of $G^{(k)}_i$, $N^{(k)}$ is the sample number in dataset $D^{(k)}$, and $N = \sum_{k=1}^{K} N^{(k)}$. Each client owns a GNN model (an $L$-layer MPNN(Gilmer et al., 2017; Rong et al., 2020c)) to learn graph-level representations. Multiple clients are interested in collaborating through a server to improve their GNN models without necessarily revealing their graphs.

![Figure 1: Formulation of FedGraphNN (Federated Graph Neural Network)](image)

MPNN performs the forward pass in two phases: a message-passing phase and a readout phase. The message passing phase contains two steps: First, the model gathers and transforms the neighbors’ messages. Then, the model uses aggregated messages to update node hidden states. Mathematically,
To formulate GNN-based FL, we define representation using some readout function $R$ for downstream tasks (e.g. graph-level). For example, we can obtain the whole graph optimization problem as follows:

$$m_{i}^{(k+1)} = \text{AGG} \left( \left\{ M_{\theta}^{(k+1)} \left( h_{i}^{(k)}, h_{j}^{(k)}, e_{i,j} \right) \mid j \in N_{i} \right\} \right), k = 0, \ldots L - 1$$

where $h_{i}^{(k,0)} = x_{i}^{(k)}$ is the $k$th client’s node features, $\ell$ is the layer index, $\text{AGG}$ is the aggregation function (e.g., in the GCN model, the aggregation function is a simple SUM operation), $N_{i}$ is the neighborhood set of node $i$ (e.g., 1-hop neighbors), and $M_{\theta}^{(k+1)}$ is the message generation function which takes the hidden state of current node $h_{i}$, the hidden state of the neighbor node $h_{j}$ and the edge features $e_{i,j}$ as inputs. $U_{\theta}^{(k+1)}$ is the state update function receiving the aggregated feature $m_{i}^{(k+1)}$. After propagating through an $L$-layer MPNN, the readout phase computes a feature vector for downstream tasks (e.g. graph-level). For example, we can obtain the whole graph representation using some readout function $R_{\theta}$ according to:

$$\hat{y}_{i}^{(k)} = R_{\theta}\left( \left\{ h_{j}^{(k,L)} \mid j \in V_{i}^{(k)} \right\} \right)$$

To formulate GNN-based FL, we define $W = \{ M_{\theta}, U_{\theta}, R_{\theta} \}$ as the overall learnable weights in client $k$. In general, $W$ is independent of graph structure (i.e., GNN models are normally inductive and generalize to unseen graphs). Consequently, we formulate GNN-based FL as a distributed optimization problem as follows:

$$\min_{W} F(W) = \min_{W} \sum_{k=1}^{K} N_{(k)} \cdot f^{(k)}(W)$$

where $f^{(k)}(W) = \frac{1}{N_{(k)}} \sum_{i=1}^{N_{(k)}} \mathcal{L}(W; X_{i}^{(k)}, Z_{i}^{(k)}, y_{i}^{(k)})$ is the $k$th client’s local objective function that measures the local empirical risk over the heterogeneous graph dataset $D_{k}$. $\mathcal{L}$ is the loss function of the global GNN model. To solve this problem, we utilize FedAvg (McMahan et al., 2017). It is important to note here that in FedAvg, the aggregation function on the server merely averages model parameters. We use GNNs inductively, i.e. the model is independent of the structure of the graphs it is trained on. Thus, no topological information about graphs on any client is required on the server during parameter aggregation. Other advanced algorithms such as FedOPT (Reddi et al., 2020) and FedGKT (He et al., 2020a) can also be applied.

### 3 FedGraphNN System Design

We develop an open source federated learning system for GNNs, named FedGraphNN, which includes implementations of standard baseline datasets, models, and federated learning algorithms for GNN-based FL research. FedGraphNN aims to enable efficient and flexible customization for future exploration. As shown in Figure 2 in the appendix, FedGraphNN is built based on FedML research library (He et al., 2020b) which is a widely used FL library, but without any GNN support as yet. To distinguish FedGraphNN over FedML, we color-coded the modules that specific to FedGraphNN. In the lowest layer, FedGraphNN reuses FedML-core APIs but further supports tensor-aware RPC (remote procedure call), which enables the communication between servers located at different data centers (e.g., different pharmaceutical vendors). An enhanced security and privacy primitive modules are added to support techniques in upper layers. The layer above supports plug and play operation of common GNN models such as GraphSage and GAT. We provide dedicated data loaders and splitters to handle non-I.I.D. nature of graph datasets. Users can either reuse our data distribution or manipulate the non-I.I.D. ness by setting hyperparameters. For details of the system design and benchmark details, we refer the readers to Appendix B and C.

### 4 Benchmark and Experiments

**Benchmarking Dataset:** In the latest release, we use MoleculeNet (Wu et al., 2018b), a molecule machine learning benchmark, as the data source to generate our non-I.I.D. benchmark datasets using the partition algorithm Latent Dirichlet Allocation (LDA) (He et al., 2020b). In addition, we provide
a new dataset, named hERG, related to the cardiac toxicity and collected from (Kim et al., 2021; Gaulton et al., 2017) with data cleaning. Table 2 summarizes all datasets we used in experiments. Figure 4 shows each dataset’s distribution.

Result of Model Accuracy on Non-I.I.D. Partitioning: Experiments were conducted on a GPU server equipped with 8 NVIDIA Quadro RTX 5000 (16GB GPU memory). We built the benchmark with FedAvg algorithm for three GNN models (GCN, GAT, and GraphSage). We run experiments on both classification and regression tasks. Hyper-parameters are tuned (sweeping) by grid search (see Section D for the search space). After hyper-parameter tuning, we report all results in Table 1 and Table 5. For each result, the optimal hyper-parameters can be found in the Appendix E. For more details, please refer to the Appendix D.

There are multiple takeaways: 1. When graph datasets are small, FL accuracy is on par with (or even better than) centralized learning. 2. But when dataset sizes grow, FL accuracy becomes worse than the centralized approach. In larger datasets, the non-I.I.D. nature of graphs leads to an accuracy drop. 3. Our results show that the best model in the centralized setting may not be the best for the non-I.I.D. federated setting. Interestingly, we find that GAT suffers the largest performance compromise on 5 out of 9 datasets. This may be due to the sensibility of the attention calculation on the non-I.I.D. settings. Hence, additional research is needed to understand the nuances of training GNNs in a federated setting and bridge this gap.

System Performance Analysis: We also present system performance analysis when using Message Passing Interface (MPI) as the communication backend. The results are summarized in Table 4. Even on large datasets, Federated training can be completed under 1 hour using only 4 GPUs, except the QM9 dataset, which requires hours to finish training. FedGraphNN thus provides an efficient mapping of algorithms to the underlying resources, thereby making it attractive for deployment. The training time using RPC is also evaluated, but results similar to using MPI. Note that RPC is useful for realistic deployment when GPU/CPU-based edge devices can only be accessed via public IP addresses due to locating in different data centers. We will provide detailed test results in such a scenario in our future work.

5 Conclusion and Future Works

In this paper, we designed a federated learning (FL) system and benchmark for federated graph neural networks (GNN), named FedGraphNN including implementations of common baseline datasets, models, and federated learning algorithms. Our system performance analysis shows that GNN-based FL research is affordable to most research labs. We hope FedGraphNN can serve as an easy-to-follow research platform for researchers to explore exciting problems in the intersection of federated learning and graph neural networks. Here we highlight some future research directions that deserve more efforts: 1. Supporting more graph datasets and GNN models for diverse applications; 2. Optimizing the system to accelerate the training speed for large-scale graph datasets; 3. Proposing advanced FL algorithms or GNN models to mitigate the accuracy gap on datasets with non-IIDness; 4. Real-world graph data often has limited labels. However, existing FL algorithms are mainly for supervised learning. Exploring semi-supervised or self-supervised learning methods is essential toward realistic GNN-based FL applications.
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### A Related Works

Federated Graph Neural Networks (FedGraphNN) lies at the intersection of graph neural networks (GNNs) and federated learning. We mainly discuss related works that train graph neural networks using decentralized datasets. (Suzumura et al., 2019) and (Mei et al., 2019) use computed graph statistics for information exchange and aggregation to avoid node information leakage. (Zhou et al., 2020) utilize Secure Multi-Party Computation (SMPC) and Homomorphic Encryption (HE) into GNN learning for node classification. (Zheng et al., 2020) train a global GNN model
for privacy-preserving node-classification under non-IID data using Shamir’s secret sharing. (Jiang et al., 2020) propose a secure aggregation method to learn dynamic representations from multi-user graph sequences. Recently, (Wang et al., 2020a) use the hybrid method of federated learning and meta-learning to solve the semi-supervised graph node classification problem in decentralized social network dataset. (Meng et al., 2021) attempt to protect the node-level privacy using a edge-cloud partitioned GNN model for spatio-temporal forecasting task using node-level traffic sensor datasets. Finally, (Wu et al., 2021) propose a federated recommendation system with GNNs.

Our library is still in its early stage. Our vision is that FedGraphNN should cover four types of GNN-based federated learning: 1. Graph level. We believe molecular machine learning is a paramount application in this setting, where many small graphs are distributed between multiple edge devices; 2. Sub-graph level. This scenario typically pertains to social networks or knowledge graphs that need to be partitioned into many small sub-graphs due to data barriers between different departments in a giant company, as demonstrated in Wu et al. (2021). 3. Node level. When the privacy of a specific node in a graph is important, node-level GNN-based FL is useful in practice. The IoT setting is a good example Zheng et al. (2020); 4. Link level is also a promising direction that is relevant when the privacy of edges (e.g. connections in a social network) is of importance.

Although the current version of FedGraphNN only contains graph-level GNN-based FL, other scenarios are also in our plan.

## B More Details of System Design

Deploying federated learning algorithms to existing internal systems in cross-silo institutes faces several challenges:

1. Both different institutes and different subsystems in an institute have heterogeneous data schemes (different feature space, different labels for the same data point, different formats);
2. Datasets or features are scattered in different subsystems in an institute;
3. The FL client software should be compatible to existing system (OS platform, system architecture, API design pattern).

In general, frequent and large-scale deployment of updates, monitoring, and debugging is challenging; running ML workloads on an edge server is hampered by the lack of a portable, fast, small footprint, and flexible runtime engine for on-device training (Kairouz et al., 2019, Section 7).

To address these deployment challenges, we plan to develop FedML Client SDK, which has three key modules, Data Collector and Manager, Training Manager, and Model...
### Table 2: Summary of Molecular Machine Learning Datasets

| Category       | Dataset                                      | # Tasks | Task Type | # Compounds | Average # of Nodes | Average # of Edges | Rec. - Metric |
|----------------|----------------------------------------------|---------|-----------|-------------|--------------------|--------------------|---------------|
| Quantum Mechanics | QM9 (Gaulton et al., 2012)                   | 12      | Regression | 13385       | 8.80               | 27.60              | MAE           |
| Physical Chemistry | 1. Freesolv(Mooney & Galbraith, 2004)      | 1       | Regression | 642         | 8.72               | 25.00              | RMSE          |
|                | 2. ESOL (Delaney, 2004)                     | 1       | Regression | 1128        | 13.29              | 40.05              | RMSE          |
|                | 3. FreeSolv (Mobley & Galbraith, 2004)      | 1       | Regression | 6290        | 27.25              | 80.05              | RMSE          |
|                | 4. Lipo (Delaney, 2004)                     | 1       | Regression | 642         | 8.72               | 25.00              | RMSE          |
|                | 5. Lipophilicity (Gaulton et al., 2012)     | 1       | Regression | 4200        | 27.04              | 86.04              | RMSE          |
| Biophysics     | hERG (Gaulton et al., 2016; Kim et al., 2021) | 1       | Classification | 10572   | 29.39              | 94.09              | ROC-AUC       |
|                | BACE (Subramanian et al., 2016)             | 1       | Classification | 1513       | 34.09              | 36.89              | ROC-AUC       |
| Physiology     | BBBP (Martins et al., 2012)                 | 2       | Classification | 2039       | 24.03              | 25.94              | ROC-AUC       |
|                | SIDER (Kuhn et al., 2016)                   | 27      | Classification | 1427       | 33.64              | 35.36              | ROC-AUC       |
|                | ClinTox (Gayvert et al., 2016)              | 2       | Classification | 1478       | 26.13              | 27.86              | ROC-AUC       |
|                | Tox21 (tox, 2017)                          | 12      | Classification | 7831       | 18.51              | 25.94              | ROC-AUC       |

Serving, as shown in Figure 2. In essence, the three modules inside FedML Client SDK builds up a pipeline that manages a model’s life cycle, from federated training to personalized model serving (inference). Unifying three modules of a pipeline into a single SDK can simplify the system design. Any subsystem in an institute can integrate FedML Client SDK with a host process, which can be the backend service or desktop application. We can create multiple replicas on multiple servers in the institute. More specially, Data Collector and Manager is a distributed computing system that can collect scattered datasets or features from multiple servers to Training Manager. Such collection can also keep the raw data in the original server with RPCs (remote procedure call), which can only access the data during training. After obtaining all necessary datasets for federated training, Training Manager will start federated training using algorithms supported by FedML-API. Once training has been completed, Model Serving can request the trained model to be deployed for inference. Under this SDK abstraction, we plan to address the aforementioned challenges (1) and (2) within the Data Collector and Manager. As for challenge (3), we plan to make FedML Client SDK compatible with any operating systems (Linux, Android, iOS) with a cross-platform abstraction interface design. Overall, we hope FedML Client SDK could be a lightweight and easy-to-use SDK for federated learning among diverse cross-silo institutes.

![Figure 3: Example code for benchmark evaluation with FedGraphNN](image-url)

### C FedGraphNN Benchmark: Datasets, Models, and Algorithms

#### Non-I.I.D. Datasets
To facilitate the research for GNN-based federated learning, we plan to support various graph datasets with non-I.I.Dness in different domains such as molecule machine learning, knowledge graph, and recommendation system. In the latest release, we use MoleculeNet (Wu et al., 2018b), a molecule machine learning benchmark, as the data source to generate our non-I.I.D. benchmark datasets. Specially, we use the unbalanced partition algorithm Latent Dirichlet Allocation (LDA) (He et al., 2020b) to partition datasets in the MoleculeNet benchmark. In addition, we provide a new dataset, named hERG, which is related to the cardiac toxicity and collected from (Kim et al., 2021; Gaulton et al., 2017) with data cleaning. Table 2 summarizes all datasets we used in experiments. Figure 4 shows each dataset’s distribution.

#### C.1 Molecular Dataset Details

Table 2 summarizes the necessary information of benchmark datasets (Wu et al., 2018b). The details of each dataset are listed below:
Molecular Classification Datasets

- **BBBP** (Martins et al., 2012) involves records of whether a compound carries the permeability property of penetrating the blood-brain barrier.
- **SIDER** (Kuhn et al., 2016), or Side Effect Resource, dataset consists of marketed drugs with their adverse drug reactions. The available
- **ClinTox** (Gayvert et al., 2016) includes qualitative data of drugs both approved by the FDA and rejected due to the toxicity shown during clinical trials.
- **BACE** (Subramanian et al., 2016) is collected for recording compounds which could act as the inhibitors of human $\beta$-secretase 1 (BACE-1) in the past few years.
- **Tox21** (tox, 2017) is a dataset which records the toxicity of compounds.

Molecular Regression Datasets

- **QM9** (Ramakrishnan et al., 2014) is a subset of GDB-13, which records the computed atomization energies of stable and synthetically accessible organic molecules, such as HOMO/LUMO, atomization energy, etc. It contains various molecular structures such as triple bonds, cycles, amide, epoxy, etc.
- **hERG** (Gaulton et al., 2017; Kim et al., 2021) is a dataset which records the gene (KCNH2) that codes for a protein known as Kv11.1 responsible for its contribution to the electrical activity of the heart to help the coordination of the heart’s beating.
- **ESOL** (Delaney, 2004) is a small dataset documenting the water solubility (log solubility in mols per litre) for common organic small molecules.
- **Lipophilicity** (Gaulton et al., 2012) which records the experimental results of octanol/water distribution coefficient for compounds.
- **FreeSolv** (Mobley & Guthrie, 2014) contains the experimental results of hydration free energy of small molecules in water.

**Dataset Splitting.** We apply random splitting as advised in (Wu et al., 2018b). Dataset partition is 80% training, 10% validation and 10% test. We plan to support the scaffold splitting (Bemis & Murcko, 1996) specifically for molecular machine learning datasets as a future work.

C.2 GNN MODELS AND FEDERATED LEARNING ALGORITHMS.

In the latest release, FedGraphNN supports GCN (Kipf & Welling, 2016), GAT (Veličković et al., 2018), and GraphSage (Hamilton et al., 2017). The readout function currently supported is a simple multilayer perceptron (MLP). Users can easily plug their customized GNN models and readout functions into our framework. For FL algorithms, besides FedAvg (McMahan et al., 2017), other advanced algorithms such as FedOPT (Reddi et al., 2020) and FedGKT (He et al., 2020a) are also supported. GNN algorithms are listed as follows:

- **Graph Convolutional Networks** (Kipf & Welling, 2016) is a GNN model which is a 1st order approximation to spectral GNN models.
- **GraphSAGE** (Hamilton et al., 2017) is a general inductive GNN framework capable of generating node-level representations for unseen data.
- **Graph Attention Networks** (Veličković et al., 2018) is the first attention-based GNN model. Attention is computed in a message-passing fashion.

C.3 FEATURE EXTRACTION PROCEDURE FOR MOLECULES

The feature extraction is in two steps:

1. Atom-level feature extraction and Molecule object construction using RDKit (Landrum, 2006).
2. Constructing graphs from molecule objects using NetworkX (Hagberg et al., 2008).
Atom features, shown in Table 3, are the atom features we used exactly same as in (Rong et al., 2020a).

| Features          | Size | Description                                                                 |
|-------------------|------|-----------------------------------------------------------------------------|
| atom type         | 100  | Representation of atom (e.g., C, N, O), by its atomic number                |
| formal charge     | 5    | An integer electronic charge assigned to atom                              |
| number of bonds   | 6    | Number of bonds the atom is involved in                                    |
| chirality         | 5    | Number of bonded hydrogen atoms                                            |
| number of H       | 5    | Number of bonded hydrogen atoms                                            |
| atomic mass       | 1    | Mass of the atom, divided by 100                                           |
| aromaticity       | 1    | Whether this atom is part of an aromatic system                            |
| hybridization     | 5    | SP, SP2, SP3, SP3D, or SP3D2                                               |

Table 3: Atom features

C.4 NON-I.I.D. PARTITION

The alpha value for latent Dirichlet allocation (LDA) in each non-IID graph dataset can be found in Table 1 and 5. The data distribution for each dataset is illustrated in Figure 4.

D MORE EXPERIMENTAL DETAILS

The hyper-parameters reported in Section E are based on the hyper-parameter sweeping (grid search). We further provide the curve of test score (accuracy) during training for each dataset with a specific model. We hope these visualized training results can be an useful reference for future research exploration.

E HYPER-PARAMETERS

| SIDER | BACE | Clintox | BBBP | Tox21 | FreeSolv | ESOL | Lipo | hERG | QM9 |
|-------|------|---------|------|-------|----------|------|------|------|-----|
| Wall-clock Time | GCN | 5m 58s | 4m 57s | 4m 40s | 4m 13s | 15m 3s | 4m 12s | 5m 25s | 16m 14s | 35m 30s | 6h 48m | 6h 48m |
| GAT   | 8m 48s | 5m 27s | 7m 37s | 5m 28s | 25m 49s | 6m 24s | 8m 36s | 25m 28s | 58m 14s | 9h 23m | 9h 23m |
| GraphSAGE | 4m 42s | 4m 26s | 3m 26s | 14m 31s | 5m 53s | 6m 54s | 15m 28s | 32m 57s | 5h 33m |

| Average FLOP | GCN | 697.3K | 605.1K | 466.2K | 427.2K | 345.8K | 142.6K | 231.6K | 480.6K | 516.6K | 153.9K |
| GAT   | 703.4K | 612.1K | 470.2K | 413K | 347.8K | 142.5K | 232.6K | 485K | 521.3K | 154.3K |
| GraphSAGE | 846K | 758.6K | 1.1M | 980K | 760.6K | 326.9K | 531.1K | 1.5M | 1.184M | 338.2K |

| Parameters | GCN | 15.1K | 13.5K | 13.5K | 14.2K | 13.5K | 13.5K | 13.5K | 13.5K | 14.2K |
| GAT   | 20.2K | 18.5K | 18.6K | 18.5K | 18.5K | 18.5K | 18.5K | 18.5K | 18.5K |
| GraphSAGE | 10.6K | 8.9K | 18.2K | 18.1K | 18.8K | 18.1K | 18.1K | 18.1K | 18.1K |

*Note that we use the distributed training paradigm where each client’s local training uses one GPU. Please refer our code for details.
For each task, we utilize grid search to find the best results. Table 6 & 7 lists all the hyper-parameters range used in our experiments. All hyper-parameter tuning is run on a single GPU. The best hyper-parameters for each dataset and model Table 8, 9, 10, & 11 For molecule tasks, batch-size is kept fixed since the molecule-level task requires us to have mini-batch is equal to 1. Also, number of GNN layers were fixed to 2 because having too many GNN layers result in over-smoothing phenomenon as shown in (Li et al., 2018). For all experiments, we used Adam optimizer.
### Table 5: Regression results (lower is better)

| Dataset  | Non-I.I.D. Partition Method | GNN Model | Federated Optimizer | Performance Metric | MoleculeNet Score for Centralized Training | MoleculeNet Score for Federated Training |
|----------|-----------------------------|-----------|---------------------|--------------------|------------------------------------------|-----------------------------------------|
| FreeSolv | LDA with $\alpha = 0.5$     | GCN       | FedAvg              | RMSE               | 1.5787                                   | 2.7470 (↑ 1.1683)                       |
|          | 4 clients                   | GraphSAGE |                     |                    | 1.2175                                   | 3.1080 (↑ 1.8905)                       |
| ESOL     | LDA with $\alpha = 2$       | GCN       | FedAvg              | RMSE               | 0.97 ± 0.01                              | 1.1690 (↑ 0.1916)                       |
|          | 4 clients                   | GraphSAGE |                     |                    | 0.9358                                   | 1.3740 (↑ 0.4382)                       |
| Lipo     | LDA with $\alpha = 2$       | GCN       | FedAvg              | RMSE               | 0.655 ± 0.036                            | 0.7078 (↑ 0.0523)                       |
|          | 8 clients                   | GraphSAGE |                     |                    | 0.7465                                   | 1.0040 (↑ 0.2575)                       |
| hERG     | LDA with $\alpha = 3$       | GCN       | FedAvg              | RMSE               | -                                        | 0.7257 (↑ 0.0087)                       |
|          | 8 clients                   | GraphSAGE |                     |                    | 0.6621                                   | 0.7322 (↑ 0.0101)                       |
| QM9      | LDA with $\alpha = 3$       | GCN       | FedAvg              | MAE                | 2.35                                     | 13.06 (↑ 10.7173)                       |
|          | 8 clients                   | GraphSAGE |                     |                    | 12.44                                    | 19.167 (↑ 6.707)                        |

*Note: to reproduce the result, please use the same random seeds we set in the library.*

### Table 6: Hyper-parameter Range for Centralized Training

| hyper-parameter       | Description                                           | Range                      |
|-----------------------|-------------------------------------------------------|----------------------------|
| learning rate         | Rate of speed at which the model learns.              | [0.00015, 0.0015, 0.015, 0.15] |
| dropout rate          | Dropout ratio                                         | [0.0, 0.2, 0.3, 0.5, 0.6]   |
| node embedding dimension | Dimensionality of the node embedding               | [16, 32, 64, 128, 256]     |
| hidden layer dimension | Hidden layer dimensionality                           | [16, 32, 64, 128, 256]     |
| readout embedding dimension | Dimensionality of the readout embedding | [16, 32, 64, 128, 256]     |
| graph embedding dimension | Dimensionality of the graph embedding              | [16, 32, 64, 128, 256]     |
| attention heads       | Number of attention heads required for GAT            | 1-7                        |
| alpha                 | LeakyRELU parameter used in GAT model                 | 0.2                        |

### Table 7: Hyper-parameter Range for Federated Learning

| hyper-parameter       | Description                                           | Range                       |
|-----------------------|-------------------------------------------------------|-----------------------------|
| learning rate         | Rate of speed at which the model learns.              | [0.00015, 0.0015, 0.015, 0.15] |
| dropout rate          | Dropout ratio                                         | [0.3, 0.5, 0.6]             |
| node embedding dimension | Dimensionality of the node embedding               | 64                          |
| hidden layer dimension | Hidden layer dimensionality                           | 64                          |
| readout embedding dimension | Dimensionality of the readout embedding | 64                          |
| graph embedding dimension | Dimensionality of the graph embedding              | 64                          |
| attention heads       | Number of attention heads required for GAT            | 1-7                        |
| alpha                 | LeakyRELU parameter used in GAT model                 | 0.2                        |
| rounds                | Number of federating learning rounds                  | [10, 50, 100]              |
| epoch                 | Epoch of clients                                      | 1                          |
| number of clients     | Number of users in a federated learning round         | 4-10                       |
### Table 8: Hyperparameters for Molecular Classification Task

| Dataset | ROC-AUC Score | Score & Parameters | GCN | GAT | GraphSAGE |
|---------|---------------|--------------------|-----|-----|-----------|
| BBBP    | 0.8705        | learning rate      | 0.0015 | 0.015 | 0.01 |
|         |               | dropout rate       | 0.2  | 0.5  | 0.2 |
|         |               | node embedding dimension | 64  | 64  | 64 |
|         |               | hidden layer dimension | 64  | 64  | 64 |
|         |               | readout embedding dimension | 64  | 64  | 64 |
|         |               | graph embedding dimension | 64  | 64  | 64 |
|         |               | attention heads    | None | 2    | None |
|         |               | alpha              | None | 0.2  | None |
| BACE    | 0.9221        | learning rate      | 0.0015 | 0.001 | 0.0015 |
|         |               | dropout rate       | 0.3  | 0.3  | 0.3 |
|         |               | node embedding dimension | 64  | 64  | 16 |
|         |               | hidden layer dimension | 64  | 64  | 64 |
|         |               | readout embedding dimension | 64  | 64  | 64 |
|         |               | graph embedding dimension | 64  | 64  | 64 |
|         |               | attention heads    | None | 2    | None |
|         |               | alpha              | None | 0.2  | None |
| Tox21   | 0.7800        | learning rate      | 0.0015 | 0.00015 | 0.00015 |
|         |               | dropout rate       | 0.4  | 0.3  | 0.3 |
|         |               | node embedding dimension | 64  | 128  | 256 |
|         |               | hidden layer dimension | 64  | 64  | 128 |
|         |               | readout embedding dimension | 64  | 128  | 256 |
|         |               | graph embedding dimension | 64  | 64  | 128 |
|         |               | attention heads    | None | 2    | None |
|         |               | alpha              | None | 0.2  | None |
| SIDER   | 0.6476        | learning rate      | 0.0015 | 0.0015 | 0.0015 |
|         |               | dropout rate       | 0.3  | 0.3  | 0.3 |
|         |               | node embedding dimension | 64  | 64  | 16 |
|         |               | hidden layer dimension | 64  | 64  | 64 |
|         |               | readout embedding dimension | 64  | 64  | 64 |
|         |               | graph embedding dimension | 64  | 64  | 64 |
|         |               | attention heads    | None | 2    | None |
|         |               | alpha              | None | 0.2  | None |
| ClinTox | 0.8914        | learning rate      | 0.0015 | 0.0015 | 0.0015 |
|         |               | dropout rate       | 0.3  | 0.3  | 0.3 |
|         |               | node embedding dimension | 64  | 64  | 64 |
|         |               | hidden layer dimension | 64  | 64  | 64 |
|         |               | readout embedding dimension | 64  | 64  | 64 |
|         |               | graph embedding dimension | 64  | 64  | 64 |
|         |               | attention heads    | None | 2    | None |
|         |               | alpha              | None | 0.2  | None |
Table 9: Hyperparameters for Federated Molecular Classification Task

| Dataset | Score & Parameters | GCN + FedAvg | GAT + FedAvg | GraphSAGE + FedAvg |
|---------|-------------------|--------------|--------------|-------------------|
| BBBP    | ROC-AUC Score     | 0.7629       | 0.8746       | **0.8935**        |
|         | number of clients | 4            | 4            | 4                 |
|         | learning rate     | 0.0015       | 0.0015       | 0.015             |
|         | dropout rate      | 0.3          | 0.3          | 0.6               |
|         | Node Embedding Dimension | 64 | 64 | 64 |
|         | Hidden Layer Dimension | 64 | 64 | 64 |
|         | Readout Embedding Dimension | 64 | 64 | 64 |
|         | Graph Embedding Dimension | 64 | 64 | 64 |
|         | attention heads   | None         | 2            | None              |
|         | alpha             | None         | 0.2          | None              |
|         | ROC-AUC Score     | 0.6594       | 0.7629       | **0.8604**        |
| BACE    | Number of Clients | 4            | 4            | 4                 |
|         | Learning Rate     | 0.0015       | 0.0015       | 0.0015            |
|         | Dropout Rate      | 0.5          | 0.3          | 0.6               |
|         | Node Embedding Dimension | 64 | 1.05 ± 0.10 | 16 |
|         | Hidden Layer Dimension | 64 | 1.05 ± 0.10 | 64 |
|         | Readout Embedding Dimension | 64 | 1.05 ± 0.10 | 64 |
|         | Graph Embedding Dimension | 64 | 1.05 ± 0.10 | 64 |
|         | attention heads   | None         | 2            | None              |
|         | alpha             | None         | 0.2          | None              |
|         | ROC-AUC Score     | 0.7128       | 0.7714       | **0.7801**        |
| Tox21   | Number of Clients | 4            | 4            | 4                 |
|         | Learning Rate     | 0.0015       | 0.15         | 0.0015            |
|         | Dropout Rate      | 0.6          | 0.6          | 0.3               |
|         | Node Embedding Dimension | 64 | 64 | 64 |
|         | Hidden Layer Dimension | 64 | 64 | 64 |
|         | Readout Embedding Dimension | 64 | 64 | 64 |
|         | Graph Embedding Dimension | 64 | 64 | 64 |
|         | attention heads   | None         | 2            | None              |
|         | alpha             | None         | 0.2          | None              |
|         | ROC-AUC Score     | 0.6266       | 0.6591       | **0.67**          |
| SIDER   | Number of Clients | 4            | 4            | 4                 |
|         | Learning Rate     | 0.0015       | 0.0015       | 0.0015            |
|         | Dropout Rate      | 0.6          | 0.3          | 0.6               |
|         | Node Embedding Dimension | 64 | 64 | 16 |
|         | Hidden Layer Dimension | 64 | 64 | 64 |
|         | Readout Embedding Dimension | 64 | 64 | 64 |
|         | Graph Embedding Dimension | 64 | 64 | 64 |
|         | attention heads   | None         | 2            | None              |
|         | alpha             | None         | 0.2          | None              |
|         | ROC-AUC Score     | 0.8784       | 0.9160       | **0.9246**        |
| ClinTox | Number of Clients | 4            | 4            | 4                 |
|         | Learning Rate     | 0.0015       | 0.0015       | 0.015             |
|         | Dropout Rate      | 0.3          | 0.6          | 0.3               |
|         | Node Embedding Dimension | 64 | 64 | 64 |
|         | Hidden Layer Dimension | 64 | 64 | 64 |
|         | Readout Embedding Dimension | 64 | 64 | 64 |
|         | Graph Embedding Dimension | 64 | 64 | 64 |
|         | attention heads   | None         | 2            | None              |
|         | alpha             | None         | 0.2          | None              |
| Dataset         | Score & Parameters | GCN | GAT | GraphSAGE |
|-----------------|--------------------|-----|-----|-----------|
| Freesolv        | RMSE Score         | 0.8705 | 0.8824 | **0.8930** |
|                 | learning rate      | 0.0015 | 0.015 | 0.01 |
|                 | dropout rate       | 0.2 | 0.5 | 0.2 |
|                 | node embedding dimension | 64 | 64 | 64 |
|                 | hidden layer dimension | 64 | 64 | 64 |
|                 | readout embedding dimension | 64 | 64 | 64 |
|                 | graph embedding dimension | 64 | 64 | 64 |
|                 | attention heads    | None | 2 | None |
|                 | alpha              | None | 0.2 | None |
| ESOL            | RMSE Score         | 0.8705 | 0.8824 | **0.8930** |
|                 | learning rate      | 0.0015 | 0.015 | 0.01 |
|                 | dropout rate       | 0.2 | 0.5 | 0.2 |
|                 | node embedding dimension | 64 | 64 | 64 |
|                 | hidden layer dimension | 64 | 64 | 64 |
|                 | readout embedding dimension | 64 | 64 | 64 |
|                 | graph embedding dimension | 64 | 64 | 64 |
|                 | attention heads    | None | 2 | None |
|                 | alpha              | None | 0.2 | None |
| Lipophilicity   | RMSE Score         | 0.8521 | 0.7415 | **0.7078** |
|                 | learning rate      | 0.0015 | 0.001 | 0.001 |
|                 | dropout rate       | 0.3 | 0.3 | 0.3 |
|                 | node embedding dimension | 128 | 128 | 128 |
|                 | hidden layer dimension | 64 | 64 | 64 |
|                 | readout embedding dimension | 128 | 128 | 128 |
|                 | graph embedding dimension | 64 | 64 | 64 |
|                 | attention heads    | None | 2 | None |
|                 | alpha              | None | 0.2 | None |
| hERG            | RMSE Score         | 0.7257 | **0.6271** | 0.7132 |
|                 | learning rate      | 0.001 | 0.001 | 0.005 |
|                 | dropout rate       | 0.3 | 0.5 | 0.3 |
|                 | node embedding dimension | 64 | 64 | 64 |
|                 | hidden layer dimension | 64 | 64 | 64 |
|                 | readout embedding dimension | 64 | 64 | 64 |
|                 | graph embedding dimension | 64 | 64 | 64 |
|                 | attention heads    | None | 2 | None |
|                 | alpha              | None | 0.2 | None |
| QM9             | RMSE Score         | 14.78 | **12.44** | 13.06 |
|                 | learning rate      | 0.0015 | 0.015 | 0.01 |
|                 | dropout rate       | 0.2 | 0.5 | 0.2 |
|                 | node embedding dimension | 64 | 64 | 64 |
|                 | hidden layer dimension | 64 | 64 | 64 |
|                 | readout embedding dimension | 64 | 64 | 64 |
|                 | graph embedding dimension | 64 | 64 | 64 |
|                 | attention heads    | None | 2 | None |
|                 | alpha              | None | 0.2 | None |
### Table 11: Hyperparameters for Federated Molecular Regression Task

| Dataset         | Parameters                  | GCN + FedAvg | GAT + FedAvg | GraphSAGE + FedAvg |
|-----------------|-----------------------------|--------------|--------------|-------------------|
|                 | RMSE Score                  | 2.747        | 3.508        | 1.641             |
| FreeSolv        | Number of Clients           | 4            | 8            | 4                 |
|                 | learning rate               | 0.0015       | 0.00015      | 0.015             |
|                 | dropout rate                | 0.6          | 0.3          | 0.6               |
|                 | node embedding dimension    | 64           | 256          | 64                |
|                 | hidden layer dimension      | 64           | 128          | 64                |
|                 | readout embedding dimension | 64           | 256          | 64                |
|                 | graph embedding dimension   | 64           | 64           | 64                |
|                 | attention heads             | None         | 2            | None              |
|                 | alpha                       | None         | 0.2          | None              |
| ESOL            | RMSE Score                  | 1.435        | 1.374        | 1.185             |
|                 | Number of Clients           | 4            | 4            | 4                 |
|                 | learning rate               | 0.0015       | 0.0015       | 0.0015            |
|                 | dropout rate                | 0.3          | 0.3          | 0.3               |
|                 | node embedding dimension    | 64           | 256          | 64                |
|                 | hidden layer dimension      | 64           | 128          | 64                |
|                 | readout embedding dimension | 64           | 256          | 64                |
|                 | graph embedding dimension   | 64           | 64           | 64                |
|                 | attention heads             | None         | 2            | None              |
|                 | alpha                       | None         | 0.2          | None              |
| Lipophilicity   | RMSE Score                  | 1.146        | 1.004        | 0.7788            |
|                 | Number of Clients           | 4            | 4            | 4                 |
|                 | learning rate               | 0.0015       | 0.0015       | 0.0015            |
|                 | dropout rate                | 0.3          | 0.3          | 0.6               |
|                 | node embedding dimension    | 64           | 256          | 256               |
|                 | hidden layer dimension      | 64           | 128          | 256               |
|                 | readout embedding dimension | 64           | 256          | 256               |
|                 | graph embedding dimension   | 64           | 64           | 256               |
|                 | attention heads             | None         | 2            | None              |
|                 | alpha                       | None         | 0.2          | None              |
| hERG            | RMSE Score                  | 0.7944       | 0.7322       | 0.7265            |
|                 | Number of Clients           | 8            | 8            | 8                 |
|                 | learning rate               | 0.0015       | 0.0015       | 0.0015            |
|                 | dropout rate                | 0.2          | 0.3          | 0.3               |
|                 | node embedding dimension    | 64           | 64           | 64                |
|                 | hidden layer dimension      | 64           | 64           | 64                |
|                 | readout embedding dimension | 64           | 64           | 64                |
|                 | graph embedding dimension   | 64           | 64           | 64                |
|                 | attention heads             | None         | 2            | None              |
|                 | alpha                       | None         | 0.2          | None              |
| QM9             | MAE Score                   | 21.075       | 23.173       | 19.167            |
|                 | Number of Clients           | 8            | 8            | 8                 |
|                 | learning rate               | 0.0015       | 0.00015      | 0.0015            |
|                 | dropout rate                | 0.2          | 0.5          | 0.3               |
|                 | node embedding dimension    | 64           | 256          | 64                |
|                 | hidden layer dimension      | 64           | 128          | 64                |
|                 | readout embedding dimension | 64           | 256          | 64                |
|                 | graph embedding dimension   | 64           | 64           | 64                |
|                 | attention heads             | None         | 2            | None              |
|                 | alpha                       | None         | 0.2          | None              |