# PyGOD: A Python Library for Graph Outlier Detection

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#### Abstract

PyGOD is an open-source Python library for detecting outliers on graph data. As the first comprehensive library of its kind, PyGOD supports a wide array of leading graph-based methods for node-, edge-, subgraph-, and graph-level outlier detection, under a unified, well-documented API designed for use by both researchers and practitioners. To overcome the scalability issue in large graphs, we provide advanced functionalities for selected models, including mini-batch and sampling. PyGOD is equipped with best practices to foster code reliability and maintainability, including unit testing, continuous integration, and code coverage. To foster accessibility, PyGOD is released under a permissive BSD-license at https://github.com/pygod-team/pygod/ and the Python Package Index (PyPI).

**Keywords:** outlier detection, anomaly detection, graph learning, graph neural networks

#### 1. Introduction

Outlier detection (OD), also known as anomaly detection, is a key machine learning task to identify the deviant samples from the general data distribution (Aggarwal, 2017; Li et al., 2022). With the increasing importance of graph data in both research and real-world applications (Ding et al., 2021b; Huang et al., 2021; Fu et al., 2021; Zhou et al., 2021; Xu et al., 2022), detecting outliers with graph-based methods such as graph neural networks (GNNs) recently have drawn much attention (Ma et al., 2021; Ding et al., 2019b, 2021a) with many applications such as detecting suspicious activities in social networks (Sun et al., 2018; Dou et al., 2020) and security systems (Cai et al., 2021).

Although there is a long list of established libraries for detecting outliers in tabular and time-series data in multiple programming languages, e.g., PyOD (Zhao et al., 2019), SUOD (Zhao et al., 2021b), PyODDs (Li et al., 2020), ELKI (Achtert et al., 2010), OutlierDetec-

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Algorithm	Supervision	Level	Backbone	Mini-batch
MLPAE (Sakurada and Yairi, 2014)	Unsupervised	Node	MLP	Yes
GCNAE (Kipf and Welling, 2016)	Unsupervised	Node	GNN	Yes
ONE (Bandyopadhyay et al., 2019)	Unsupervised	Node	MF	No
DOMINANT (Ding et al., 2019a)	Unsupervised	Node	GNN	Yes
DONE (Bandyopadhyay et al., 2020)	Unsupervised	Node	GNN	Yes
AdONE (Bandyopadhyay et al., 2020)	Unsupervised	Node	GNN	Yes
AnomalyDAE (Fan et al., 2020)	Unsupervised	Node	GNN	In progress
GAAN (Chen et al., 2020)	Unsupervised	Node	GAN	Yes
OCGNN (Wang et al., 2021)	Unsupervised	Node	GNN	Yes
GUIDE (Yuan et al., 2021)	Unsupervised	Node	GNN	Yes
CONAD (Xu et al., 2022)	Unsupervised/SSL	Node	GNN	In progress
CoLA (Xu et al., 2022)	Unsupervised/SSL	Node	GNN	In progress

Table 1: Select outlier detection models in PyGOD V0.2.0

tion.jl (Muhr et al., 2022), PyTOD (Zhao et al., 2021a), TODS (Lai et al., 2021), Telemanom (Hundman et al., 2018), a specialized library for graph outlier detection is absent.

To tap this gap, we design the first comprehensive **Py**thon **G**raph **O**utlier **D**etection library called PyGOD, with a couple of key technical advancement and contributions. First, it covers a wide array of algorithms from node to graph level detection, with varying availability of labels/supervision. Table 1 shows that PyGOD already supports more than ten leading algorithms. Second, PyGOD streamlines the accessibility of detection models with a unified API design. From the user perspective, one only needs to prepare the data into a predefined graph format—all outlier detectors in PyGOD are then capable of processing and handling it. Third, PyGOD supports large-scale detection via mini-batch and sampling, which can facilitate detection on large graphs. With code clarity and quality in mind, we offer detailed API documentation and examples, and enable unit testing with cross-platform continuous integration along with code coverage and maintainability checks.

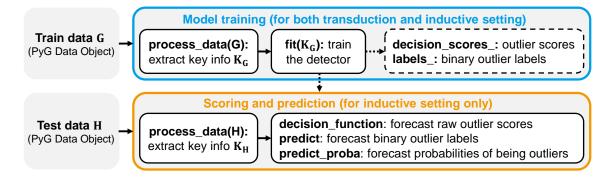


Figure 1: Demonstration of PyGOD's unified API design

### 2. Library Design and Implementation

Dependency. PyGOD builds for Python 3.6+, and depends on popular Pytorch (Paszke et al., 2019) and Pytorch Geometric (PyG) (Fey and Lenssen, 2019) for effective graph learning on both CPUs and GPUs. Additionally, it uses numpy (Harris et al., 2020), scipy (Virtanen et al., 2020), and scikit-learn (Pedregosa et al., 2011) for data manipulation. API Design. Inspired by the API design of scikit-learn (Buitinck et al., 2013) and PyOD (Zhao et al., 2019), all detection algorithms in PyGOD inherit from a base class with the same API interface: (i) fit trains the detection model, gets the outlier scores (the higher, the more outlying) and labels on the input data, and generates necessary statistics for prediction (in the inductive setting); (ii) decision\_function leverages the trained model to predict the raw outlier scores of the incoming data (in the inductive setting); (iii) predict returns the binary prediction using the trained model (0 for normal samples and 1 for outliers); and (iv) predict\_proba returns the probability of samples being outlier using the leading method (Kriegel et al., 2011). Meanwhile, we also include the recent advance in providing the confidence score in outlier detection (Perini et al., 2020) for the above prediction methods. The usage of the above APIs is demonstrated in Code demo 1.

```
from torch_geometric.datasets import Planetoid # import data from PyG
     from pygod.utils import gen_attribute_outliers # import injection func
2
3
     data = Planetoid("Cora")[0]
                                                     # load data in PyG format
4
     data, y = gen_attribute_outliers(data, n=100) # inject outliers
6
     from pygod.models import DOMINANT
                                                     # import the model
     model = DOMINANT(num_layers=2)
                                                     # init. detection model
                                                     # fit with data
     model.fit(data)
LO
     pred_label = model.predict(data)
                                                     # predict binary labels
     pred_scores = model.decision_function(data)
                                                     # predict outlier scores
     pred_proba = model.predict_proba(data)
                                                     # predict probability
13
15
     from pygod.utils.metric import eval_recall_at_k, eval_precision_at_k
     eval_recall_at_k(y.numpy(), pred_scores)
                                                     # eval. by recall
     eval_precision_at_k(y.numpy(), pred_scores)
                                                     # eval. by precision
```

Code demo 1: Using Dominant (Ding et al., 2019a) on Cora data (Morris et al., 2020)

Streamlined Graph Learning with PyG. We choose to develop PyGOD on top of the popular PyG Llibrary for multiple reasons. First, this reduces the complexity in processing graph data for users. That is, PyGOD only requires the input data to be in the standard graph data format in PyG¹. Notably, different detection models need distinct information from a PyG graph. Within the implementation of each detection model, we design an abstract process\_graph method to extract necessary information, e.g., the adjacency matrix, node, and edge attributes, etc., for the underlying detection algorithm. Second, most of the

<sup>1.</sup> PyG data object: https://pytorch-geometric.readthedocs.io/en/latest/modules/data.html

detection algorithms share common backbones (see Table 1) like graph convolutional neural networks (GCN) (Kipf and Welling, 2017) and graph autoencoders (Kipf and Welling, 2016), where PyG already provides optimized implementation. Third, PyG is the most popular GNN libraries with advanced functions like graph sampling and distributed training. Under the PyG framework, we enable and implement mini-batch and/or sampling for selected models to accommodate the learning with large graphs as shown in Table 1.

In addition to the detection models, a set of helpful utility functions is designed to facilitate graph outlier detection. Evaluation-wise, PyGOD provides common metrics for graph OD in the utils.metric module. Data-wise, PyGOD offers outlier injection methods for both structure and attribute settings (Ding et al., 2019a) in utils.outlier\_generator, as a solution to model evaluation and benchmarking.

### 3. Library Robustness and Accessibility

Robustness and Quality. While building PyGOD, we follow the best practices of system design and software development. First, we leverage the continuous integration by *GitHub Actions*<sup>2</sup> to automate the testing process under various Python versions and operating systems. In addition to the scheduled daily test, both commits and pull requests trigger the unit testing. Notably, we enforce all code to have at least 90% coverage<sup>3</sup>. By following the PEP8 standard, we enforce a consistent coding style and naming convention, which facilitates the community collaboration and code readability.

Accessibility. PyGOD comes with detailed API documentation rendered by Read the Docs<sup>4</sup>. Within the documentation, installation guide and interactive examples in Jupyter notebooks are provided. To facilitate community contribution, the project is hosted on GitHub with friendly contribution guide and issue reporting mechanism.

## 4. Conclusion and Future Plans

In this paper, we present the first comprehensive library for graph outlier detection, called PyGOD. Uniquely, it supports a wide range of detection algorithms with unified APIs, rich documentation, and robust code design, which are readily useful for both academic research and industry applications. The development plan of PyGOD will focus on multiple aspects: (i) including more algorithms for different sub-tasks, e.g., outlier detection in edges and sub-graphs; (ii) collaborating with industries to make PyGOD more practical and tailor the needs of practitioners; (iii) optimizing its accessibility and scalability with the latest advancement in graph (Jia et al., 2020); and (iv) incorporate automated machine learning to enable intelligent model selection and hyperparameter tuning (Zhao et al., 2021c).

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<sup>2.</sup> Continuous integration by GitHub Actions: https://github.com/pygod-team/pygod/actions

<sup>3.</sup> Code coverage by Coveralls: https://coveralls.io/github/pygod-team/pygod

<sup>4.</sup> Documentation: https://docs.pygod.org/

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