A Comprehensive Study for Anomaly Detection on Graphs

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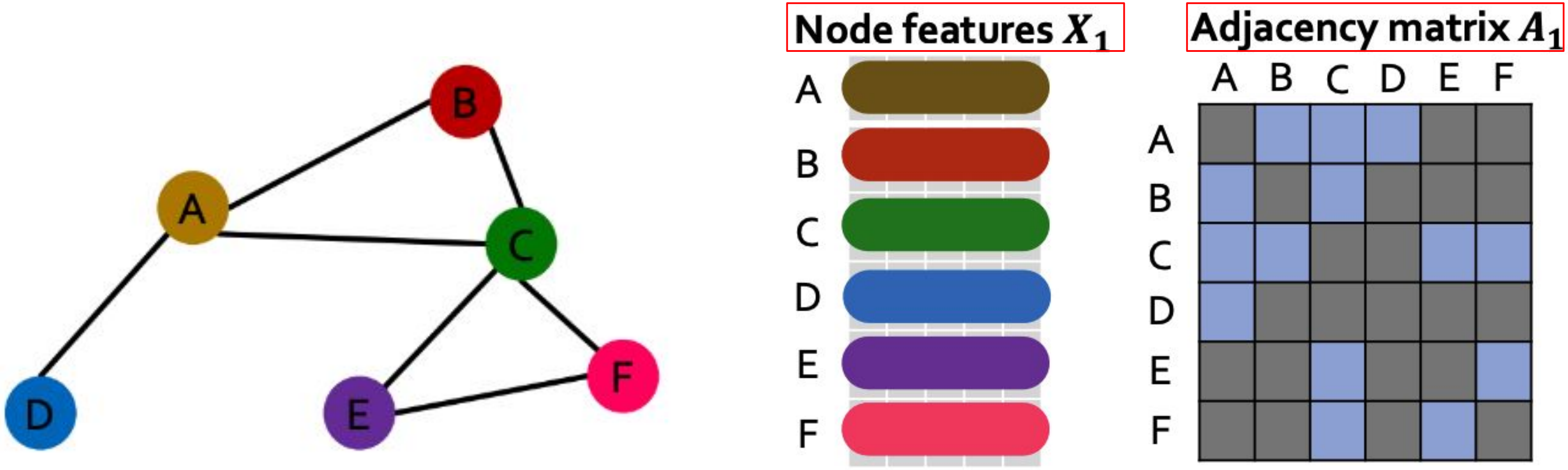
Contributions

Contributions:

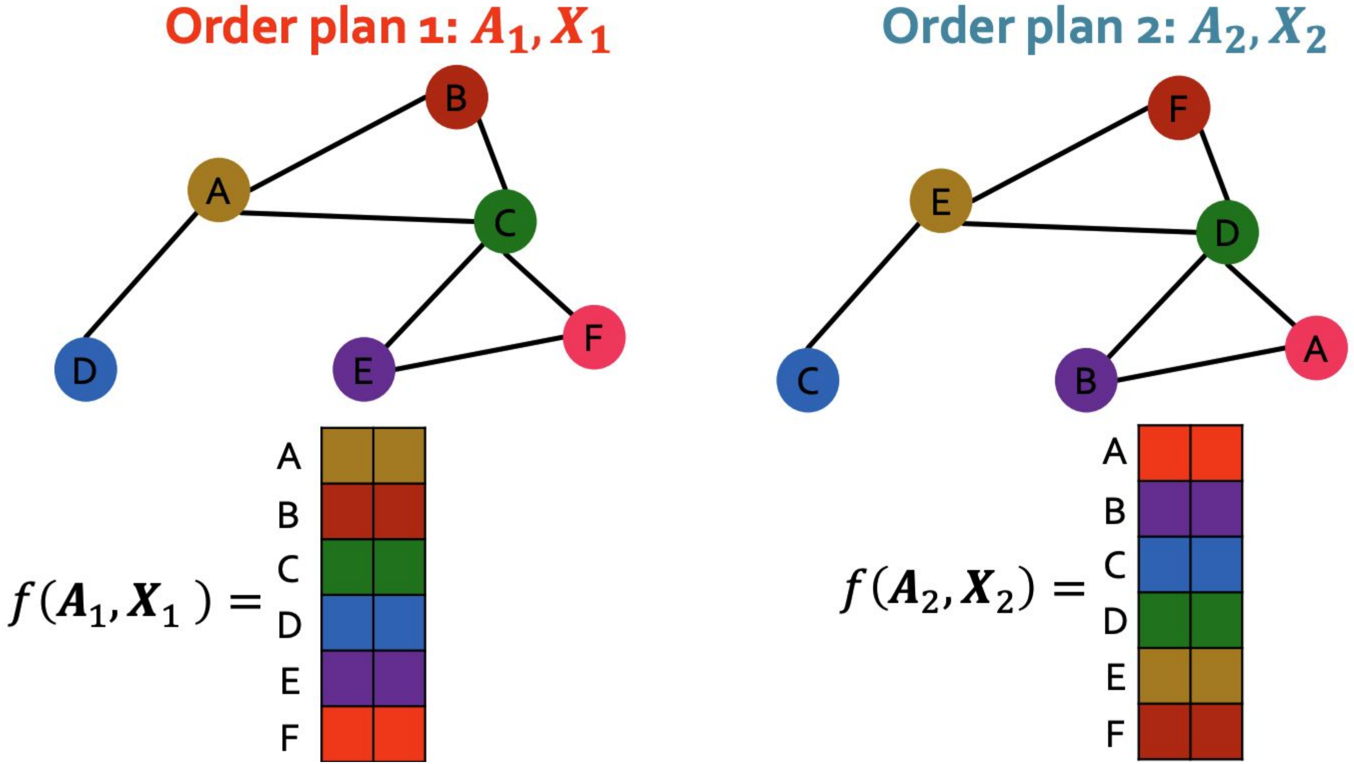
1. Analyze graph anomaly detection frameworks from the perspective of **model architectures**.

2. Analyze graph anomaly detection frameworks from the perspective of **data.**

Background: What is a Graph?



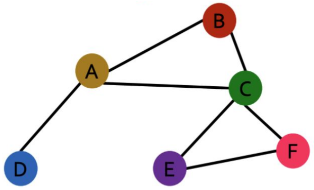
Background: Permutation Equivariance for Learning on Graph

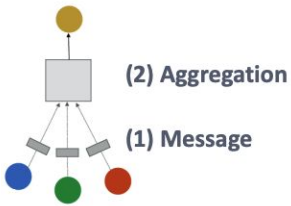


$$f(A_1, X_1) = f(A_2, X_2)$$

f() should be permutation equivariance

Background: Achieve Permutation Equivariance on Architecture





- **(1) Graph Convolutional Networks (GCN)**

$$\mathbf{h}_v^{(l)} = \sigma\left(\mathbf{W}^{(l)} \sum_{u \in N(v)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}\right)$$

- **(2) GraphSAGE**

$$\mathbf{h}_v^{(l)} = \sigma\left(\mathbf{W}^{(l)} \cdot \mathrm{CONCAT}\left(\mathbf{h}_v^{(l-1)}, \mathrm{AGG}\left(\left\{\mathbf{h}_u^{(l-1)}, \forall u \in N(v)\right\}\right)\right)\right)$$

- **(3) Graph Attention Networks**

$$\mathbf{h}_v^{(l)} = \sigma\left(\textstyle\sum_{u \in N(v)} \boxed{\alpha_{vu}} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)}\right)$$

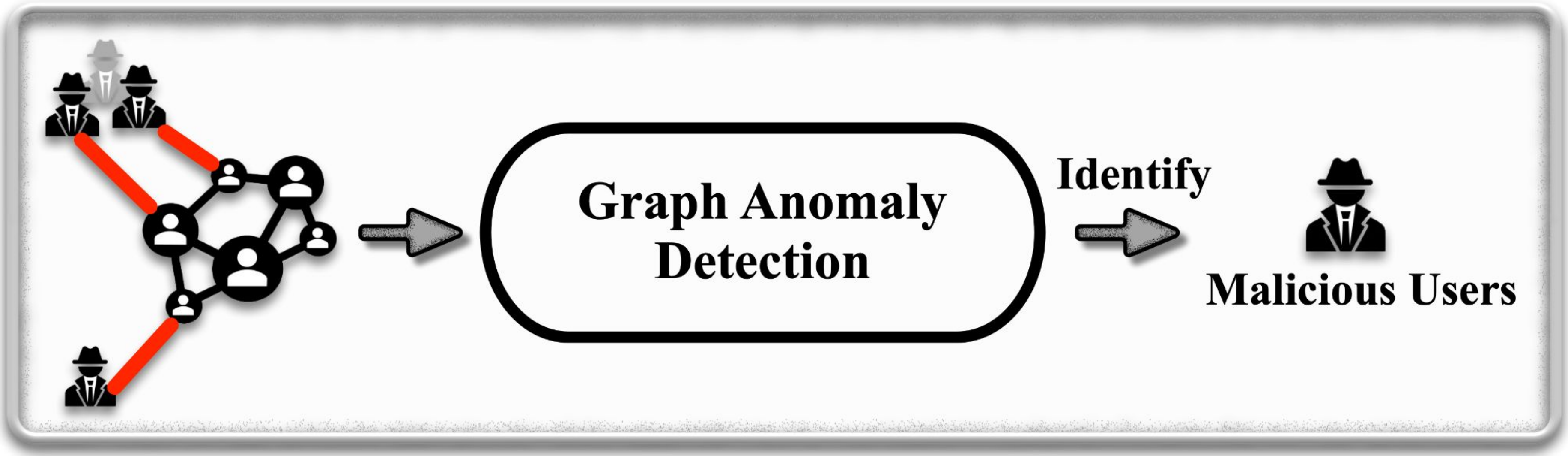
Attention weights

1. Kipf, Thomas N., and Max Welling. "Semi-supervised classification with graph convolutional networks." *arXiv preprint arXiv:1609.02907* (2016).

2. Brody, S., Alon, U., & Yahav, E. (2021). How attentive are graph attention networks?. arXiv preprint arXiv:2105.14491.

3. Hamilton, Will, Zhitao Ying, and Jure Leskovec. "Inductive representation learning on large graphs." Advances in neural information processing systems 30 (2017).

Anomaly Detection on Graph



Application: Filter fake news or malicious users out

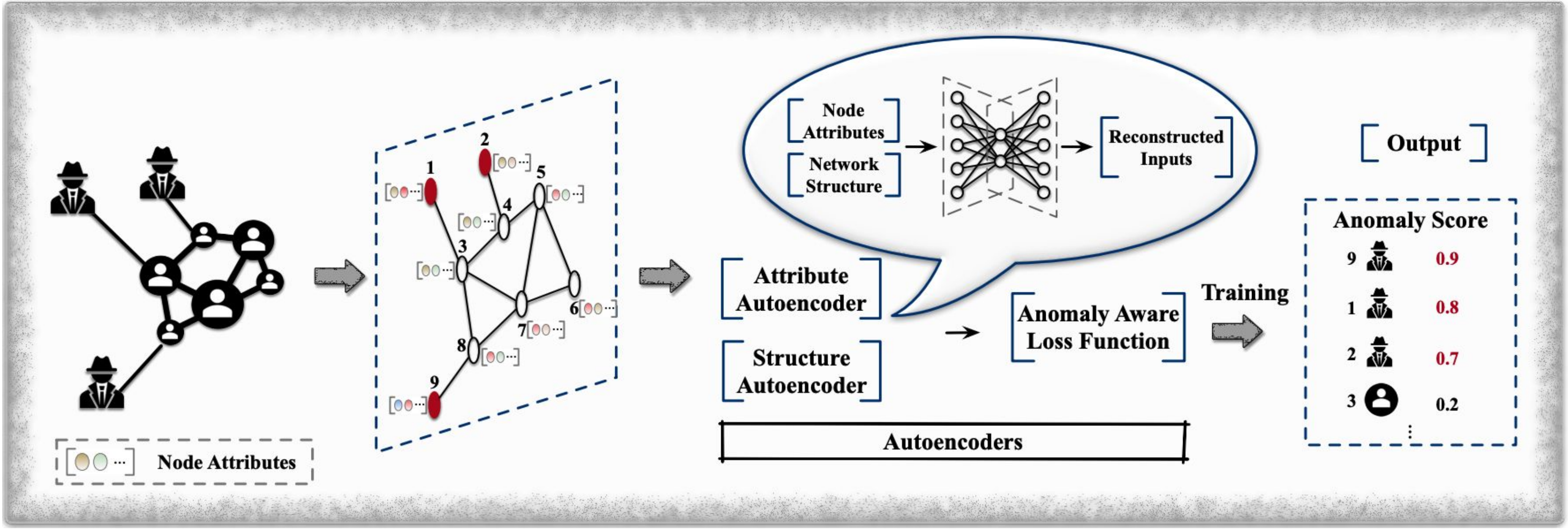
1. Ma, Xiaoxiao, Jia Wu, Shan Xue, Jian Yang, Chuan Zhou, Quan Z. Sheng, Hui Xiong, and Leman Akoglu. "A comprehensive survey on graph anomaly detection with deep learning." IEEE Transactions on Knowledge and Data Engineering 35, no. 12 (2021): 12012-12038.

What are anomalous nodes?

1. Context anomalous nodes:
   a. Anomalous on Node Features.

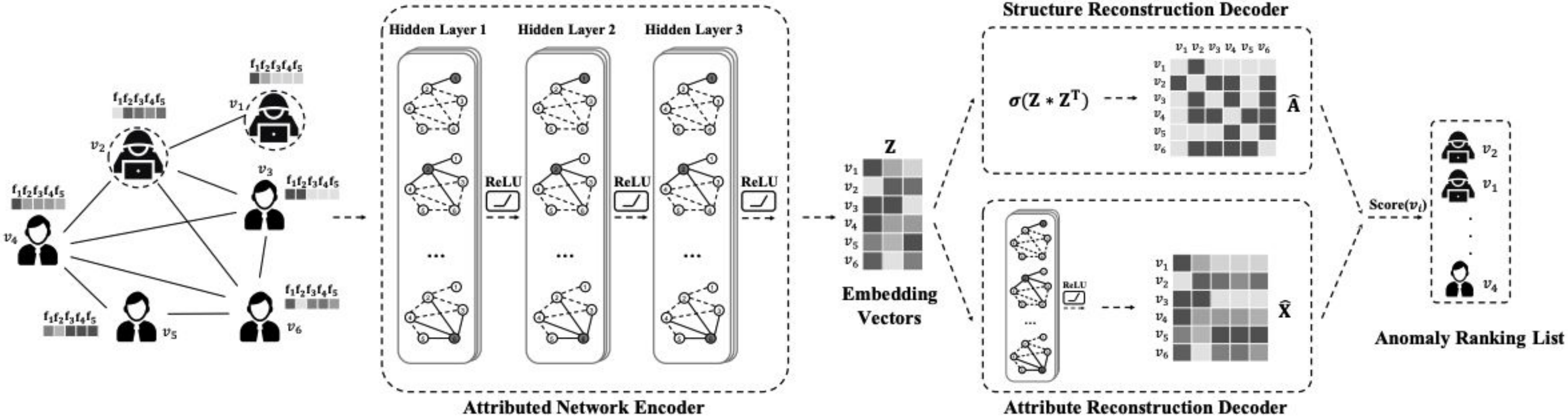
2. Structure anomalous nodes:
   a. Anomalous on the connections with other nodes.

Unified Framework for AD on Graph



Key Motivation: Anomalous nodes are hard to be reconstructed

Baseline: DOMINANT



$$score(\mathbf{v}_i) = (1-\alpha)||\mathbf{a} - \widehat{\mathbf{a}}_i||_2 + \alpha||\mathbf{x}_i - \widehat{\mathbf{x}}_i||_2$$

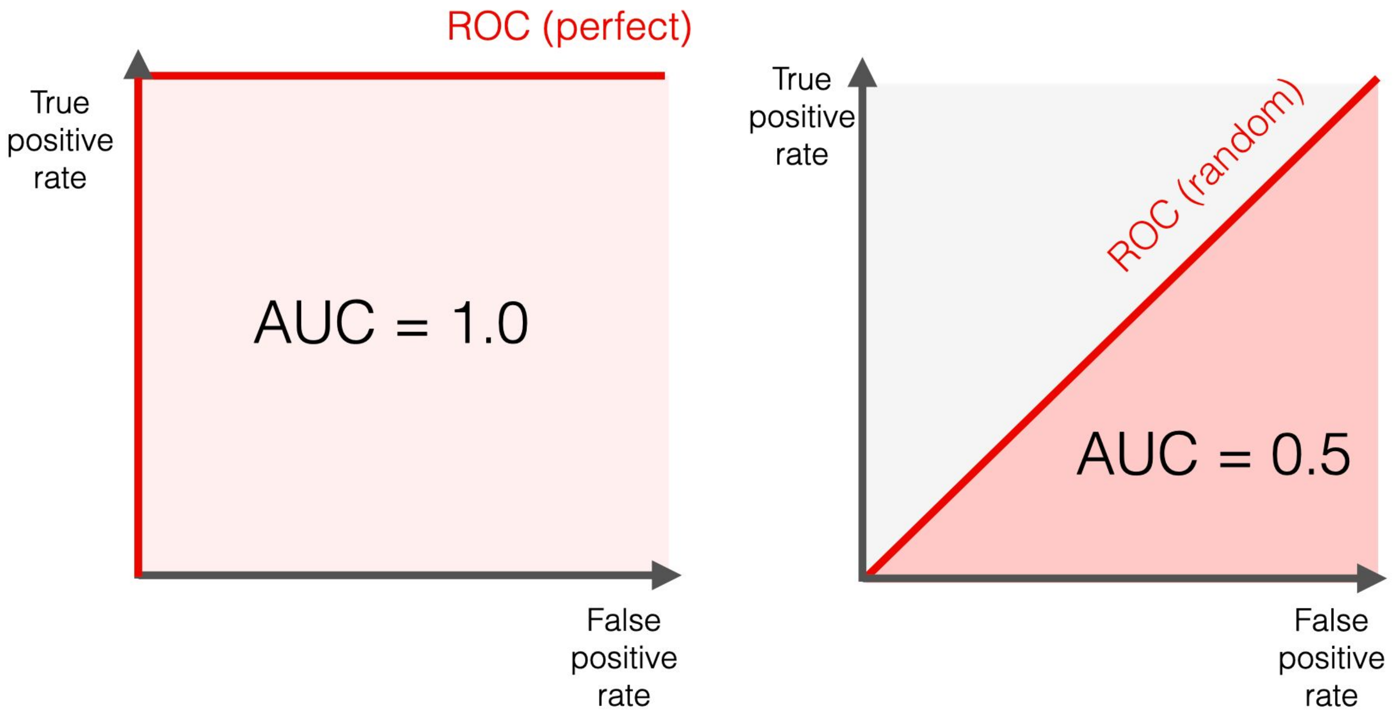
The details of more baselines (e.g. GAE, CoLA) are shown in the appendix

1. Ding, Kaize, et al. "Deep anomaly detection on attributed networks." Proceedings of the 2019 SIAM International Conference on Data Mining. Society for Industrial and Applied Mathematics, 2019.

AD Benchmarks

Dataset	#Nodes	#Edges	#Feat	Avg. Degree	#Outliers	Outlier Ratio
'disney'	124	335	28	2.7	6	4.8%
'books'	1,418	3,695	21	2.6	28	2.0%
'enron'	13,533	176,987	18	13.1	5	0.04%

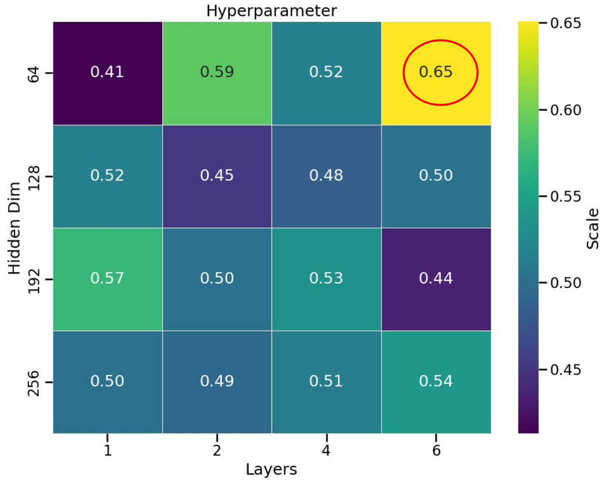
Evaluation Metric: AUC Score

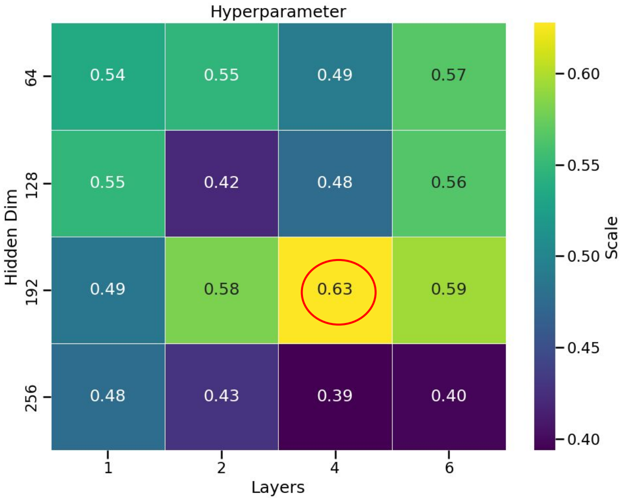


The Effect of Model Architecture - Experimental Setup

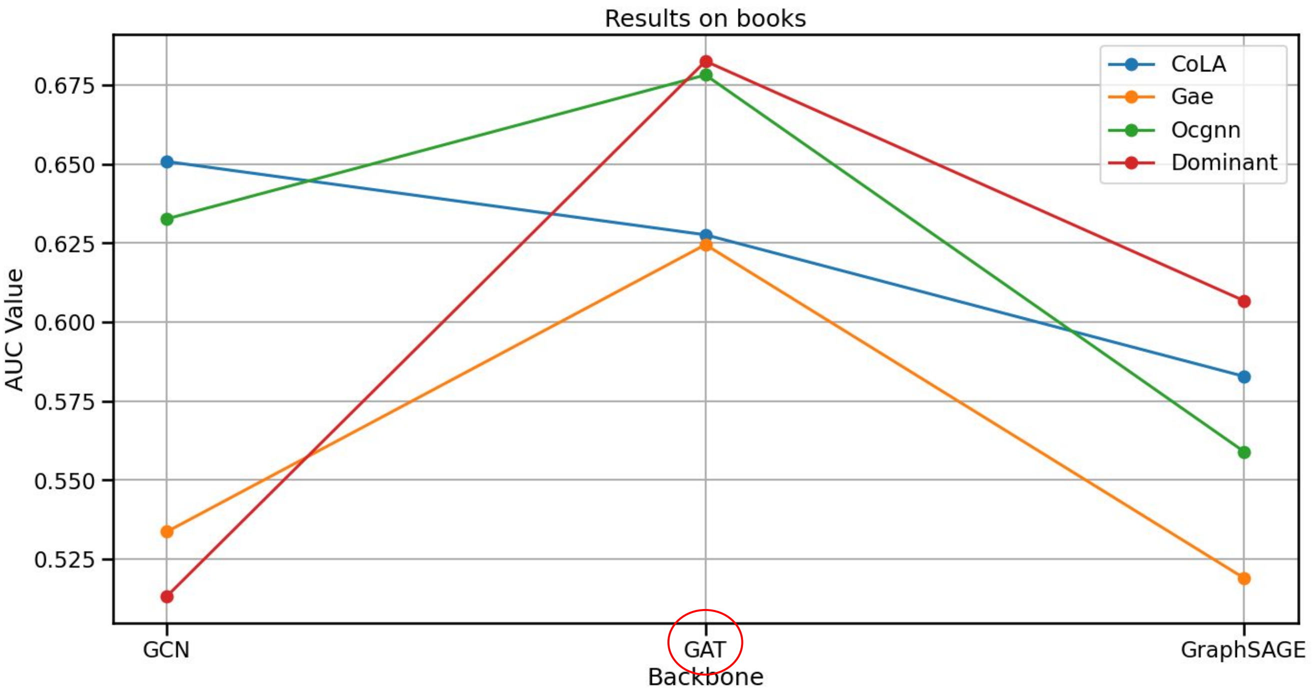
Run different node AD frameworks with different model architectures (backbones). For example, Dominant with GCN.

For each group, I tune the model on two hyperparameters as hidden dimensions and number of layers to find the best results.



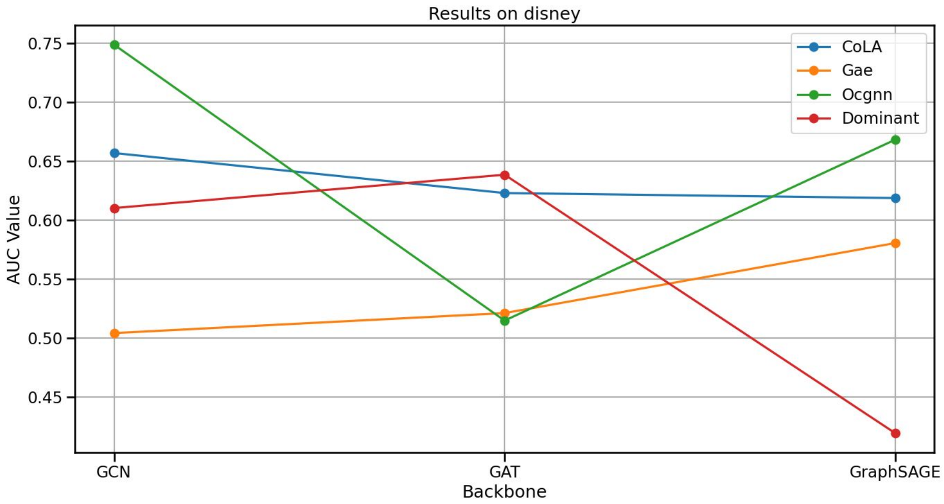


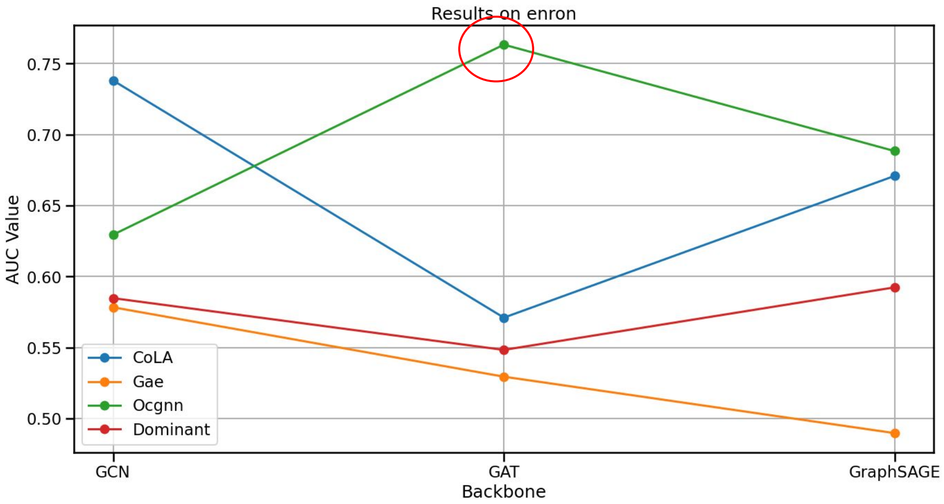
The Effect of Model Architecture



For books data, GAT is the best backbone for all AD frameworks!

The Effect of Model Architectures





1. For disney and enron data, the line is quite fluctuated. There is no dominant backbone on these two datasets.
2. There is a performance gap between Ocgnn with GAT on enron and other methods.

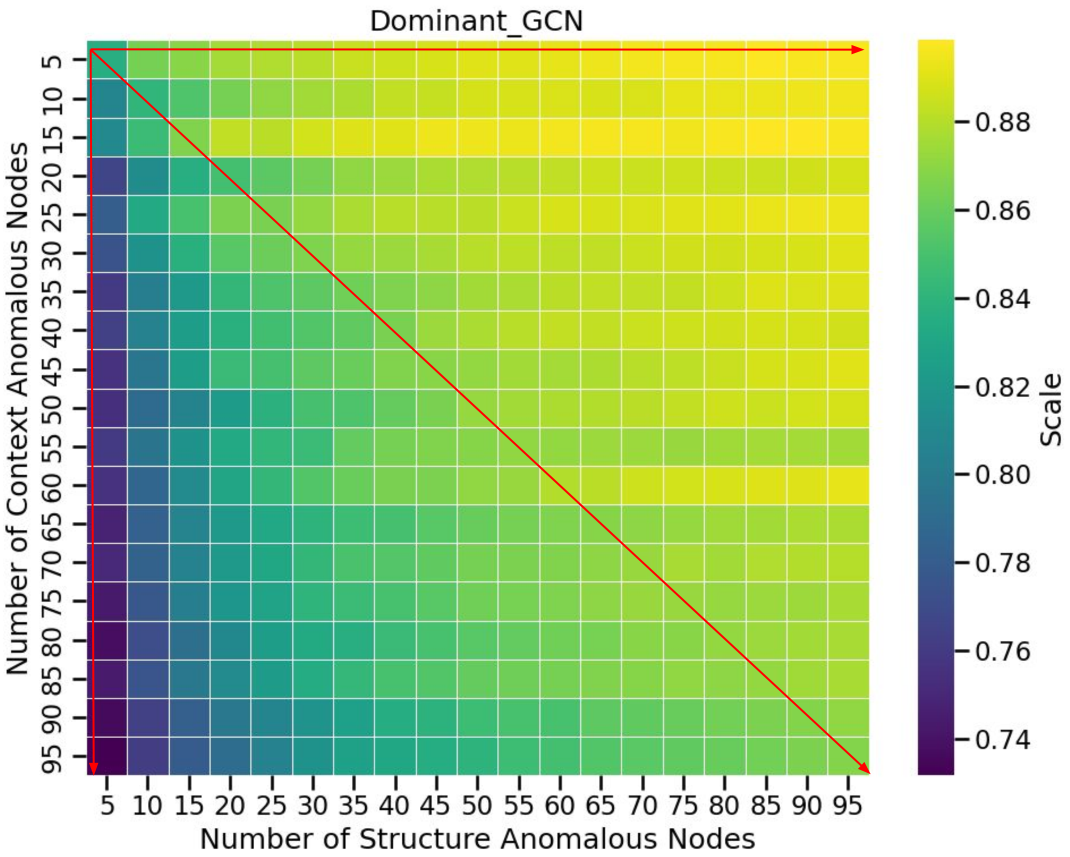
The Effect of Data - Experimental Setup

1. Context anomalous nodes:
   a. Anomalous on Node Features.

2. Structure anomalous nodes:
   a. Anomalous on the connections with other nodes.

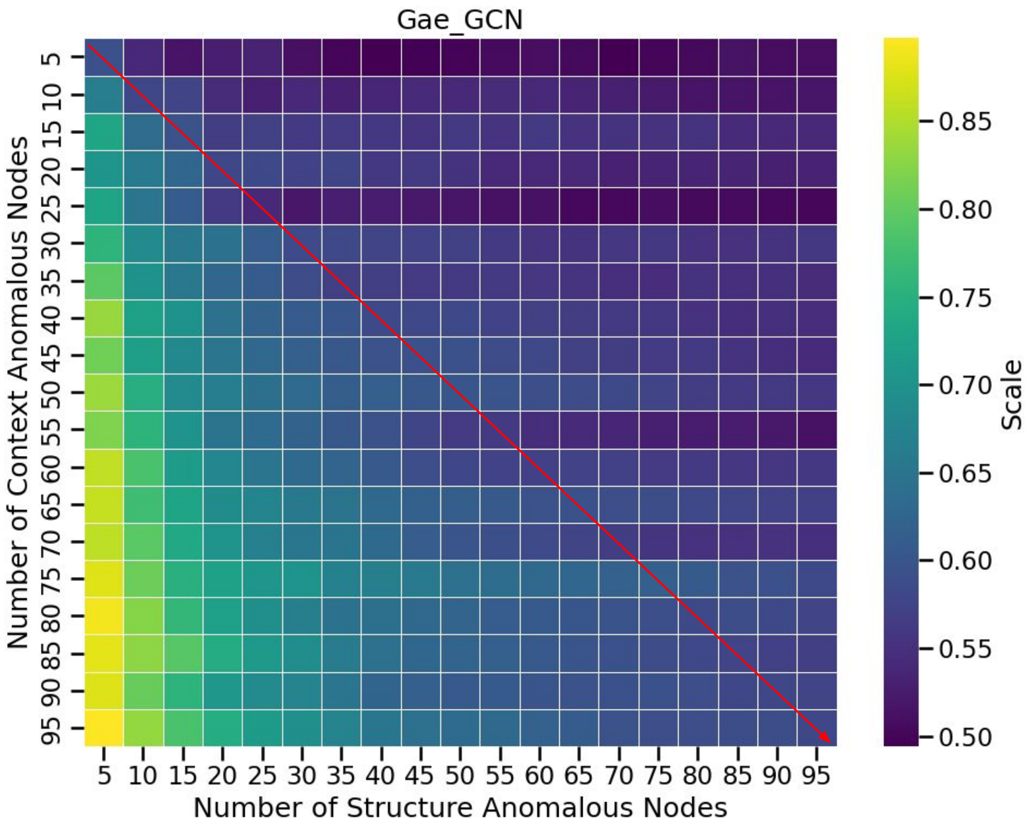
3. I manually add context/structure nodes to the cora dataset.

The Effect of Data



DOMINANT performs well in detecting structure anomalous nodes, but it is not good at handling a large number of context anomalous nodes.

The Effect of Data



GAE can work if and only if:

1. A large number of context anomalous nodes.
2. A small number of structure anomalous nodes

Implementation

Codes for ECE594N Project

Preparation

Create the Environment

```
conda env create -f environment.yml
```

Reproduce the Experimental Results

Results for different model architecures

```
python main_arch.py --save_path <YOUR_PATH_FOR_SAVING>
```

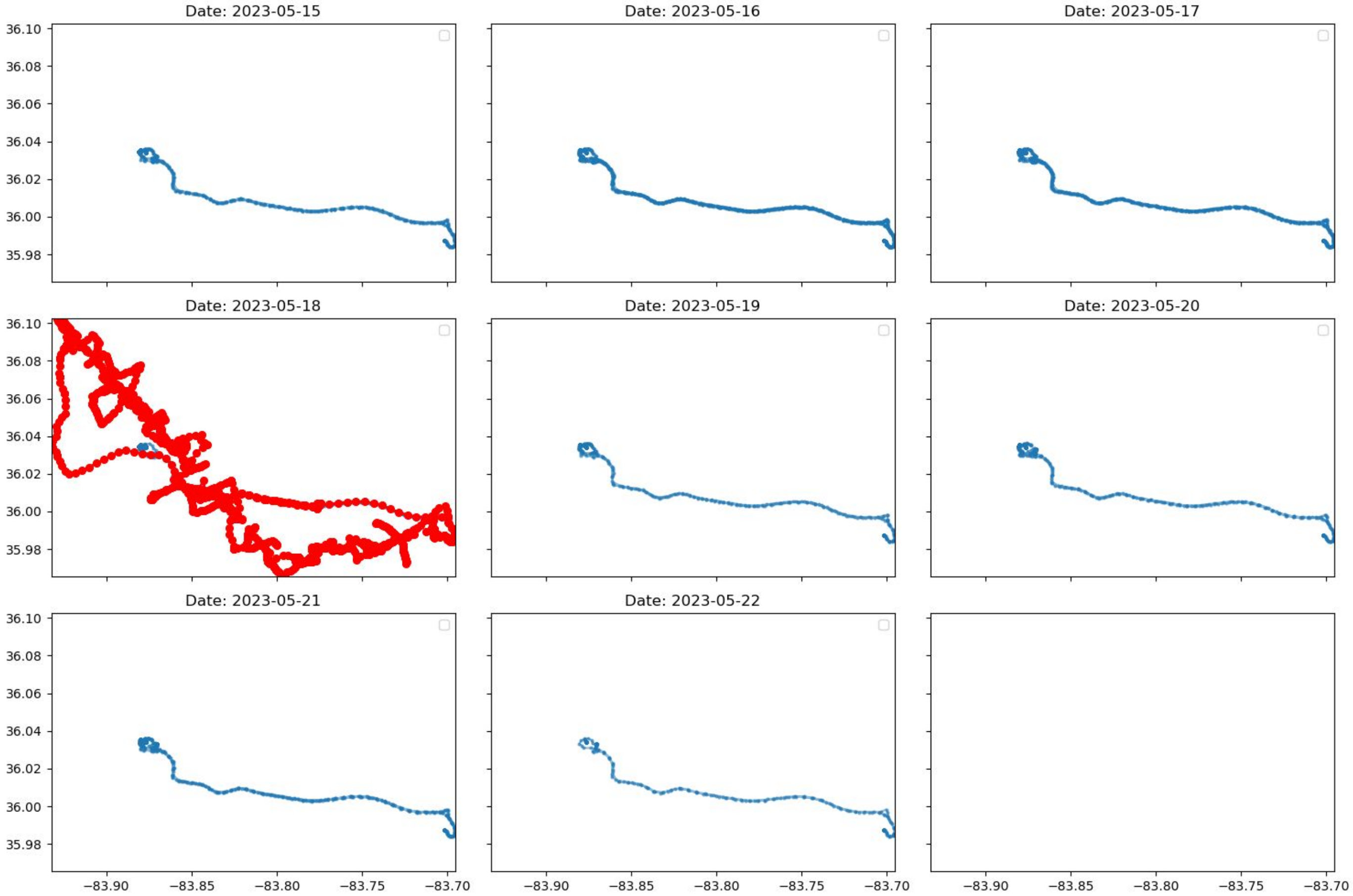
Results for different anomalous data

```
python main_data.py --save_path <YOUR_PATH_FOR_SAVING>
```

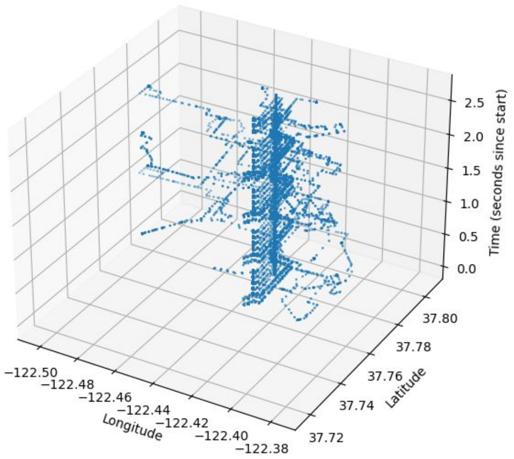
Visualize the Results

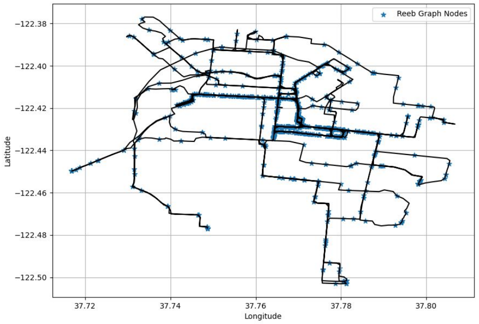
Check vis.ipynb

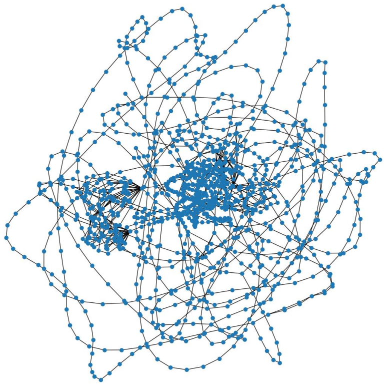
Future Work: Anomaly Detection on Trajectory Data



Future Work: Anomaly Detection on Trajectory Data





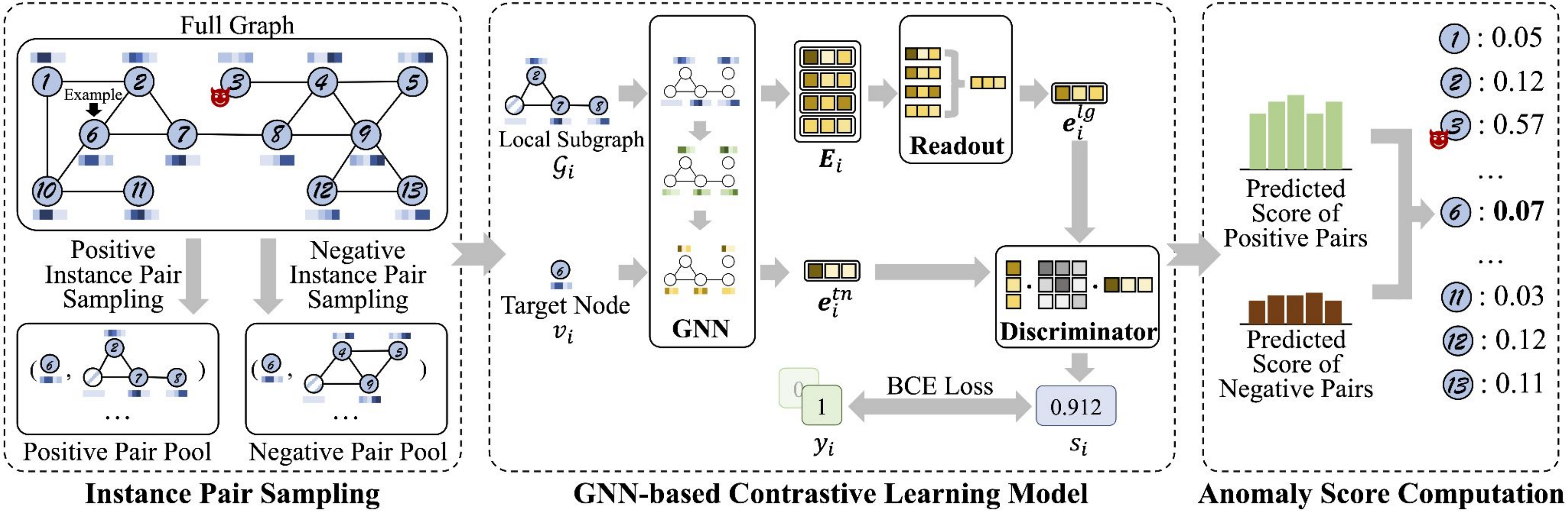


Key Challenge: How to Construct the Graph based on Trajectory.

Thank you for listening!
Q&A

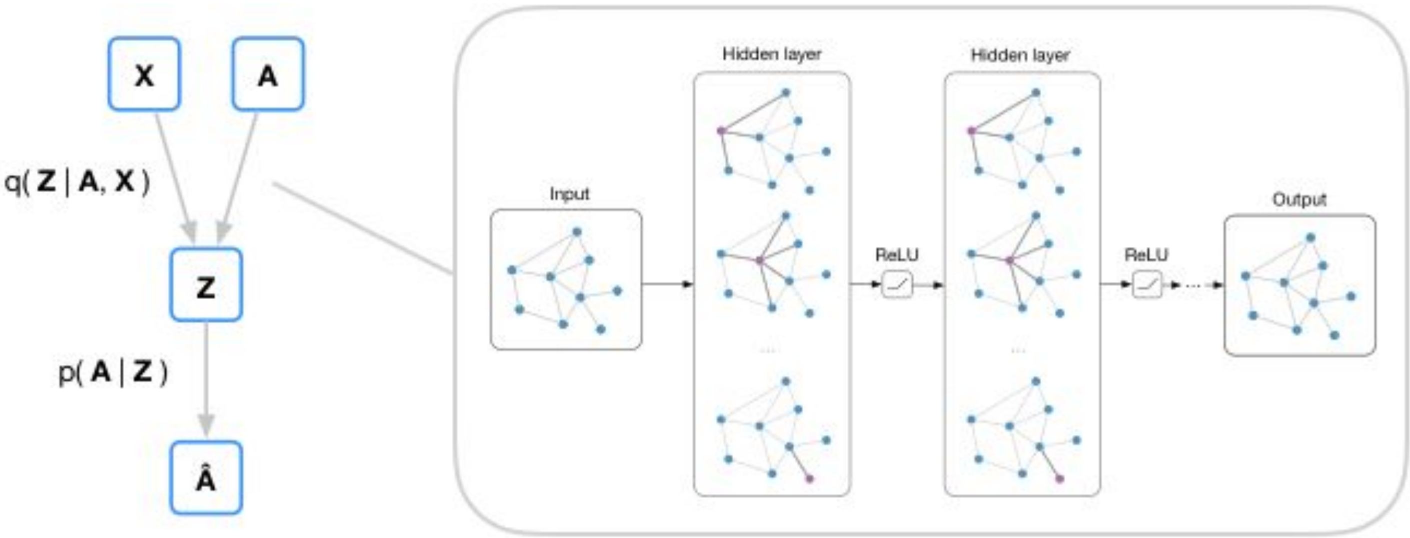
Appendix

Baseline: CoLA



1. Liu, Yixin, et al. "Anomaly detection on attributed networks via contrastive self-supervised learning." IEEE transactions on neural networks and learning systems 33.6 (2021): 2378-2392.

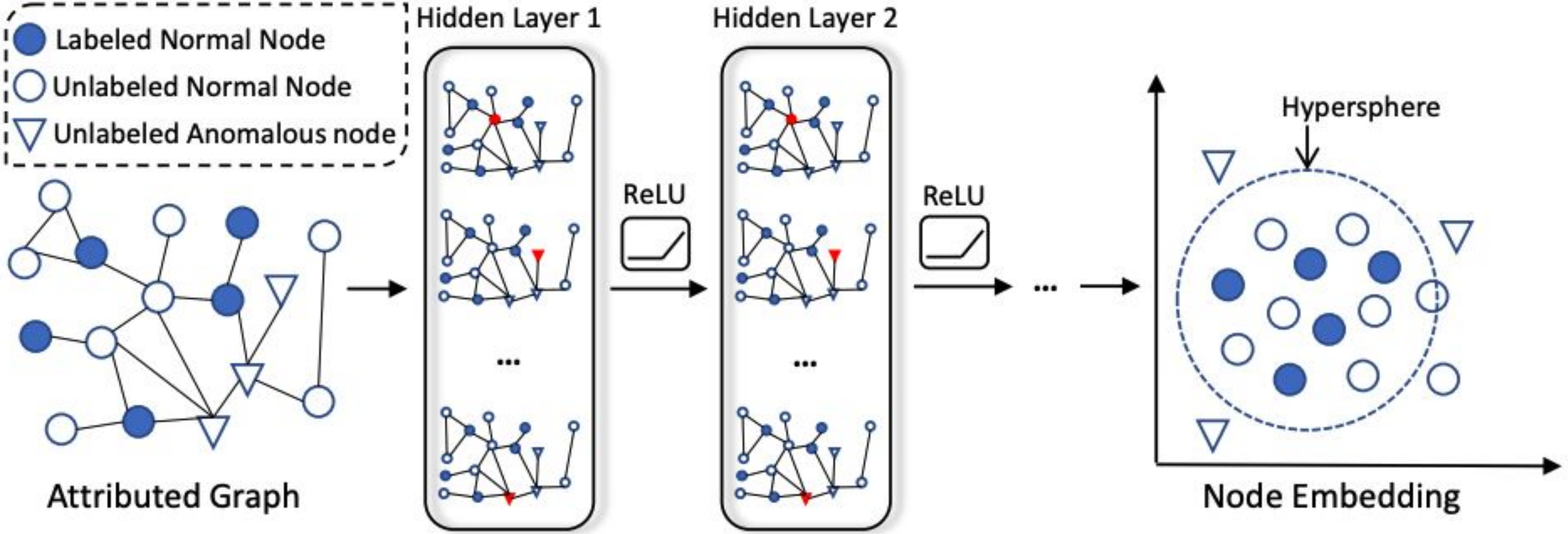
Baseline: GAE



VGAE **Graph Convolutional Network (GCN)**

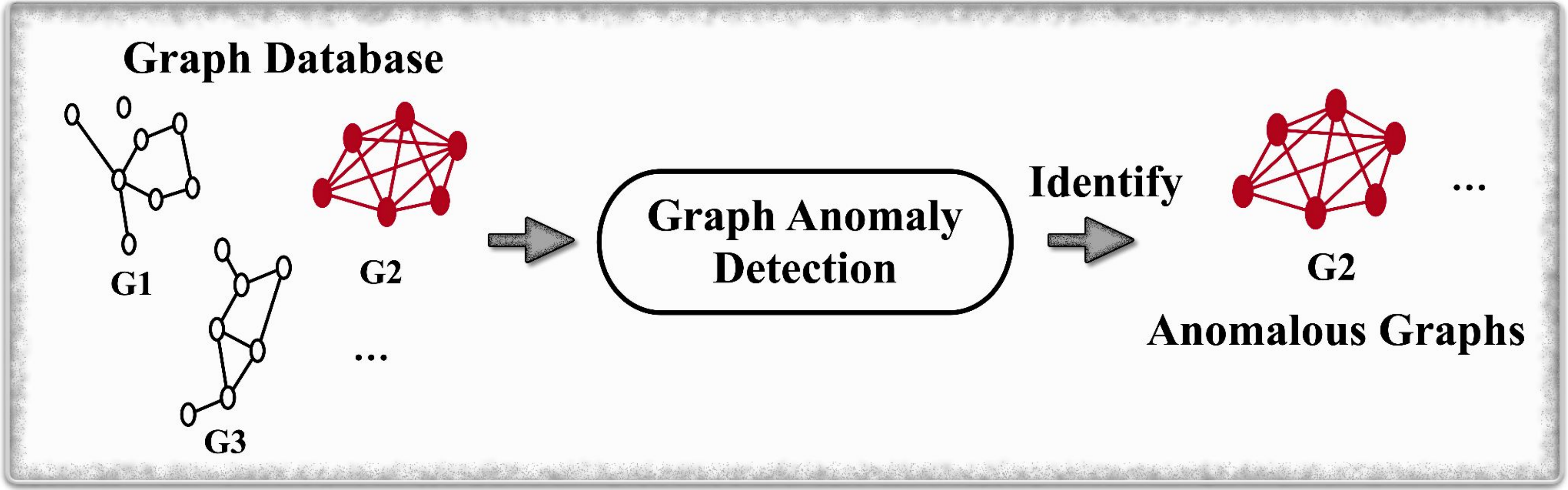
1. Kipf, Thomas N., and Max Welling. "Variational graph auto-encoders." arXiv preprint arXiv:1611.07308 (2016).

Baseline: OCGNN



1. Wang, Xuhong, et al. "One-class graph neural networks for anomaly detection in attributed networks." Neural computing and applications 33 (2021): 12073-12085.

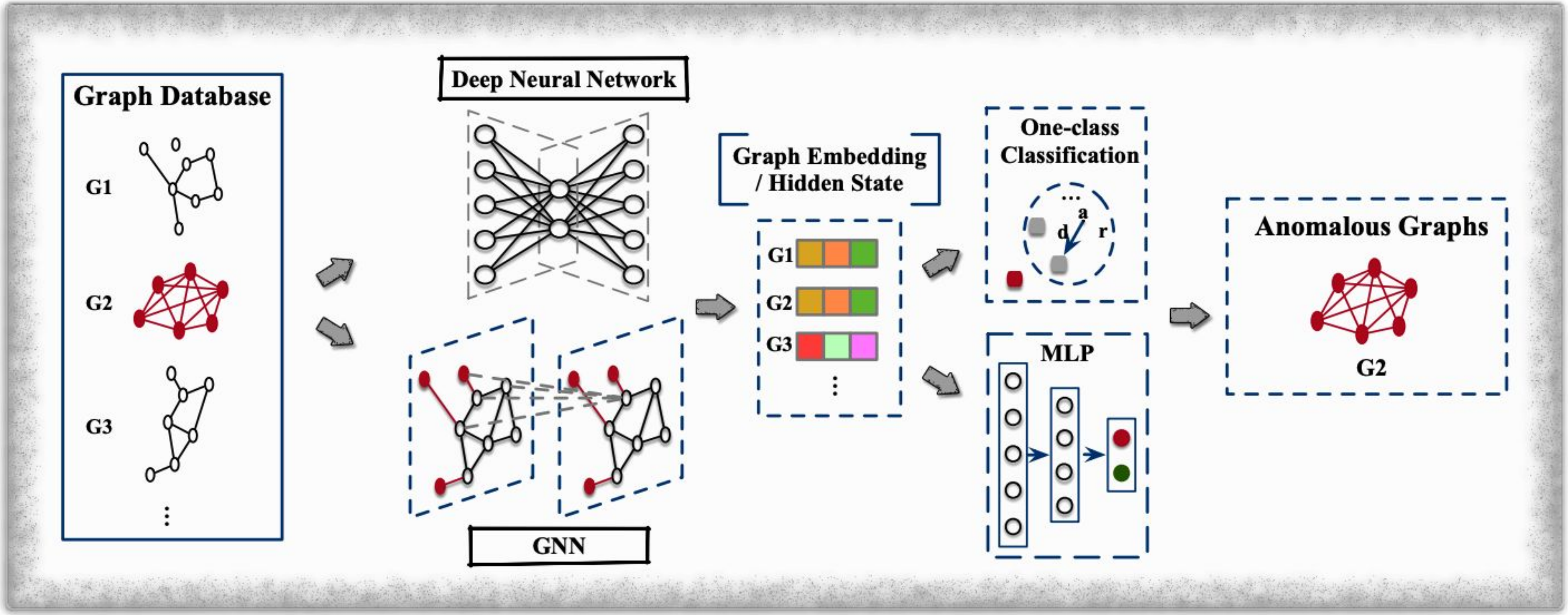
Graph-Level Anomaly Detection



Application: Unusual Molecule Detection

1. Ma, Xiaoxiao, Jia Wu, Shan Xue, Jian Yang, Chuan Zhou, Quan Z. Sheng, Hui Xiong, and Leman Akoglu. "A comprehensive survey on graph anomaly detection with deep learning." IEEE Transactions on Knowledge and Data Engineering 35, no. 12 (2021): 12012-12038.

Framework for Anomaly Detection on Graphs



1. Ma, Xiaoxiao, Jia Wu, Shan Xue, Jian Yang, Chuan Zhou, Quan Z. Sheng, Hui Xiong, and Leman Akoglu. "A comprehensive survey on graph anomaly detection with deep learning." IEEE Transactions on Knowledge and Data Engineering 35, no. 12 (2021): 12012-12038.