

Datasets

| | (M) | (M) | (M) | (P) | (S) | (M) | (M) | (M) | (M) | (M) |
|---------------|--------|--------|--------|---------|-------|-------|--------|--------|-------|-------|
| Datasets | BZR | DHFR | COX2 | ENZYMES | IMDB | AIDS | NCI1 | MMP | HSE | p53 |
| Nodes | 35.75 | 42.43 | 41.22 | 32.63 | 19.77 | 15.69 | 29.87 | 17.62 | 16.89 | 17.92 |
| Edges | 38.36 | 44.54 | 43.45 | 62.14 | 96.53 | 16.2 | 32.3 | 17.98 | 17.23 | 18.34 |
| Graphs | 405 | 467 | 467 | 600 | 1,000 | 2,000 | 4,110 | 7,558 | 8,417 | 8,903 |
| Anomaly ratio | 21.23% | 39.02% | 21.84% | 16.67% | 50% | 20% | 49.95% | 17.76% | 5.2% | 8.74% |

Table 1. Statistics and properties of graph anomaly datasets.

- Molecule anomaly graphs (M)
- Protein anomaly graphs (P)
- Social network anomaly graphs (S)

Datasets cont.

- Attributed graphs
 - Node attribute information
 - BZR, DHFR, COX2, ENZYMES and AIDS
- Plain graphs
 - Node feature information derived from the degree information of each node (number of edges)

Datasets cont.

File structure

- **DS_A.txt** (m lines): adjacency matrix for all graphs (node_id, node_id)
- **DS_graph_indicator.txt** (n lines): node to graph mapping (value in the i-th line is the graph_id of the node with node_id i)
- **DS_graph_labels.txt** (N lines): class labels for each graph (0 or 1, normal or abnormal)

n = total number of nodes

m = total number of edges

N = number of graphs

Experiment

- Five-fold cross-validation method (around 4/5ths for training and 1/5th for testing) (except for MMP, HSE and p53)
 - This process repeats 5 times to ensure that every graph becomes part of the testing set once
 - * Note that all abnormal graphs are removed from the training set to learn only normal ones
- Parameters:
 - Optimizer: Adam -> $\text{lr} = 0.0001$ (0.00001 on MMP, HSE and p53)
 - Encoder and decoder: 2 graph convolution layers before each pooling ($d - 256 - 128$) ($128 - 256 - d$)
 - Batch size: 300 (2000 on MMP, HSE and p53)

Experiment cont.

- 'main.py'
 - 2 linear layers before each pooling
 - Sets default lr to 0.0001
 - 5 fold
- 'main_1.py'
 - 2 graph conv layers before each pooling
 - Appears to be tailored for the Tox21_ datasets (some hard coding going on)
 - HSE
 - MMP
 - P53
 - Sets default lr to 0.00001 as stated before
 - Taking train-test split as it comes with dataset (no fold)
 - Requires running 5 times to match paper results (made some changes in the code to automate this)
 - 31:1 train-test ratio

Results

| Datasets | GLADC | | |
|----------|-------------------------------------|---|-------------------------------------|
| MMP | 0.696 ± 0.042 | → | 0.508 ± 0.138 |
| HSE | 0.618 ± 0.110 | → | 0.587 |
| p53 | 0.649 ± 0.216 | → | 0.497 ± 0.122 |
| BZR | 0.715 ± 0.067 | → | 0.618 ± 0.048 |
| DHFR | 0.612 ± 0.041 | → | 0.399 ± 0.038 |
| COX2 | 0.615 ± 0.044 | → | 0.578 ± 0.062 |
| ENZYMES | 0.583 ± 0.035 | → | 0.465 ± 0.042 |
| IMDB | 0.656 ± 0.023 | → | |
| AIDS | 0.993 ± 0.005 | → | 0.993 ± 0.005 |
| NCI1 | 0.683 ± 0.011 | → | 0.330 ± 0.016 |

Results cont.

```
● mambo@mambo-build:~/repos/GLADC$ /bin/python3 /home/mambo/repos/GLADC/main.py --DS NCI1
No node attributes
Graphs in current dataset: 4110
Normal vs abnormal graphs: 2053 2057

Fold 0 (train-test split): 3288 822
Fold 0 (train-test split after abnormal removal): 1646 822

semi-supervised abnormal detection: auroc_ab: 0.31339501897336625
semi-supervised abnormal detection: auroc_ab: 0.3134838178793637
semi-supervised abnormal detection: auroc_ab: 0.35480490880352356
semi-supervised abnormal detection: auroc_ab: 0.3134778979522972
semi-supervised abnormal detection: auroc_ab: 0.3134778979522972
semi-supervised abnormal detection: auroc_ab: 0.3133950189733662
semi-supervised abnormal detection: auroc_ab: 0.31338909904629975
semi-supervised abnormal detection: auroc_ab: 0.3161892245487536
semi-supervised abnormal detection: auroc_ab: 0.3135252573688292
semi-supervised abnormal detection: auroc_ab: 0.31348381787936375

Fold 1 (train-test split): 3288 822
Fold 1 (train-test split after abnormal removal): 1646 822
```

Results cont.

```
mambo@mambo-build:~/repos/GLADC$ /bin/python3 /home/mambo/repos/GLADC/main_1.py --DS Tox21_MMP
No node attributes
No node attributes
Number of graphs: 7558
Trial 1:
Train-test split: 1142 238

Epoch 10 semi-supervised abnormal detection, auroc_ab: 0.6738815789473683
Epoch 20 semi-supervised abnormal detection, auroc_ab: 0.675921052631579
Epoch 30 semi-supervised abnormal detection, auroc_ab: 0.6755263157894738
Epoch 40 semi-supervised abnormal detection, auroc_ab: 0.6767105263157894
Epoch 50 semi-supervised abnormal detection, auroc_ab: 0.6748684210526317
Epoch 60 semi-supervised abnormal detection, auroc_ab: 0.6755263157894736
Epoch 70 semi-supervised abnormal detection, auroc_ab: 0.6760526315789475
Epoch 80 semi-supervised abnormal detection, auroc_ab: 0.6776315789473684
Epoch 90 semi-supervised abnormal detection, auroc_ab: 0.6749999999999999
Epoch 100 semi-supervised abnormal detection, auroc_ab: 0.6740131578947368
Max AUC: 0.6776315789473684

Trial 2:
Train-test split: 1142 238

Epoch 10 semi-supervised abnormal detection, auroc_ab: 0.39434210526315794
Epoch 20 semi-supervised abnormal detection, auroc_ab: 0.39473684210526316
Epoch 30 semi-supervised abnormal detection, auroc_ab: 0.3217763157894737
```