

BIONETDatasets

What is it?

- A repository of biological datasets in TUD format
- A set of python wrappers
 - for using graphs in TUD format within the more popular graph deep learning libraries: DGL, PyTorch, Spektral, Grakel
- Available at: [Github](#)

The TU Datasets format file

Results: GIN-0

- 5-fold stratified cross validation
- learning rate: 0.001, 100 epochs, batch size: 10, 3 layers, 64 channels

dataset	loss	acc
MUTAG	0.51	0.85
PROTEINS	0.59	0.72
ogbg-molbbbp	0.43	0.86
ogbg-molbace	0.63	0.76

Results: HGP-SL

- one-random split: 80 train, 10% val, 10% test
- learning rate: 0.001, 1000 epochs with self stop, batch size: 512, 3 layers, 128 channels

dataset	loss	acc	batch	stopped at	struct learn	sparse att	pool_ratio
MUTAG	0.389	0.850	32	322	✗	✗	0.5
PROTEINS	0.381	0.857	512		✓	✓	0.5
Mutagenicity			512		✓	✓	0.8
ogbg-molbbbp	0.43	0.86	512	224	✓	✓	0.5
ogbg-molbace	0.522	0.743	512		✓	✓	0.5