

1). FreeSolv Dataset without path info:

num\_layers: 2

hidden\_dim: 361

pow\_dim: 0

dropout: 0.3452039813522458

weight\_decay: 6.0419833079684976e-15

batch\_size: 8

lr: 0.11019359201526167

2). FreeSolv Dataset with path info:

num\_layers: 1

hidden\_dim: 208

pow\_dim: 2

dropout: 0.5196842037821313

weight\_decay: 2.767099305559158e-18

batch\_size: 5

lr: 0.15479631120975956

3). ESOL Dataset without path info:

num\_layers: 3

hidden\_dim: 168

pow\_dim: 0

dropout: 0.52

weight\_decay: 1.302768700471842e-12

batch\_size: 5

lr: 0.023504521841891612

4). ESOL Dataset with path info:

num\_layers: 3

hidden\_dim: 297

pow\_dim: 4

dropout: 0.32237108467149417

weight\_decay: 8.866739110758421e-18

batch\_size: 6

lr: 0.029569723377469003

5). Lipophilicity Dataset without path info:

num\_layers: 3

hidden\_dim: 165

pow\_dim: 0

dropout: 0.0005789312483251083

weight\_decay: 3.415131374396533e-10

batch\_size: 10

lr: 0.002154844550078915

6). Lipophilicity Dataset with path info:

num\_layers: 1

hidden\_dim: 180

pow\_dim: 2

dropout: 0.4219960959598102

weight\_decay: 5.968202723677461e-20

batch\_size: 9

lr: 0.015812919139792124

7). BACE Dataset without path info:

num\_layers: 2

hidden\_dim: 198

pow\_dim: 0

dropout: 0.29690381882578476

weight\_decay: 2.587714005614795e-12

batch\_size: 6

lr: 0.0009437528771705722

8). BACE Dataset with path info:

num\_layers: 2  
hidden\_dim: 202  
pow\_dim: 1  
dropout: 0.7479123228381995  
weight\_decay: 2.6753837502739997e-17  
batch\_size: 7  
lr: 0.03976907015630966

9). BBBP Dataset without path info:

num\_layers: 3  
hidden\_dim: 243  
pow\_dim: 0  
dropout: 0.6962156787142889  
weight\_decay: 7.460646579829558e-17  
batch\_size: 8  
lr: 0.023663507801800314

10). BBBP Dataset with path info:

num\_layers: 1  
hidden\_dim: 324  
pow\_dim: 3  
dropout: 0.6104535457955884

weight\_decay: 2.545413999847812e-17

batch\_size: 4

lr: 0.08955851643035374

11). ClinTox Dataset without path info:

num\_layers: 1

hidden\_dim: 303

pow\_dim: 0

dropout: 0.38927567112685557

weight\_decay: 1.8365272549658533e-14

batch\_size: 8

lr: 0.02476945340075211

12). ClinTox Dataset with path info:

num\_layers: 2

hidden\_dim: 340

pow\_dim: 4

dropout: 0.7123844457157064

weight\_decay: 1.1839905103876106e-14

batch\_size: 10

lr: 0.0021488524554826825

13). Example Usage:

```
python train_t_hop.py --use_gpu 1 --dataset ClinTox
--repitition 3 --epochs 200
--use_path_info 1 --add_noise 1 --noise_factor 0.1
--num-layers 2 --hidden_dim 340 --pow_dim 4
--dropout 0.71 --weight_decay 1.18399051038761e-14 --batch-size 10
--lr 0.002148852455 --dir_to_save_model /path/to/t_hop_models/
```