Supplementary manuscript of

Identifying personalized driver genes of cancer individual patients with semi-supervised graph neural network

Han-Wen Wan1,2†, Meng-Han Wu3†, Wen-Shan Zhao3, Han Cheng3, Xiang-Rui Zhang3, Yan Li4, Wei-Feng Guo1,5\*

1 School of Electrical Engineering, Zhengzhou University, Zhengzhou 450001, China

2 School of International College, Zhengzhou University, Zhengzhou 450001, China

3 School of Life Sciences, Zhengzhou University, Zhengzhou 450001, China

4 Key Laboratory of Information Fusion Technology of Ministry of Education, School of Automation, Northwestern Polytechnical University, Xian, 710072, China

5 State Key Laboratory of Oncology in South China, Collaborative Innovation Center for Cancer Medicine, Sun Yat-sen University Cancer Center, Guangzhou 510060, China

\* To whom correspondence should be addressed.

[Tel:86-0371-677810](Tel:86-21-54920100)18; Fax: [86-0371-677810](Tel:86-21-54920100)18; Email: [guowf@zzu.edu.cn](mailto:liangjing@zzu.edu.cn,)

† The authors should be regarded as Joint First Authors.

1. **The parameters in PersonalizedGNN**

Table S1 The parameters of PersonalizedGNN on cancer driver gene prediction

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| The number of layers | The number of nodes in each layer | weight decay | learn rate | coefficient of Dropout | coefficient of DropEdge | coefficient of DropAttention | The number of attention heads | epoch |
| 3 | 750 | 1E-7 | 0.02 | 0.25 | 0.75 | 0.75 | 5 | 2000 |

1. **Parameters in other methods**

ChebNet: the graph convolution kernel size is 2; the number of layers is 3; the size of each hidden layer is 750; the number of epochs is 2000; bias in graph convolution is enabled, the activation function is ReLU; the dropout rate is 0.25; the learning rate is 0.02, and the optimizer is Adam.

GraphSAGE: the number of layers is 3; the size of each hidden layer is 750; the number of epochs is 2000; the number of sampled neighbors is 10; the batch size is 50; and the learning rate is 0.02.

GCN: the number of layers is 3; the size of hidden layers is 750; the num of epochs is 2000; the the dropout rate is 0.25; learning rate is 0.02; and the weight decay is 1e-7.

GAT without label reuse: the heads of attention mechanism is 5; the number of layers is 3; the size of each hidden layer is 500; the number of epochs is 2000; the coefficient of Dropout, DropEdge and DropAttention is 0.25, 0.75 and 0.75 respectively; the learning rate is 0.02; the weight decay is 1e-7; and the activation function is LeakyReLU with the slope alpha equals 0.2.

1. **The statistic information of positive and negative genes in PGIN**

Table S2 The statistic information of positive and negative genes in PGIN

|  |  |  |  |
| --- | --- | --- | --- |
|  | BRCA | LUSC | LUAD |
| #posi | 18.4602+-1.5749 | 27.7292+-3.0479 | 29.4286+-3.7005 |
| #neg | 191.9115+-15.8389 | 419.7292+-23.0389 | 412.5000+-24.4861 |

## 4 Experimental parameters sensitivity analysis

To further demonstrate the effectiveness of the setting parameters in our PersonalizedGNN, we tuned one of the parameters over suitable ranges of parameter values while we fixed other parameters in BRCA, LUSC, LUAD data sets. For each cancer data set, we used the same parameters among all individual patients and calculated the average gene ranking score among all individual patients for each cancer data. Based on the average gene ranking score of the cancer data, we obtained the gene ranking result and calculated the *Average* *Precision* of different parameter choices on each cancer data. The parameter setting results on BRCA, LUAD, and LUSC were shown in **Fig S1 of Additional file 1**. As shown in Figure S1, PersonalizedGNN has the best performance for our setting parameters in PersonalizedGNN.

## 5 Supplementary results of PersonalizedGNN

**para check**

**Fig S1** The error bar in terms of *Average* *Precision* for different parameter choices among top *k* (*k*=1, 2, ..., 30) ranking genes on BRCA, LUSC, LUAD data sets.

342b84516eba339c4ea137fec87cc6a4

**Fig.S2** Enrichment pathway results of NPDGs on different subtypes of BRCA cancer patients.

770023a6d07613f2e38a5fa451d25461

**Fig.S3** Enrichment pathway results of NPDGs on different subtypes of LUNG cancer patients.