Supplementary manuscript of

A novel graph neural network method with label reuse in personalized gene interaction network for prioritizing cancer driver genes

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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.