

Supporting Information

Graph Attention Mechanism-based Deep Tensor Factorization for Predicting disease-associated miRNA-miRNA pairs

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1 Data and parameters for baseline methods

2 Network input and output of GraphTF

1 Data and parameters for baseline methods

CANDECOMP/PARAFAC(CP) [24]: A classical tensor factorization model without any auxiliary information which decomposes a tensor as a sum of rank-one tensors via alternating least squares (ALS) rules. The rank R is set as 4.

DrugCom [25]: We use miRNA sequence similarity, miRNA functional similarity and disease semantic similarity to train the model. The parameters we used are the default values in the original paper, where the latent factor R is set to 30.

TDRC [5]: We utilize miRNA functional similarity and disease semantic similarity to train the model the same way as the original paper. The parameters we used are the default values in the original paper, where the latent factor $r=4$, $\alpha=0.125$, $\beta=0.25$, $\lambda=0.001$.

DeepSynergy [26]: We take miRNA sequence similarity, miRNA functional similarity and disease semantic similarity as the input feature for miRNA and disease in the comparison. We apply DeepSynergy with two hidden layers and the units are 933, 4096, 2048, 1 for input features, two units for each hidden layer and outputs, respectively.

DTF [10]: We use miRNA sequence similarity, miRNA functional similarity and disease semantic similarity as latent features of miRNAs and diseases for prediction. We apply DTF with three hidden layers and the units are 3000, 2048, 1024, 512, 1 for input features, three units for each hidden layer and outputs, respectively.

2 Network input and output of GraphTF

For GAT, the input features and output features of miRNAs and diseases are 128 and 384, respectively. For the three-layer MLP, the input units and output are 384, 128 and 128, respectively.