**Table1**

The results comparison with other baseline models in dataset1

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Metrics | Methods | | | | | |
| Our | CNNMDA | PADLMHOOI | LDAformer | DFELMDA | HGCNMDA |
| AUC | **99.83** | 94.17 | 83.62 | 95.82 | 94.33 | 95.71 |
| AUPR | **99.84** | 94.21 | 81.92 | 95.83 | 93.60 | 95.78 |
| ACC | **98.19** | 86.04 | 75.42 | 89.11 | 87.77 | 88.80 |
| F1 | **98.18** | 85.64 | 75.09 | 89.05 | 87.59 | 88.56 |

The results comparison with other baseline models in dataset2

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Metrics | Methods | | | | | |
| Our | CNNMDA | PADLMHOOI | LDAformer | DFELMDA | HGCNMDA |
| AUC | **98.70** | 96.82 | 94.47 | 92.84 | 97.10 | 94.38 |
| AUPR | **98.78** | 96.56 | 93.61 | 92.61 | 96.75 | 94.27 |
| ACC | **93.43** | 90.87 | 87.63 | 85.90 | 90.09 | 87.85 |
| F1 | **93.21** | 90.83 | 87.58 | 86.06 | 89.97 | 87.92 |

Table2

The influence of the node sizes in subgraph

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Metrics | Number of nodes in subgraph | | | | | |
| nodes=1 | nodes=2 | nodes=3 | nodes=4 | nodes=5 | nodes=6 |
| Time cost (s/epoch) | 10.927 | 10.985 | 11.038 | 11.071 | 11.097 | 11.114 |
| AUC | 95.36 | 98.75 | 99.68 | 99.75 | 99.91 | **99.97** |
| AUPR | 95.47 | 98.92 | 99.72 | 99.79 | 99.91 | **99.97** |
| ACC | 87.44 | 94.91 | 97.84 | 97.43 | 98.63 | **99.28** |
| F1 | 86.93 | 94.86 | 97.83 | 97.46 | 98.62 | **99.28** |

Table3

The results of different feature aggregation methods

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Metrics | Feature aggregation way | | | |
| E(element-weight) MLP | Weight-multiply and sum up | Concatenate and using MLP | None process of feature aggregation |
| AUC | **95.36** | 94.59 | 94.15 | 93.64 |
| AUPR | **95.47** | 94.73 | 94.33 | 94.02 |
| ACC | **87.44** | 86.89 | 86.41 | 84.50 |
| F1 | 86.93 | **87.29** | 86.72 | 82.74 |

Table 4

The ACC of different fine-tune model in the last epoch:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Metric | Different fine-tune models | | | |
| Origin BertNDA | BertNDA+MLP | BertNDA+CNN | BertNDA+AE |
| ACC |  |  |  |  |

Table 5

The average ACC of different size of layers in encoder network in each epochs (1-20):

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ACC | The number of layers | | | | |
| Layers=1 | Layers=2 | Layers=4 | Layers=8 | Layers=16 |
| Epoch=1 | 0.4375 | 0.4375 | **0.5938** | 0.2813 | 0.3000 |
| Epoch=2 | 0.6563 | 0.6563 | **0.7188** | 0.5781 | 0.4000 |
| Epoch=3 | 0.7292 | **0.7708** | 0.7604 | 0.6875 | 0.5792 |
| Epoch=4 | 0.7578 | **0.7734** | **0.7734** | 0.7422 | 0.6219 |
| Epoch=5 | 0.8000 | 0.8063 | **0.8125** | 0.7813 | 0.6788 |
| Epoch=6 | 0.7969 | 0.8333 | **0.8438** | 0.7969 | 0.7219 |
| Epoch=7 | 0.8214 | **0.8482** | 0.8393 | 0.8259 | 0.7214 |
| Epoch=8 | 0.8242 | **0.8555** | 0.8516 | 0.8438 | 0.7406 |
| Epoch=9 | 0.8299 | **0.8681** | 0.8507 | 0.8611 | 0.7660 |
| Epoch=10 | 0.8375 | **0.8750** | 0.8531 | 0.8719 | 0.7863 |
| Epoch=11 | 0.8466 | **0.8807** | 0.8608 | 0.8750 | 0.7972 |
| Epoch=12 | 0.8542 | **0.8854** | 0.8698 | 0.8828 | 0.8089 |
| Epoch=13 | 0.8582 | **0.8918** | 0.8798 | 0.8846 | 0.8164 |
| Epoch=14 | 0.8639 | **0.8973** | 0.8862 | 0.8906 | 0.8250 |
| Epoch=15 | 0.8688 | **0.9021** | 0.8896 | 0.8979 | 0.8325 |
| Epoch=16 | 0.8731 | **0.9063** | 0.8965 | 0.9043 | 0.8410 |
| Epoch=17 | 0.8768 | **0.9099** | 0.8971 | **0.9099** | 0.8504 |
| Epoch=18 | 0.8837 | 0.9132 | 0.9010 | **0.9149** | 0.8587 |
| Epoch=19 | 0.8865 | 0.9145 | 0.9030 | **0.9194** | 0.8628 |
| Epoch=20 | 0.8891 | 0.9188 | 0.9063 | **0.9219** | 0.8697 |

Table6

The AUC/AUPR of different models without data leakage:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Metrics | models | | | | | |
| Ours | CNNMDA | PADLMHOOI | LDAformer | HGCNMDA | GraphSAGE |
| AUC | 87.3 | 84.8 | 84.2 | 83.5 | 84.9 | 81.7 |
| AUPR | 86.9 | 84.0 | 83.7 | 82.8 | 84.8 | 79.0 |

The ACC of five-fold cross-validation without data leakage

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Models | ACC value of different folds | | | | | |
| Fold\_0 | Fold\_1 | Fold\_2 | Fold\_3 | Fold\_4 | Average |
| Ours | 78.45 | 78.40 | 77.05 | 77.15 | 78.40 | 77.89 |
| CNNMDA | 76.15 | 76.35 | 76.85 | 76.25 | 76.25 | 76.37 |
| PADLMHOOI | 76.00 | 76.80 | 75.35 | 75.70 | 76.35 | 76.04 |
| LDAformer | 76.80 | 74.05 | 75.95 | 75.40 | 76.65 | 75.77 |
| HGCNMDA | 77.50 | 77.25 | 75.70 | 75.95 | 76.10 | 76.50 |
| GraphSAGE | 73.40 | 75.50 | 74.35 | 73.65 | 71.65 | 73.71 |
| DEFLMDA | 77.35 | 76.75 | 73.25 | 77.95 | 77.65 | 76.59 |

Figure1

The t-SNE of origin feature and WL-embedding

Figure2

The heatmap of Association-matrix (a), Similarity matrix (b), Laplacian matrix (c) and WL-embedding matrix (d) in dataset1:

