Supplementary Materials for

"Predicting Human Microbe-Disease Associations via Graph Attention Networks with Inductive Matrix Completion"

Experiment results

Comparison performance between our model with seven state-of-the-art methods

To evaluate the effectiveness of our model, we compare our proposed model of GATMDA with seven state-of-the-art methods on two datasets, i.e., HMDAD and Disbiome under the setting CVS1. Table S1 and Table S2 show the results of 2-fold CV, 5-fold CV and 10-fold CV for HMDAD and Disbiome, respectively. It indicates that our model consistently outperforms all baseline methods in terms of AUC and AUPR for both datasets. Therefore, we can conclude that our model is effective and promising in inferring potential microbe-disease associations.

Table S1. Comparison performance between our method and state-of-the-art methods under the setting CVS1 based on HMDAD dataset. The best results are marked in bold and the second best is underlined.

Methods	2-fold CV		5-fold CV		10-fold CV	
	AUC	AUPR	AUC	AUPR	AUC	AUPR
KATZHMDA	0.8599±0.0064	0.8755±0.0103	0.8703±0.0199	0.8807±0.0167	0.8654±0.0352	0.8855±0.0336
NTSHMDA	0.8615±0.0151	0.8534±0.0188	<u>0.8982±0.0312</u>	<u>0.9087±0.0294</u>	<u>0.9012±0.0354</u>	<u>0.9086±0.0393</u>
BiRWHMDA	0.8799±0.0120	<u>0.8921±0.0116</u>	0.8890±0.0194	0.8969±0.0146	0.8744±0.0362	0.8850±0.0298
NGRHMDA	<u>0.8929±0.0059</u>	0.8870±0.0183	0.8921±0.0327	0.8720±0.0844	0.8844±0.0506	0.8988±0.0428
BRWMDA	0.8663±0.0030	0.8753±0.0084	0.8916±0.0029	0.9064±0.0152	0.8973±0.0025	0.9031±0.0123
WMGHMDA	0.8547±0.0086	0.8754±0.0121	0.8745±0.0296	0.8895±0.0296	0.8547±0.0594	0.8800±0.0500
GRNMFHMDA	0.8756±0.0164	0.8891±0.0179	0.8806±0.0156	0.8914±0.0162	0.8750±0.0373	0.8880±0.0310
GATMDA	**0.9538±0.0049**	**0.9377±0.0176**	**0.9554±0.0184**	**0.9334±0.0417**	**0.9467±0.0117**	**0.9135±0.0435**

Table S2. Comparison performance between our method and state-of-the-art methods under the setting CVS1 based on Disbiome dataset. The best results are marked in bold and the second best is underlined.

Methods	2-fold CV		5-fold CV		10-fold CV	
	AUC	AUPR	AUC	AUPR	AUC	AUPR
KATZHMDA	0.6696±0.0058	0.6650±0.0052	0.6779±0.0141	0.6785±0.0163	0.6850±0.0210	0.6852±0.0172
NTSHMDA	0.8086±0.0058	0.7701±0.0076	0.8294±0.0071	0.7881±0.0099	0.8378±0.0097	0.7928±0.0098
BiRWHMDA	0.8139±0.0060	0.7924±0.0071	0.8344±0.0089	0.8104±0.0103	0.8291±0.0165	0.8034±0.0187
NGRHMDA	0.8233±0.0046	0.8175±0.0033	0.8313±0.0052	0.8202±0.0043	0.8419±0.0092	0.8343±0.0096
BRWMDA	0.8114±0.0026	0.8232±0.0041	0.8266±0.0031	0.8365±0.0121	0.8337±0.0032	0.8450±0.0153
WMGHMDA	0.7050±0.0108	0.7490±0.0108	0.7176±0.0076	0.7567±0.0062	0.7248±0.0115	0.7748±0.0134
GRNMFHMDA	<u>0.8501±0.0017</u>	<u>0.8527±0.0032</u>	<u>0.8609±0.0047</u>	<u>0.8669±0.0060</u>	<u>0.8701±0.0117</u>	<u>0.8797±0.0083</u>
GATMDA	**0.9296±0.0154**	**0.9172±0.0208**	**0.9307±0.0079**	**0.9211±0.0088**	**0.9388±0.0101**	**0.9223±0.0121**