

Learning characteristics of graph neural networks predicting protein–ligand affinities

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Supplementary Table 1

Supplementary Table 1. Edges determining predictions.

	Edges			RMSE
Set	Protein	Ligand	Interaction	
GCN				
Low-affinity	4.8% (5.0)	75.0% (69.8)	20.2% (25.2)	1.735
Medium-affinity	8.8% (7.2)	64.2% (47.0)	27.0% (45.8)	0.531
High-affinity	7.0% (10.8)	70.6% (36.0)	22.4% (53.2)	1.561
Average	6.9% (7.6)	69.9% (50.9)	23.2% (41.4)	1.276
GAT				
Low-affinity	10.4% (6.5)	72.8% (67.5)	16.8% (26.0)	1.570
Medium-affinity	11.2% (9.2)	60.6% (62.0)	28.2% (28.8)	0.541
High-affinity	13.0% (8.2)	63.4% (61.0)	23.6% (30.8)	1.563
Average	11.5% (8.0)	65.6% (63.5)	22.9% (28.5)	1.225
GIN				
Low-affinity	10.8% (7.9)	72.4% (68.0)	16.8% (24.1)	1.667
Medium-affinity	14.8% (7.0)	58.4% (67.6)	26.8% (25.4)	0.902
High-affinity	22.4% (6.2)	47.6% (71.6)	30.0% (22.2)	1.544
Average	16.0% (7.0)	59.5% (69.1)	24.5% (23.9)	1.372
GINE				
Low-affinity	6.7% (3.6)	65.3% (77.9)	28.0% (18.5)	1.583
Medium-affinity	11.8% (4.2)	59.4% (68.8)	28.8% (27.0)	0.900

High-affinity	10.6% (5.4)	62.2% (65.2)	27.2% (29.4)	1.729
Average	9.7% (4.4)	62.3% (70.6)	28.0% (25.0)	1.404
GraphSAGE				
Low-affinity	10.3% (7.1)	70.2% (70.8)	19.5% (22.1)	1.471
Medium-affinity	9.8% (7.6)	67.6% (59.4)	22.6% (33.0)	0.667
High-affinity	10.2% (8.6)	69.8% (56.4)	20.0% (35.0)	1.564
Average	10.1% (7.8)	69.2% (62.2)	20.7% (30.0)	1.234
GC-GNN				
Low-affinity	11.1% (6.9)	55.2% (52.3)	33.7% (40.8)	1.607
Medium-affinity	12.0% (6.4)	42.6% (40.4)	45.4% (53.2)	0.831
High-affinity	11.8% (6.2)	36.6% (35.6)	51.6% (58.2)	1.622
Average	11.6% (6.5)	44.8% (42.8)	43.6% (50.7)	1.353

Reported are the mean proportions (%) of protein, ligand, and interaction edges among the top-25 edges determining test set predictions as prioritized by EdgeSHAPer and GNNExplainer (in parentheses). Edge proportions are reported for test instances falling into three different potency subranges. The average at the bottom is calculated for all three affinity sub-ranges. In addition, the RMSE for each GNN model and sub-range is reported (right-most column). All models were derived using identical training sets and tested on the same test set (hold-out set). Predictions were then separately analyzed for test instances falling into different affinity sub-ranges.