

Hyperparameter	Values
Number of graph convolutional layers	1, 2, 3
Number of linear layers	1, 2, 3
Graph convolutional layer embedding sizes	64, 128, 256, 384
Linear layer sizes	Keep sizes of all linear layers constant; alternatively, for each subsequent layer, divide size by 2
Activation function after graph convolutional layers	Include; alternatively, do not include

Table S1: Hyperparameter combinations used for tuning in grid search. A grid search was conducted by varying the following hyperparameters: number of graph convolutional layers, number of linear layers, embedding size for graph convolutional layers, linear layer sizes, and inclusion/exclusion of activation function after the graph convolutional layers.

that match that of the graph convolutional layers, and using an activation function (ReLU) after all graph convolutional layers and all linear layers except for the last.