Random Walk Graph Neural Network Summary

Most GNNs we've covered in Math 189 are examples of message-passing neural networks (MPNNs). MPNNs use representation learning to embed nodes in a low-dimensional space and iteratively update each node's embedding using information from its neighbors. One drawback of the MPNN approach to graph deep learning is that the approach has many constituent parts and the learning process is somewhat hard to understand and draw human-readable insights from. The goal of the authors of this paper was to develop a framework that applies a function directly to a graph without transforming its information. The authors developed a new GNN called the Random Walk Graph Neural Network (RWNN). The RWNN uses a random walk kernel to make representations of the graph, and contains several trainable "hidden graphs" that are compared to the ground-truth graph. The outputs from this step are passed into a FCNN, which then produces the final output.

To define the problem explicitly, the RWNN's goal is to perform graph-level classification by learning a vector representation of a graph G, **h_G,** that can be passed into a function F to predict the class label of a graph. The model compares input graphs against N hidden graphs G_1, … , G_N. Instead of creating a vector representation of each graph, the model uses the similarity between input graphs and hidden graphs based on a kernel (in this case, a random walk kernel that is differentiable) to produce output classes. The goal of the model is to learn hidden graphs that can help distinguish between the available classes.

The random walk kernel the authors employ is fairly simple. The p-step kernel compares two graphs based on the number of shared available walks of length p between the two during a simultaneous random walk on both. Different values of p contain different similarities, so the RWNN takes random walks of length p in the range {0,P} as components in a vector and passes the output of the kernel to a FCNN to perform classification.

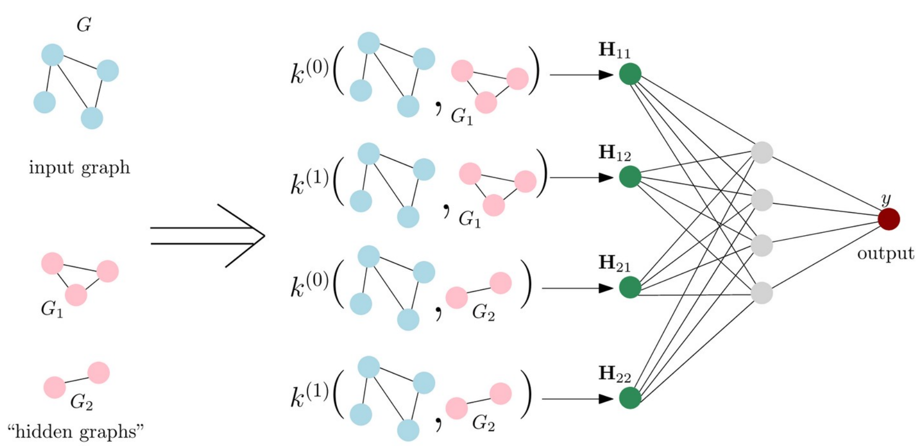

Figure 1: Overview of the proposed RWNN model (biases are omitted for clarity).

This architecture cannot deal with graphs that have real-valued multidimensional feature vectors at each node, so the authors developed a generalization that handles such graphs by learning feature vectors for the hidden graphs. To compare graphs, the model takes the direct product between two graphs and applies the random walk kernel to the resulting graph. To construct an adjacency matrix for the direct product graph, the authors use the Kronecker product of the two adjacency matrices.

The authors present results on a few sample bio-informatics, chemistry and social interaction graph classification tasks:

	MUTAG	D&D	NCI1	PROTEINS	ENZYMES
SP	80.2 (± 6.5)	**78.1** (± 4.1)	72.7 (± 1.4)	**75.3** (± 3.8)	38.3 (± 8.0)
GR	80.8 (± 6.4)	75.4 (± 3.4)	61.8 (± 1.7)	71.6 (± 3.1)	25.1 (± 4.4)
WL	84.6 (± 8.3)	**78.1** (± 2.4)	**84.8** (± 2.5)	73.8 (± 4.4)	50.3 (± 5.7)
DGCNN	84.0 (± 6.7)	76.6 (± 4.3)	76.4 (± 1.7)	72.9 (± 3.5)	38.9 (± 5.7)
DiffPool	79.8 (± 7.1)	75.0 (± 3.5)	76.9 (± 1.9)	73.7 (± 3.5)	59.5 (± 5.6)
ECC	75.4 (± 6.2)	72.6 (± 4.1)	76.2 (± 1.4)	72.3 (± 3.4)	29.5 (± 8.2)
GIN	84.7 (± 6.7)	75.3 (± 2.9)	80.0 (± 1.4)	73.3 (± 4.0)	**59.6** (± 4.5)
GraphSAGE	83.6 (± 9.6)	72.9 (± 2.0)	76.0 (± 1.8)	73.0 (± 4.5)	58.2 (± 6.0)
1-step RWNN	**89.2** (± 4.3)	77.6 (± 4.7)	71.4 (± 1.8)	74.7 (± 3.3)	56.7 (± 5.2)
2-step RWNN	88.1 (± 4.8)	76.9 (± 4.6)	73.0 (± 2.0)	74.1 (± 2.8)	57.4 (± 4.9)
3-step RWNN	88.6 (± 4.1)	77.4 (± 4.9)	73.9 (± 1.3)	74.3 (± 3.3)	57.6 (± 6.3)

	IMDB BINARY	IMDB MULTI	REDDIT BINARY	REDDIT MULTI-5K	COLLAB
SP	57.7 (± 4.1)	39.8 (± 3.7)	89.0 (± 1.0)	51.1 (± 2.2)	**79.9** (± 2.7)
GR	63.3 (± 2.7)	39.6 (± 3.0)	76.6 (± 3.3)	38.1 (± 2.3)	71.1 (± 1.4)
WL	**72.8** (± 4.5)	**51.2** (± 6.5)	74.9 (± 1.8)	49.6 (± 2.0)	78.0 (± 2.0)
DGCNN	69.2 (± 3.0)	45.6 (± 3.4)	87.8 (± 2.5)	49.2 (± 1.2)	71.2 (± 1.9)
DiffPool	68.4 (± 3.3)	45.6 (± 3.4)	89.1 (± 1.6)	53.8 (± 1.4)	68.9 (± 2.0)
ECC	67.7 (± 2.8)	43.5 (± 3.1)	OOR	OOR	OOR
GIN	71.2 (± 3.9)	48.5 (± 3.3)	89.9 (± 1.9)	**56.1** (± 1.7)	75.6 (± 2.3)
GraphSAGE	68.8 (± 4.5)	47.6 (± 3.5)	84.3 (± 1.9)	50.0 (± 1.3)	73.9 (± 1.7)
1-step RWNN	70.8 (± 4.8)	47.8 (± 3.8)	**90.4** (± 1.9)	51.7 (± 1.5)	71.7 (± 2.1)
2-step RWNN	70.6 (± 4.4)	48.8 (± 2.9)	90.3 (± 1.8)	51.7 (± 1.4)	71.3 (± 2.1)
3-step RWNN	70.7 (± 3.9)	47.8 (± 3.5)	89.7 (± 1.2)	53.4 (± 1.6)	71.9 (± 2.5)