Paper(s) discussed

(1) GRAND: Graph Neural Diffusion; Ben Chamberlain, James Rowbottom, Maria I Gorinova, Michael Bronstein, Stefan Webb, Emanuele Rossi Proceedings of the 38th International Conference on Machine Learning, PMLR 139:1407-1418, 2021.

Summary

(1) The GRAND (Graph Neural Diffusion) paper introduces a novel graph neural network (GNN) model that uses a diffusion process to propagate information throughout a graph. The model is designed to perform graph classification tasks, where the goal is to predict a label for an entire graph based on its node and edge attributes.

In GRAND, each node in the graph is represented by a feature vector, which is updated through a diffusion process that involves aggregating information from neighboring nodes. The diffusion process is controlled by a set of learnable parameters that are optimized during training.

Pros

- The model achieves competitive or better performance than other state-of-the-art GNN models on most benchmark datasets, particularly in cases where the graphs have a large number of nodes or edges.
- The diffusion process used in GRAND is simple and computationally efficient, making it scalable to larger graphs and allowing for faster training times.

Cons

- The diffusion process used in GRAND may not be suitable for all types of graphs, particularly those that have a high degree of sparsity or disconnected components.

Questions for discussion

- How does the diffusion process used in GRAND compare to other methods for capturing long-range dependencies in graphs, such as message-passing or attention mechanisms?
- Do you think there are certain types of graph classification tasks where these non-GNN models might be more effective than GRAND?
- Why different methods were used for different experiments?

Presentation and Discussion Feedback

Name of Presenters: Andrew, Vishal, Owen

How was the presentation? Did it help you?

The presentation was very well-structured, the thermodynamics-related parts were made to understand in very good way, I studied physics during undergrad and I know how good of a job they did on this part! They looked at the presentation with the perspective of teaching what they learned to the class.

Feedback for the presenters:

- Maybe dividing the presentation in a way that all three could present the same amount could help improve everyone's presentation skill.

Novel points raised during the presentation or discussion that you thought were crucial. Carefully consider all issues raised and list only those you feel were most important.

- Using PDE in a way to make the model efficient, even though the analytical solution might not exist.
- While GNNs have been used extensively for node classification tasks, GRAND focuses on graph classification tasks, where the goal is to predict a label for an entire graph based on its node and edge attributes.
- GRAND can provide insights into how the model makes its predictions. This is achieved by visualizing the diffusion process and examining the importance of each node in the graph.