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Chapter 6 Reflection

1. Please give a brief summary of the chapter?

The use of convolutional and recurrent neural networks are for encoding regular grid-like data. However, many real-world problems are represented as graphs. Graph Neural Networks (GNNs) are neural networks designed for processing graphs, with many use cases such as molecular representations, spatiotemporal networks, drug-drug interaction networks, protein-protein interaction networks, gene expression networks, and biomedical knowledge graphs. GNNs are good at modeling complex relationships among entities in these graphs, making them useful for understanding patterns and extracting information.

A notable application of GNNs is in drug discovery, where they can predict properties of prospective drugs by representing them as graphs. This allows GNNs to predict characteristics such as solubility or toxicity, thereby accelerating the drug discovery process. Various versions of GNNs, including graph convolutional networks (GCN), graph attention networks (GAT), and message passing neural networks (MPNN), are discussed to solve different parts of graph processing. In addition, two practical GNN applications are discussed: drug property prediction and clinical predictive tasks.

2. What improvements do you want to see in this chapter? Please elaborate on them

While it presents a significant challenge, exploring improved visual representations of graphs could be good. The current charts and images are easy to implement and decent for individuals who can mentally visualize mathematical concepts effectively. However, given the graphical nature of the topic, investing in more compelling graphics would be highly valuable. A set of meticulously crafted high-quality graphics illustrating the process of the GNN would greatly enhance the clarity of the lesson. This is particularly important for individuals who struggle with matrices of numbers, onto other matrices.

3. What are the typos in this chapter?

- Pg 140 “Equation (7.13) take the last-layer… and aggregated” has a typo. It should be “takes” and “aggregates”.

Otherwise no other typos were noticed.

4. Which part of the chapter do you like most

I quite liked the applications of GNNs showing how other topics at UIUC can be related to DLH. And also to see how there are options for Deep Learning strategies to help out in the real world.

5. What are the most useful things you learned from this chapter?

The code blocks and numerous examples provided in this chapter were particularly beneficial, offering readers practical demonstrations of the concepts discussed. The final example, which guides through a complete process, is especially effective in illustrating how PyTorch can be utilized to implement an GNN with things such as attention mechanism. The chapter effectively builds up to this demonstration by thoroughly explaining the components and workings involved.

6. Could you find at least one research papers that use GNNs for handling healthcare predictive tasks? Use one sentence to summarize the paper and add citation.

[1] is a paper on graph neural networks that predicts patient treatments from a synthetic database to show their effectiveness over other models.

References

[1] Diaz Ochoa JG, Mustafa FE. Graph neural network modelling as a potentially effective method for predicting and analyzing procedures based on patients' diagnoses. Artif Intell Med. 2022 Sep;131:102359. doi: 10.1016/j.artmed.2022.102359. Epub 2022 Jul 19. PMID: 36100347.

[2] Xiao, C., Sun, J. (2021). Introduction. In: Introduction to Deep Learning for Healthcare. Springer, Cham. https://doi-org.proxy2.library.illinois.edu/10.1007/978-3-030-82184-5_1