696DS Course Project IBM 1

Revisiting Graph Neural Networks

IBM Mentors: Veronika Thost, Tengfei Ma

Ph.D. Mentor: Shib Sankar Dasgupta

Who are we, who are you?

- Why did you choose this project?
- Any special goals you have for the project?
- What is your ML / programming experience?
- Do you have plans for the time after your Master’s?
- Anything else you want to let you know

Why this project?

- The new Open Graph Benchmark provides a reasonable and challenging set of datasets and tasks for GNNs.
- It also gives a lot of first results (GNNs and Non-GNNs) which people can use to compare to but …
- These results are a bit too bad.
- OGB Google group: "*I also agree that we should update the results of the basic GNN models from time to time. I encourage the community to re-evaluate the basic models when necessary*."

  https://groups.google.com/g/open-graph-benchmark
- Many researchers do not care and are happy that they only have to beat these results. This is not good research practice!
- This does not really help us with research. We would want to learn the actual performance to derive valid conclusions for new research.

Datasets

ogbn-…
- proteins
- arxiv
- mag

ogbl-…
- ppa
- collab
- ddi
- biokg

ogbg-…
- molhiv
- molpcba
- ppa
- code

- Let’s focus on datasets that fit into GPU
- Start with ogbn or ogbl
- Get a full set of results for 2-3 GNNs as we want to have them in the paper
- Then consider other models and datasets

We consider a few more GNNs

- GCN – better than in ogb?
- GraphSAGE – better than in ogb?
- SGC – simple + deep
- GIN – expressive
- GAT – attention
- GGNN – recurrent
- CompGCN – combi with link predictor

And more Parameters

- batch size
- learning rate: [0.0001, 0.1] (Check what is useful)
- num layers: 1 - 8? (Check until not improving anymore)
- num hidden channels (Check what is useful)
- model-specific: GAT num heads, GraphSAGE pooling, CompGCN link predictor type, ...
- See also https://ogb.stanford.edu/docs/leader_overview/

(Record all required there to be able to submit results to the board later)

A lot of Research Questions

- Compare to non-GNN baselines MLP, Node2Vec (also tune those!)
- Large differences in best parameters for different models?
- Any great differences between GCN/SAGE/GAT/GIN, which are rather similar models?
- SGC vs. other GNNs with many layers?
- Effects of training on less (10-70%) or noisy data (5-20% of training labels wrong)
- Results: are all models good on same instances or can we cluster models?
- Compare to leaderboard numbers and models (& try to explain differences)
- Look into specifics of models: does attention provide interpretation?
- Verify special hypotheses: e.g., ogbl-ppa: GNN would need position info? -> check if number for recent position-aware GNN is better?

Questions / Ideas from you?

Final goal:
NeurIPS conference paper
https://neurips.cc/
(deadline usually in May)

Week 1

- Do we meet weekly on Wed 11 am?
- Send me your GitHub IDs
- Look into OGB paper
  (No need to read later parts on all experiments, start with ones we begin with)
- Checkout code on GitHub: https://github.com/vthost/ogb-revisited
- Checkout access to resources (university cluster?)
- Understand & run ogbn-proteins example experiment
- Week 2-3: Project report, but better get an idea about the task first
- Further questions, items, …?