Tuning Graph Neural Networks with Bayesian Optimisation

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Scientific Question

Are Graph Neural Networks appropriate for large scale graph-data optimisation jobs? (**in present**)

Motivation

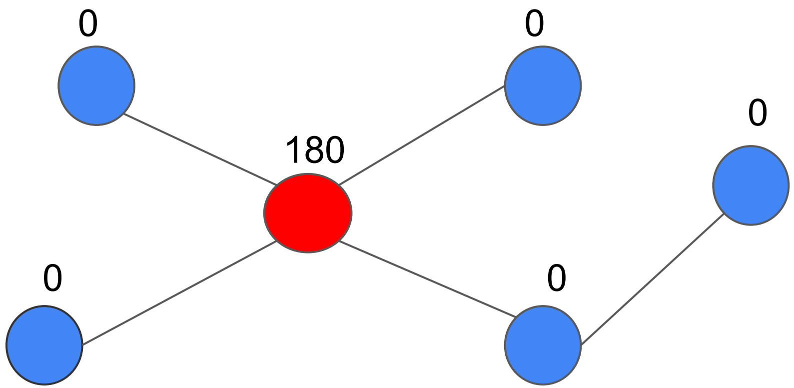
- Frameworks like REGAL use **16 layers deep** GNNs in the learning pipeline [1]

Conclusion: Depth is needed for such jobs

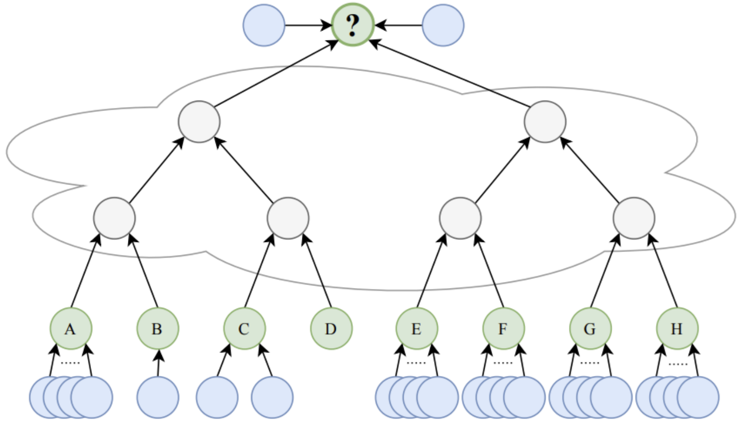
Background

Graph Neural Network face two big issues => cannot afford depth

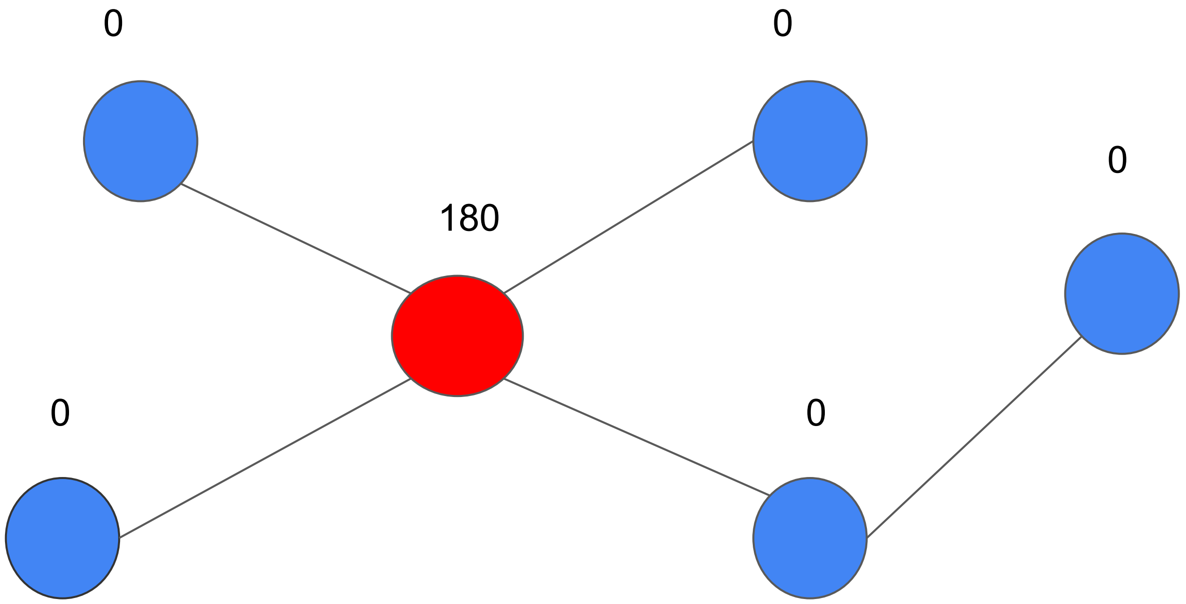
Oversmoothing



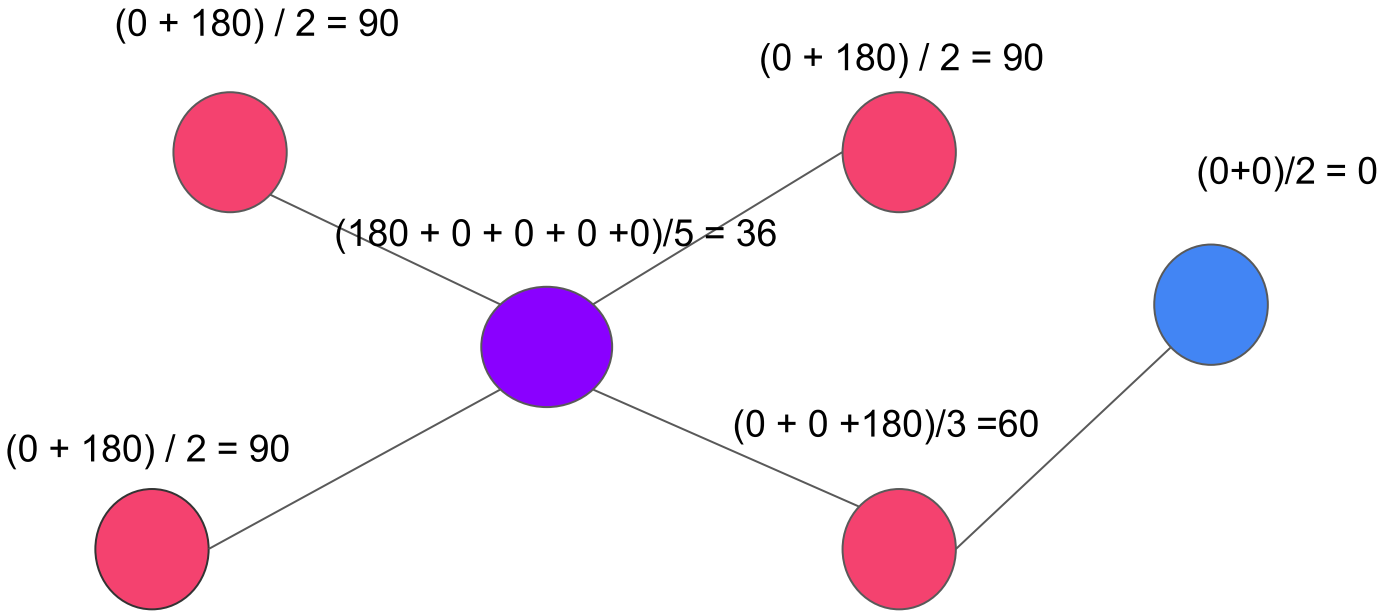
Oversquashing



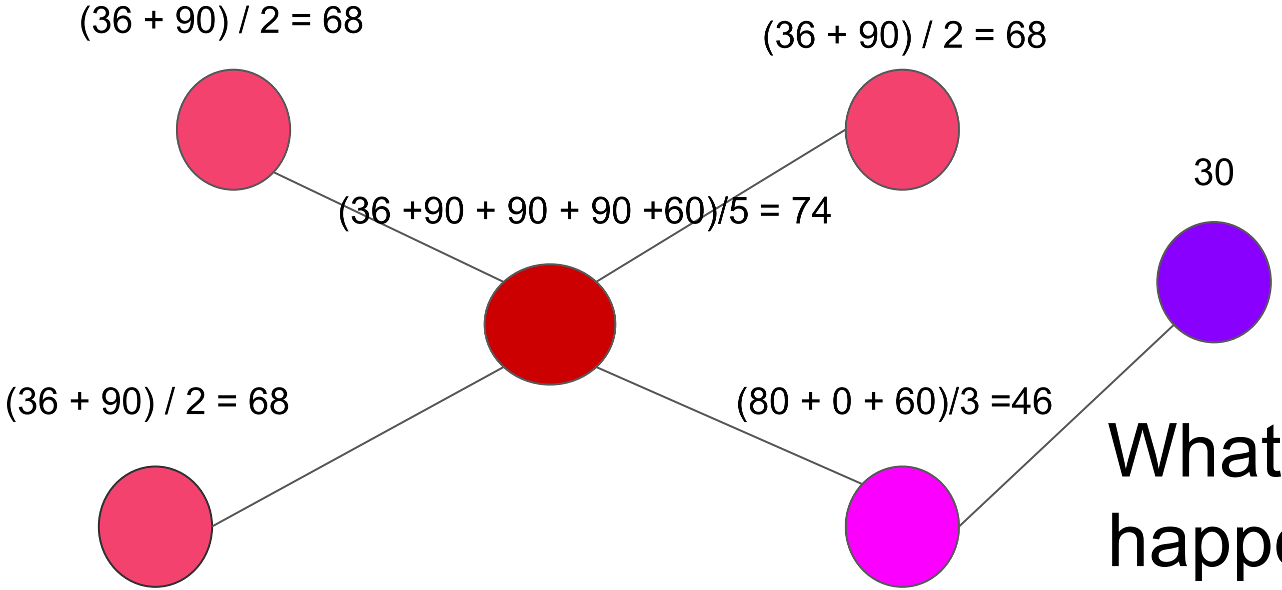
Oversmoothing - Iteration 0



Oversmoothing - Iteration 1



Oversmoothing - Iteration 2 - Observing a trend ?



What would happen for 16 layers (iterations)?

Methodology

Pick models from PyTorch-Geometric library:

- GCN [2]
- SSGConv (tackles oversmoothing) [3]
- ChebConv [4]

Benchmark graph dataset:

- Cora (aprox. 3000 nodes), PubMed [5] (aprox. 19000 nodes)

Apply Bayesian Optimisation Algorithm to find Best Depth on a Benchmark Classification Task:

- Question: What will be the best depth possible for these datasets? (varying from 1 to 100)

Analysis

Best depth:

- is it **3** or **20**? (my guess is 3)

What is the longest path in the current graph dataset (diameter):

- is it **20** or **100** or **500**? (my guess is 100)

If best accuracy for classification task on graphs is obtained with layers with depth 3 are GNNs really appropriate for Large Scale Data Optimisation jobs where ideally nodes would hold information about their furthest neighbours?

Results & Takeaways

- Will Tune GNNs with Bayesian Optimisation (varying depth) and add contribution to Pytorch Geometric
- Obtain results on what the ideal depth of GNN classifier for benchmark graph dataset
- Compare depth with how wide the initial graph was (its diameter)

What does this means for optimisation methods that leverage GNNs and need depth in order to function properly?

Citations

[1] Paliwal, A., Gimeno, F., Nair, V., Li, Y., Lubin, M., Kohli, P., & Vinyals, O. (2019). Regal: Transfer learning for fast optimization of computation graphs. arXiv preprint arXiv:1905.02494.

[2] Kipf, T. N., & Welling, M. (2016). Semi-supervised classification with graph convolutional networks. arXiv preprint arXiv:1609.02907.

[3]Wu, F., Souza, A., Zhang, T., Fifty, C., Yu, T., & Weinberger, K. (2019, May). Simplifying graph convolutional networks. In International conference on machine learning (pp. 6861-6871). PMLR.

[4] Defferrard, M., Bresson, X., & Vandergheynst, P. (2016). Convolutional neural networks on graphs with fast localized spectral filtering. Advances in neural information processing systems, 29.

[5] Yang, Zhilin, William Cohen, and Ruslan Salakhudinov. "Revisiting semi-supervised learning with graph embeddings." *International conference on machine learning*. PMLR, 2016.

Thank you for listening!

Questions?