Machine Learning with graphs - Project Defense

Delaunay Graph: Addressing Over-Squashing and Over-Smoothing Using Delaunay Triangulation
by Attali H., Duscaldi D. and Pernelle N. [1]

Edwin Roussin and Tristan Waddington

Supervised by Jhony H. Giraldo
IP-Paris, CEMST

26/03/2025

Introduction

Delauney triangulation

Reconstruct a graph completely from features using the Delaunay triangulation.
$\Rightarrow$ Avoid over-smoothing and over-squashing.

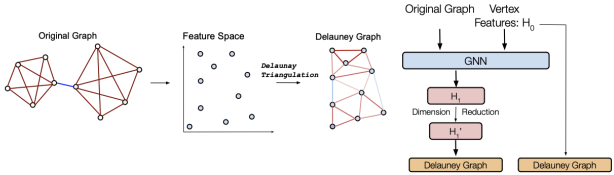

Figure: Illustration of the Delaunay [Attali al., 2024] [1]

Outline

Issues with graph rewiring
- Over-Squashing
- Over-Smoothing

Key technical novelty of the paper
- Theoretical Analysis

Experimental Evaluation
- Methodology
- Results
- Discussion

Conclusion

Issues with graph rewiring

Over-Squashing

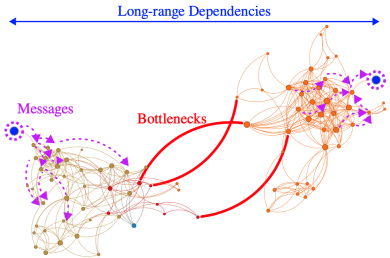

Figure: Illustration of Bottlenecks
[Giraldo, Lecture GNNs, 2025]

Over-Smoothing

Avoid over-smoothing in preventing the embedding to become the same::

- **Normalization** with PairNorm [Zaho, 2020][5].
- **Rewiring** Drop edges, at random [Rong, 2019][3] or in finding the potential good ones [Giraldo, 2023][2]

Over-smoothing and over-squashing are intrinsically related

Inevitable trade-off between these two issues, as they cannot be alleviated simultaneously.

Key technical novelty of the paper

Theoretical analysis

Delaunay rewiring

- Is an extreme 2 steps rewiring method.
- Where all edges are rebuilt during training from a umap embedding to triangles.
- Then mixed with the original edges of the graph.

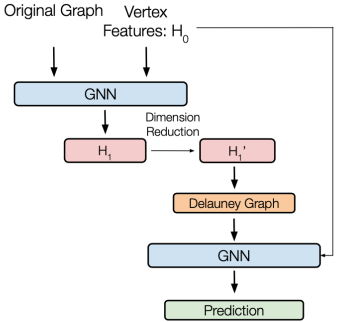

Figure 2: Illustration of the rewiring method using the features obtained by a GNN.

Theoretical analysis

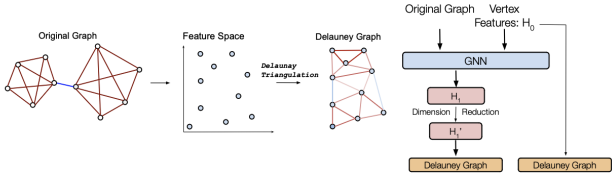

Figure: Illustration of the Delaunay [Attali al., 2024] [1]

Experimental Evaluation

Methodology

Aim to reproduce as closely as possible the experiments of the authors.

- Get same datasets, and preprocess them.
- Train the models with the same hyperparameters.
- Finally, we evaluate the models with the same metrics.

Results

Text Dataset preparation

- Text8 (English Wikipedia) processed.
- OpenWebText (GPT2 training material) processed in 18 hours.
- train/validation/test split according to experimental methodology.

We were unable to run the models

- Training impossible on our machines (size of model).
- Does not work on Colab (tensorflow numpy2 incompatibilities).
- No trained model shared by the authors.

Discussion

We faced huge challenges

- Graphs

Future paper that will be explored in the report:

- *Cayley Graph Propagation* by JJ Wilson, Maya Bechler-Speicher, Petar Veličković [4]

Conclusion

Conclusion

- Cannot confirm the results o
- Not able to reproduce.
- Hard time digging in code and documentation.

Do you have any question?

References

Hugo Attali, Davide Buscaldi, and Nathalie Pernelle.
Delaunay graph: Addressing over-squashing and over-smoothing using delaunay triangulation.
In *Forty-first International Conference on Machine Learning*, 2024.

Jhony H. Giraldo, Konstantinos Skianis, Thierry Bouwmans, and Fragkiskos D. Malliaros.
On the trade-off between over-smoothing and over-squashing in deep graph neural networks.
In *Proceedings of the 32nd ACM International Conference on Information and Knowledge Management*, CIKM '23, page 566–576. ACM, October 2023.

Y. Rong, W. Huang, T. Xu, and J. Huang.
Dropedge: Towards deep graph convolutional networks on node classification.
In *International Conference on Learning Representations*, 2019.

JJ Wilson, Maya Bechler-Speicher, and Petar Veličković.
Cayley graph propagation, 2024.

Lingxiao Zhao and Leman Akoglu.
Pairnorm: Tackling oversmoothing in gnns.
In *International Conference on Learning Representations*, 2020.