



Machine Learning with graphs - Project Defense

**Delaunay Graph: Addressing Over-Squashing and Over-Smoothing Using
Delaunay Triangulation**
by Attali et al. [1]

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Delayney triangulation

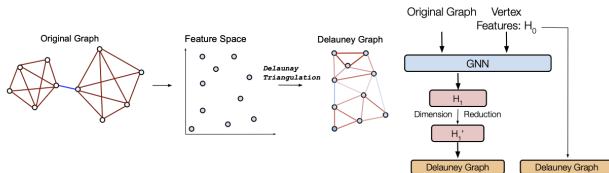


Figure: Illustration of the Delaunay [Attali al., 2024] [1]

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

Applications already exists on diverse fields such as *graph generation*, *text-to-sound generation* or *protein design*.

No access to heavy computing ressources:

Focus on text generation to understand and reproduce the results of authors.

2 models in paper:

- ❖ **MD4** (S/L) simple masked diffusion model.
- ❖ **GenMD4** Generalized state-dependent model (more complex).

Key technical novelty of the paper

State Dependent Masked Schedule:

Idea: time-dependent probability of masking a token to also depend on the token value. To be learned by NN.

In practice: polynomial schedules are described in the paper but on their code, the authors only relies on the cosine masking schedule¹.

¹ Class MaskingSchedule in <https://github.com/google-deepmind/md4/blob/main/md4/models/diffusion/md4.py>

Experimental Evaluation

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.

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.

We faced huge challenges

- ❖ Unknown flax framework
- ❖ Outdated dependencies in their GitHub
- ❖ Huge model size
- ❖ No trained model shared
- ❖ Students no competent in computer vision at the time.

Future paper that will be explored in the report:

- ❖ *Cayley Graph Propagation* by JJ Wilson, Maya Bechler-Speicher, Petar Veličković [2]

Conclusion

Conclusion

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

Do you have any question?



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.



JJ Wilson, Maya Bechler-Speicher, and Petar Veličković.

Cayley graph propagation, 2024.