Prof. Dr. Christian L. Müller
Ludwig-Maximilians-Universität München
Institut für Statistik
Ludwigstr. 33
80539 München
christian.mueller@stat.uni-muenchen.de

M.Sc. Thesis Proposal: *Interpretable chemical representations via sparsified Graph Attention Networks*

Objective: The main objective of this M.Sc. thesis proposal is to explore the use of the SparseMax [1] function in the graph attention network (GAT) [2] framework to generate an interpretable representation of molecular structures to predict a certain outcome. The main objectives include: i) incorporate SparseMax in the GAT framework, ii) train and evaluate sparsified GAT predictors on various molecular property prediction tasks, and iii) determine if there are improvements in predictive performance, training time, and interpretability of models trained with SparseMax.

To accomplish this, we will make use of the GAT implementation available in Geometric PyTorch and the SparseMax implementation made available by the authors. Benchmarks will include various regression and classification tasks from MoleculeNet. We will also apply the model to the task of predicting antimicrobial activity in the microbiome.

Plan and deliverables: A successful completion of the M.Sc. thesis requires the following computational and scientific advances. Firstly, the thesis should deliver a workflow that allows for the training of GAT-based predictive models with the optional use of SparseMax. Secondly, the student will determine if the use of SparseMax improves predictive performance over regular GATs.

A possible outcome of this analysis would be the determination sparsified GATs result in a better generalizability of GAT-based predictive models. Furthermore, the resulting attention weights accurately identify molecular substructures that contribute to the outcome of interest. When applying this strategy to the task of antimicrobial activity in the microbiome, we find certain substructures are more predictive of activity against specific bacterial species.

References

[1] Martins, A., & Astudillo, R. (2016, June). From softmax to sparsemax: A sparse model of attention and multi-label classification. In *International conference on machine learning* (pp. 1614-1623). PMLR.

[2] Veličković, P., Cucurull, G., Casanova, A., Romero, A., Lio, P., & Bengio, Y. (2017). Graph attention networks. *arXiv preprint arXiv:1710.10903*.