M2 Internship / PhD

# On optimization of Graph Neural Networks

Graph Neural Network (GNN) [4] are state-of-the-art deep models that can perform a wide range of Machine Learning task on graph data, with many applications in chemistry, biology, or recommender systems, to name a few [1]. Most GNN architectures are built by stacking layers of functions that perform *Message-Passing* (MP) along the edges of the graph, where each node receive messages from its neighbors and aggregate them to progressively build discriminative node representations.

Recently, it has been observed that *optimization* for GNNs may be subjected to phenomena [2, 3] that may be specific to them (compared to classical deep neural nets). Despite this, optimization remains a key aspect of GNNs that is relatively under-explored, both theoretically and empirically.

In this Master internship, potentially followed by a PhD, we will explore various optimization strategies for GNNs and how to improve them. Balance between theory and experimentation will depend on the candidate.

**Infos.** IRISA, Rennes, France. Starting date in 2026.

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## References

[1] Michael M. Bronstein, Joan Bruna, Taco Cohen, and Petar Veličković. Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges. *arXiv:2104.13478*, 2021.

[2] Nicolas Keriven. Backward Oversmoothing: why is it hard to train deep Graph Neural Networks? pages 1–20, 2025.

[3] MoonJeong Park and Dongwoo Kim. Taming Gradient Oversmoothing and Expansion in Graph Neural Networks. pages 1–19, 2024.

[4] Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and Philip S. Yu. A Comprehensive Survey on Graph Neural Networks. *IEEE Transactions on Neural Networks and Learning Systems*, pages 1–21, 2020.