

Master Internship / PhD: Local hyperbolicity and GNNs

Keywords

Gromov δ -Hyperbolicity, Graph Neural Network

Context

Ricci curvature, originally a concept from Riemannian geometry, has recently found applications in graph-based machine learning, including graph neural networks [TGC⁺22], and theoretical analysis of deep learning [BBC⁺24]. It provides a way to capture local and global structural properties of a manifold. Its interplays with optimal transport are numerous and arise mainly in foundational theoretical papers (e.g., [LV09]). In the case of a finite graph, the Ollivier-Ricci curvature, which is a discrete analogue of the Ricci curvature defined through the Wasserstein distance [Oll07], helps GNNs by improving connectivity-aware message passing, reducing over-smoothing or over-squashing [TGC⁺22], by detecting potential bottlenecks, and providing ways to weight or even rewire graph connections. Here, we plan to follow a similar path by examining other notions of curvature, notably the δ -Gromov hyperbolicity [Gro87], which is a measure of how closely a metric space resembles a tree-like structure, and hence is intimately linked to the fundamental *over-squashing problem* of GNNs [AY21]. One difficulty lies in adapting the combinatorial nature of δ -Gromov hyperbolicity in differentiable approximations that can be leveraged in optimization problems

In [HCMB⁺25], we recently proposed a solution to this last problem by defining a differentiable surrogate of δ -Gromov hyperbolicity that can be leveraged in gradient based optimization. However, the computational cost of this quantity, which is a global characteristic of the graph, still scales prohibitively ($O(n^4)$) with respect to the number n of nodes in the graph.

Expected outputs

In this internship, potentially followed by a PhD, we will focus on a novel notion of local hyperbolicity, which will be computed on a neighboring area of a node. By doing so, we will define a new local measure of how the graph looks locally like a tree. The multiscale property, obtained by varying the size of the neighborhood, will be considered from a practical standpoint and theoretically analyzed in a context of random graph. Ultimately, we will try to use this information to detect and eventually mitigate the oversquashing problem in GNNs.

Supervision

The research project of this internship will be conducted in the context of the IRISA laboratory (<http://www.irisa.fr/>), which is a joint research unit between CNRS, INRIA and several Universities and Engineering schools in Brittany (West of France). IRISA conducts research in computer science, applied mathematics and signal and image processing.

The Internship / PhD will be jointly supervised by **Nicolas Keriven**¹ (CR CNRS), **Prof. Laetitia Chapel**² (Professor Institut Agro Rennes) and **Prof. Nicolas Courty**³ (Professor UBS, located in Vannes), and funded by ERC MALAGA nkeriven.github.io/malaga/.

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Info.

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