Master 2 Internship Proposal (Spring 2022): Random Graphs in Machine Learning

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Context. In the last decade, machine learning (ML) on *graph data* has known a rapid growth, with the advent of kernel methods on graphs [6], Graph Neural Networks [1, 7] (GNNs), benchmark datasets [3], and numerous applications ranging from the analysis of social networks to molecular classification or protein interface prediction.

Despite this, generalization bounds and sample complexities, which characterize the amount of training data needed to ensure a low prediction error on new test data, are missing in the graph setting. This is especially true for *node-level tasks* such as Semi-Supervised Learning (SSL) [2], where the goal is to predict node labels on one or several graphs from partially labelled training nodes. This is often due to the lack *statistical modelling* of the graph structure: indeed, when no assumption is made on the graph-generating process to characterize unseen test data, the very notion of generalization becomes ill-defined.

On the other hand, *random graph* (RG) models represent a vast field of study in statistics and graph theory, but have hardly been explored in ML, despite immediate connections. In particular, *Latent Position Models* [4] (LPM: each nodes is associated to an unknown latent variable, and edges are randomly generated according to these variables) such as Stochastic Block Models, graphons or ϵ-graphs, offer striking similarities with classical ML settings, with the significant difference that latent variables are unobserved and must be indirectly deduced from the graph structure. Nevertheless, LPMs allow for instance to study some properties of GNNs in the infinite number of nodes limit [4, 5], but the generalization capacities of GNNs and other models are still mostly unknown.

Goals. The goal of this internship is the explore the use of RG models in ML, and to study quantities such as generalization bounds, sample complexities, and so on, in this context. We will compare several ML models including GNNs, and, depending on the progress of the candidate, several RG models, such as LPMs and preferential attachment models.

Profile sought The internship requires some background in machine learning or computational/theoretical statistics. Some prior knowledge of graph theory is useful but not necessary. Applicants need to be familiar with one of the following languages: Python, Julia or R.

The internship. This internship will take place at Gipsa-lab in Grenoble, France, and may involve a number of visits to the nearby city of Lyon. A "gratification de stage" (compensation) of approx. 500€/month will be provided to the intern. The usual duration of an M2 internship is 6 months, starting in the Spring of 2022. **The internship may be followed by a 3-years PhD funded by the ANR project GRANDMA**[1].

Application, contact. Please send a CV and short statement of interest to
`nicolas.keriven@cnrs.fr`; `simon.barthelme@grenoble-inp.fr`; `yohann.de-castro@ec-lyon.fr`
Do not hesitate to contact us if you have any question.

[1] `https://nkeriven.github.io/grandma/`

References

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