Internship:
(Deep) Graph Neural Networks for Fundamental Physics:
the case of Glassy liquids

Key words: Machine Learning - Graph Neural Networks (GNN) - application to Fundamental Physics - Structural Glasses - Glassy Liquids

Genereal context:

In the last decade (since 2012), Deep Neural Networks (DNN) have become an iconic success of Machine Learning, renewing the interest for the subject, to say the least. Particular attention has been paid to Convolutional Neural Networks (CNN), which are very well suited to visual data, and have yield impressive results. However, this recent success also comes from the automation of the algorithms (automated differentiation performed by libraries), the availability of large datasets and the development of GPGPUs. These last three features can be put at use in the more recent Graph Neural Networks (GNNs). GNNs are able to handle graph-based data: the key idea is to perform local operations (as in convolutions) that can adapt to the variety of nodes' geometry (variable degree, as opposed to the constant geometry seen in an image). This makes GNNs able to handle, for instance, molecular data [CYZ+19].

In fundamental Physics, a crucial and unsolved problem is that of understanding the behavior of structural glasses (also called glassy liquids). For these materials, there is no known function that can infer the local state (liquid/solid) from the local geometry of particles. This task can be attacked using Machine Learning, and in particular, using GNNs.

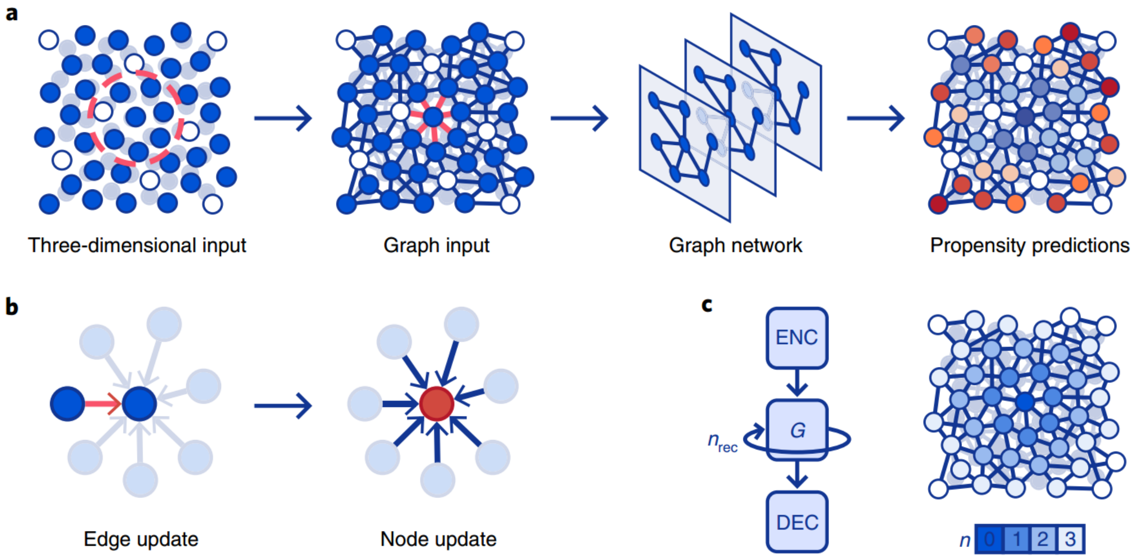

Figure 1: Essential steps involded in the GNN procedure.

Internship details and goals:

The idea of using Machine Learning to attack the problem of Structural Glasses is rather recent, the first works dating from 2015 [SCS+15] and more recently, [LBD+20]. However most of these works rely on simple, yet robust ML technology: concretely, binary classification using SVMs (shallow learning). In a previous (short) internship, it has been shown that a regression approach performed equally well as the corresponding binary classification approach. This opens the way to methodological changes in the approach. Independently and very recently, GNNs have been demonstrated to perform better than previous models to predict the local state (liquid/solid) in supercooled liquids [BKGB+20].

The internship's goal is to understand and critically assess the performance of past GNNs, and ultimately design new ones, taking into account the specificities of the problem at hand. Depending on the interests and abilities of the trainee, this task may be attacked more or less directly. At first, the trainee will be expected to get acquainted with the physics literature on glassy dynamics (for this, the previous internship report may help, along with more thorough reviews). To get a grasp of the concrete problem, one may then use the available software and data (from our team, [LBD+20]) of Molecular Dynamics simulations, which may also help in strengthening the knowledge of fundamentals of ML. Then, before designing novel GNNs architectures, one may use the available code from literature [BKGB+20] to get acquainted with GNNs (and DNNs in general) and reproduce past experiments. Using this vanilla GNN as a base, the trainee will be able to propose more advanced or entirely novel architectures to better tackle the problem. This goal is ambitious, and if it is reached it may of course lead to a publication.

References

[BKGB+20] V. Bapst, T. Keck, A. Grabska-Barwińska, C. Donner, E. D. Cubuk, S. S. Schoenholz, A. Obika, A. W. R. Nelson, T. Back, D. Hassabis, and P. Kohli. Unveiling the predictive power of static structure in glassy systems. *Nature Physics*, 16(4):448–454, April 2020.

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[LBD+20] François P. Landes, Giulio Biroli, Olivier Dauchot, Andrea J. Liu, and David R. Reichman. Attractive versus truncated repulsive supercooled liquids: The dynamics is encoded in the pair correlation function. *Physical Review E*, 101(1):010602, January 2020. arXiv: 1906.01103.

[SCS+15] Samuel S. Schoenholz, Ekin D. Cubuk, Daniel M. Sussman, Efthimios Kaxiras, and Andrea J Liu. A structural approach to relaxation in glassy liquids. *Nature Physics*, 12(5):469–471, February 2015. arXiv: 1506.07772 ISBN: 1745-2473.

Expected abilities:
The internship is open to candidates from both ML (Machine Learning) or Physics backgrounds. In any case, the trainee is expected to be proficient in python, and/or C++ (an imperative language).
In any case, strong proficiency is expected in mathematics (algebra, calculus, etc).
For physicists, a good knowledge of Machine Learning, and a strong interest in it, is needed. The ideal candidate will have some prior knowledge of Deep Learning, and of a standard library (TensorFlow or PyTorch). Of course a Physics background implies advanced understanding of Statistical Physics.
For Computer Scientists, some knowledge of basic Statistical Physics (statistical equilibrium, entropy, etc) is a great plus, since it's important to understand the underlying application problem. The ideal candidate will have some more advanced knowledge of Statistical Physics (phase transitions, order parameter, disordered media, out-of-equilibrium dynamics, etc). Of course a CS/ML-background implies advanced understanding of Deep Learning and related techniques.

Duration: The preferred duration would be of at least 4 months.
Lab: LRI (to become LISN), Université Paris-Saclay
Team: TAU (TAckling the Underspecified)
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