(M1) TER:
Graph Neural Networks for Glasses

Key words: Machine Learning - Graph Neural Networks (GNN)

Motivation:

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.

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.

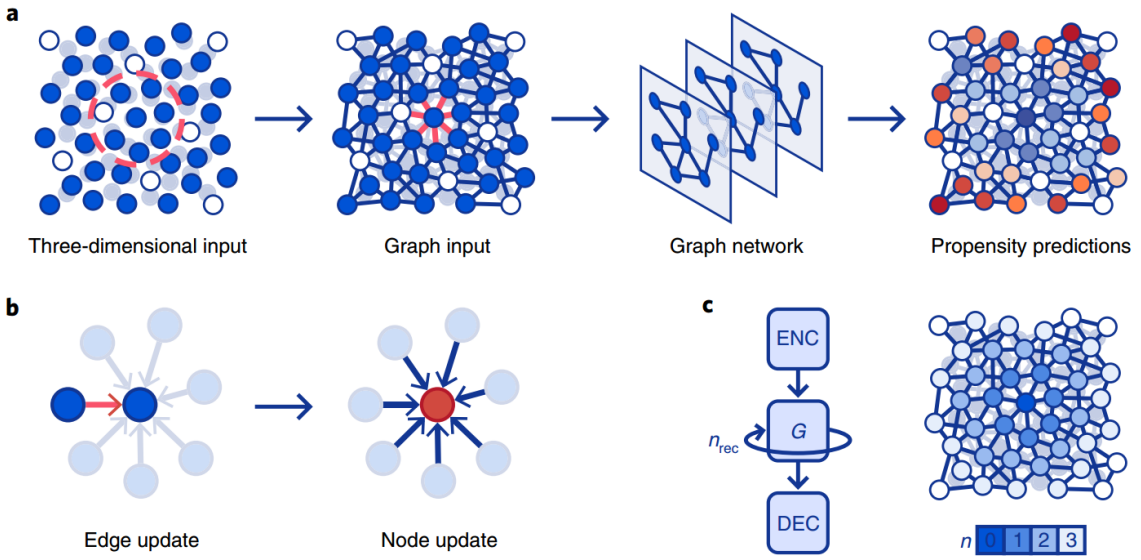

Figure 1: Essential steps involded in the GNN procedure.

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].

TER details:

In the view of a possible internship working on our network for glasses [PCL22], the student could get acquainted with GNNs and how they work, ultimately building a simple one, understanding the key concepts well.

- Before going to GNNs, getting acquaited with Pytorch is good, e.g. using https://pytorch.org/tutorials/beginner/basics/intro.html
- About theory of GNN, one may start with tutorials as e.g. : https://distill.pub/2021/gnn-intro/ and the pedagogical summary in https://webthesis.biblio.polito.it/secure/20440/1/tesi.pdf
- Then, it should be straightforward to use PyTorch Geometric, https://pytorch-geometric.readthedocs.io/en/latest/,
- To ge deeper in the theory, one could read parts of [BHB+18], that contains a lot of meta-reasoning (not fully needed), but where the part of the message passing is well explained; and also read [GSR+17], the first paper that introduces the idea of message-passing networks and shows that a lot of different architectures can be re-framed in this framework.

References

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[PCL22] Francesco Saverio Pezzicoli, Guillaume Charpiat, and François P. Landes. SE(3)-equivariant Graph Neural Networks for Learning Glassy Liquids Representations, November 2022. arXiv:2211.03226 [cond-mat].

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