Thesis Proposal: Deep Graph Representation Learning on non-uniform 3D objects

Location: Computer science Research Institute of Lens (CRIL), Lens, France

Project context:

Machine learning involves leveraging data to extract mathematical models capable of generalizing or describing this data according to predefined objectives. This data comes in various forms, ranging from well-defined structures like images and matrices to semi-structured formats such as text and graphs. However, dealing with entirely unstructured data, such as non-uniform 3D objects, poses a challenge for traditional methods that primarily focus on geometric analysis.

The development of artificial intelligence, particularly deep learning, has greatly improved performance compared to conventional learning methods, especially when it comes to textual data, images, graphs, sequences, and more. However, learning on non-uniform 3D objects remains a significant challenge. This field is garnering increasing interest in various applications such as predicting molecular properties based on their 3D structures rather than textual features [2].

In the field of bioinformatics, protein annotation based on their 3D interactions is an example [1], as is the use of 3D structures in physics to simulate objects [3] or body parts to analyze their behavior. These applications demonstrate the utility of analyzing or learning on non-uniform 3D objects, thus sparking considerable interest within the scientific community.

Objectives of the thesis

This thesis focuses on deep learning, with an emphasis on learning graph representations. Graphs are widely used in many applications, providing a versatile representation for non-regular objects, including 3D meshes, as an alternative to traditional methods such as CNNs or image segmentation models like U-net. This thesis explores graph neural networks (GNNs) for modeling non-regular 3D objects, such as 3D meshes. Unlike CNNs, GNNs are designed to handle graph-type data, making them more suitable for representing 3D meshes. They have demonstrated superior performance in modeling such data, offering a promising alternative to existing methods. However, despite their effectiveness, GNNs face scalability challenges, especially with complex meshes. This thesis proposes solutions to overcome these challenges by exploring mesh-specific pooling methods and other strategies to simplify learning. It also considers approaches for constructing graphs from 3D meshes to enhance learning efficiency. In addition to the static aspect of data, this thesis addresses the application of GNNs to data with temporal patterns or

features. It explores their uses in domains such as fluid simulation, weather modeling, and 3D medical imaging, as well as in physical simulation of 3D meshes. This highlights the temporal evolution of meshes in both space and time.

Profile:
Ideally, the recruited person will hold a Master's degree in computer science and have theoretical and practical knowledge in deep learning. Experience of machine learning on graphs is also desirable but not essential. The candidate must demonstrate:

- Programming skills, such as proficiency in Python, for example
- Experience in Deep Learning, data mining
- Synthesis and writing skills allowing for clear and effective reporting of work done

The thesis will start in October 2024, and funding will last for three years.

Application submission:
Applications should be submitted by email until April 25, 2024, to Wissem Inoubli (inoubli@cril.fr) and Said Jabbour (jabbour@cril.fr). Please submit in a single PDF:

- A detailed CV of your past activities (with possibly a list of publications)
- A letter presenting your motivations, qualifications, and experiences related to the topic
- University certificates
- Contact details or letters of recommendation (a minimum of 2 appreciated)

Please note that all documents should be in English or French.

References

[1] Laveglia, V., Giachetti, A., Sala, D., Andreini, C., & Rosato, A. (2022). Learning to Identify Physiological and Adventitious Metal-Binding Sites in the Three-Dimensional Structures of Proteins by Following the Hints of a Deep Neural Network. Journal of Chemical Information and Modeling, 62(12), 2951-2960.
[2] Yang, Y., Yao, K., Repasky, M. P., Leswing, K., Abel, R., Shoichet, B. K., & Jerome, S. V. (2021). Efficient exploration of chemical space with docking and deep learning. Journal of Chemical Theory and Computation, 17(11), 7106-7119.
[3] Atz, K., Grisoni, F., & Schneider, G. (2021). Geometric deep learning on molecular representations. Nature Machine Intelligence, 3(12), 1023-1032.
[4] Cao, Y., Chai, M., Li, M., & Jiang, C. (2023, July). Efficient learning of mesh-based physical simulation with bi-stride multi-scale graph neural network. In International Conference on Machine Learning (pp. 3541-3558). PMLR.
[5] Fahim, G., Amin, K., & Zarif, S. (2022). Enhancing single-view 3D mesh reconstruction with the aid of implicit surface learning. Image and Vision Computing, 119, 104377.