Generative Graph Convolutional Neural Networks applied to Materials Science Problems

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Over the last decade or so, Machine Learning (ML) Techniques have found widespread applicability both in industry and science. Particularly, Deep Learning (DL), the branch of ML that is concerned with the design, training and deployment of Artificial Neural Networks (ANN), has demonstrated the ability to address problems that were previously intractable, such as near-human image classification, speech recognition, autonomous driving, etc. However, conventional ANNs have traditionally worked with structured data, such as a matrix of pixels in an image, while very often one is confronted with relational information that cannot be easily cast into a structured data form. This limitation has motivated the development of so-called *Graph Neural Networks* (GNN). Graphs provide a more general way of representing interrelated data structures which is free of the constraints inherent to structured data. Typically, a graph consists of nodes, encoding items of information or node properties, and edges, representing relations between the nodes in the graph; edges themselves can encode information, such as properties of the relation between the pair of linked nodes. GNNs can take graphs as their input both to be trained and to address a number of graph-related problems, such as node classification, property prediction (at the node or graph level), etc.

To the physicist, chemist or biologist, a graph is an ideal way of representing a crystal, a molecule, a disordered array of atoms (amorphous material), or even a complex bio-molecule. It is therefore not surprising that one can envisage many ways in which graph-based AI strategies may be useful in Condensed Matter and Molecular Physics, and Materials Sci-

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ence. In this project we aim to use *Graph Convolutional Neural Networks* to accelerate the design and theoretical analysis of crystalline, amorphous and molecular materials. Specifically, our aim is to design generative systems such as Variational Auto-Encoders (VAE) or Generative Adversarial Networks (GAN) capable of working with graphs, that can be trained on existing materials databases, and used in order to create new crystal or molecular structures with desirable structural or chemical/physical properties. This field of research is at the cutting edge of the application of Artificial Intelligence techniques to Materials Science and Condensed Matter Physics.