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A Hands-on Introduction to Geometric Deep Learning, with Examples in PyTorch Geometric

A minitutorial at the SIAM Conference on Computational Science and Engineering, February 26 - March 3, 2023

Abstract

Neural Networks and Deep Learning have started only recently to become standard tools in simulation and computational sciences, and they have already enabled significant advances, becoming a viable option for the data-driven solution of possibly high-dimensional and parametric PDEs. In the deep learning literature, recent years have seen a growing interest for the development of Geometric Deep Learning (GDL) and Graph Neural Networks (GNNs), which are deep learning techniques applicable to graph-structured inputs. This field is particularly relevant to address the typical mesh-based problems that are often encountered in the numerical solution of PDEs, and indeed initial results in this direction are being investigated. The aim of this tutorial is to provide an hands-on introduction to this novel field of machine learning, addressed to an audience with a computational science background. We will recall some basic facts on graph theory, introduce the fundamental ideas underlying the functioning of GNNs and describe their common mathematical formulation, and provide several concrete examples of the most common GNN layers. These ideas will be complemented by a series of example notebooks implementing working examples in PyTorch Geometric, which is a standard library for GDL in Python. At the end of the tutorial, the audience will be able to load custom graph-based data and train simple GNN models for regression and classification of nodes and graphs.

Organization and material

The tutorial is divided in two parts:

- **Part I:** Thursday, March 2, 2:35 PM - 4:15 PM, Room G103
  - Presenter: Gabriele Santin
  - Goals: Motivations, Intro of basic concepts, definition of GNNs
  - Material: Slides and Notebooks.
- **Part II:** Thursday, March 2, 4:45 PM - 6:25 PM, Room G103
  - Presenter: Antonio Longa
  - Goals: Practical session, self-contained code for GNN training
  - Material: Slides and Notebooks.