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Graph-informed neural network and discontinuity learning

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In several applications related to rather complex problems, the availability of reliable surrogate models is of paramount importance. This is the case, for example, of multi-query tasks, such as uncertainty quantification analyses or optimization problems. In order to reduce the computational complexity of such processes, recent literature shows that it is worth considering the application of neural networks (NN) to perform regression tasks.

In several applications (such as transportation systems, epidemic spread, and social interactions), network analyses come into play, and graphs have a key role in such frameworks. Recently, new key contributions have been proposed by the neural network (NN) community, extending deep learning (DL) approaches to graphs via the so-called graph neural networks (GNNs) and the more recent graph convolutional networks (GCNs). Despite the good results of GCNs in many applications, some challenges still exist: (i) building deep GCNs with good performances; (ii) building GCNs scalable for large graphs.

In this talk, we present a new type of layer designed for regression tasks on graphs, a framework for which GCNs are not well suited and the use of multi-layer perceptrons (MLPs) is usually preferred. The new graph layer exploits the graph structure to improve the NN training (compared to an MLP). Moreover, it allows the building of deep NNs and it is scalable for large graphs. This new layer is called graph-informed (GI) layer [1]. Numerical experiments show the potentiality of the graph-informed NNs (GINNs), highlighting in particular improved regression abilities of the GINNs on maximum-flow regression problems, with respect to MLPs' performances on the same problem.

GI-layers have been recently exploited also to develop a new algorithm based on sparse grids for detecting discontinuity interfaces of n-dimensional piece-wise continuous functions; this task is of interest for example in UQ analyses, as in some applications the Quantity of Interest may be a discontinuous function in the space of stochastic parameters, thus preventing from the effective application of stochastic collocation strategies.

REFERENCES

[1] Berrone, S., Della Santa, F., Mastropietro, A., Pieraccini, S., and Vaccarino, F. (2022). Graph-Informed Neural Networks for Regressions on Graph-Structured Data. Mathematics, 10, 786.