GRAPH CALCULUS NEURAL NETWORKS

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ABSTRACT

Universal approximation theorems have advanced the use of Neural networks for parametric interpolation of functions. Among them, Graph Neural Networks (GNNs) are the popular choice for data-driven physics problems for their ability to naturally treat unstructured data. However, many of these physical problems admit to a partial differential equation model, requiring the approximation of differential operators in addition to algebraic functions. The errors in the traditional GNNs due to this limitation are typically mitigated by making the network larger to enrich its representation capacity. The obvious downside of this approach is the inflated demand for training data for these complex networks. In this work, we introduce the Graph Calculus Neural Network (GCNN) that builds upon a non-local calculus on finite weighted graphs to approximate differential quantities within the network layers. We first demonstrate the representation capability of GCNNs with regard to differential operators. Systematic proofs of convergence of the GCNN representations to local differential operators, the ability to tune their order of accuracy [1] via sampling of graph nodes and of the further convergence with density of sampling will be presented. Finally, we present three example applications of this differential representation in learning (1) reduced order models for PDEs, (2) representations for differentiable quantities of interest, and (3) surrogate models for the evolution of PDEs.

REFERENCES

[1] M. Duschenes, S. Srivastava and K. Garikipati, Numerical analysis of non-local calculus on finite weighted graphs, with application to reduced-order modelling of dynamical systems, *Computer Methods in Applied Mechanics and Engineering*, **402**, 115513, 2022.