A physics-informed DeepONet model for the solution of quantum graphs

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In this talk we focus on a machine learning approach for quantum graphs, i.e. metric graphs with an associated differential operator. In our case the differential equation is a drift-diffusion model. Computational methods for quantum graphs require a careful discretization of the differential operator that also incorporates the node conditions, in our case Kirchhoff-Neumann conditions. Traditional numerical schemes are rather mature but have to be tailored manually when the differential equation becomes the constraint in an optimization problem. Recently, physics informed deep operator networks (DeepONets) have emerged as a versatile tool for the solution of partial differential equations from a range of applications. We train physics-informed DeepONet models on a simple reference graph and show how to combine them for the solution of quantum graphs.

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