Non-linear activation using Variational Quantum Splines in Quantum Physics-Informed Neural Networks

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Abstract

Partial differential equations are often used to model physical phenomena, like wave propagation in fluid dynamics and electromagnetics, traffic flow, heat conduction etc. Given their complexity, the governing equations are solved numerically, to obtain discrete solutions in space and time. An emerging approach in this endeavour, utilizes parameterized quantum circuits as physics-informed neural networks, that function by minimizing the error, or loss incurred, in satisfying the governing equations[1]. Quantum neural networks enable a feature space where quantum kernels can explicitly be used to map data to a higher-dimensional feature Hilbert space [2].
A key constituent that highly effective classical neural networks utilize to capture complex patterns, is the use of non-linear activation functions. Recently, the idea of employing a variational version of quantum splines has been proposed to approximate non-linear quantum activation functions [3], as a near-term measure to eliminate the otherwise required use of the HHL. We demonstrate and assess the use of non-linear quantum operations in the form of variational quantum splines, as activation in QPINN-driven solutions to representative problems in computational fluid dynamics. The findings also yield requisites for other potential approaches to non-linear activation routines, in the more generalized scope of quantum neural networks. We also address the issue of scaling to larger problem sizes, aimed at practical relevance in the near-term.

Keywords: *Non-linear Activation, Variational, QPINN.*

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