Enhancing differentiable quantum circuits for solving complex PDEs: A battery simulation perspective

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Many scientific problems can be formulated in terms of conservation laws and rates of changes, which can be mathematically represented as systems of Partial Differential Equations (PDEs). However, the inherent scale and complexity of these systems of PDEs present formidable obstacles when attempting to solve them using conventional computational approaches, including mesh-based algorithms like the Finite Element Method. As a result, finding solutions for such systems often becomes arduous or even intractable. Quantum Scientific Machine Learning (QSciML) has recently emerged as a new paradigm to solve complex problems in science and engineering, including the solution of intricate Partial Differential Equations.

A prominent method proposed for solving PDEs involves the utilization of Differentiable Quantum Circuits (DQCs), as introduced by Kyriienko et al. in their work [1]. This approach draws inspiration from Physics-Informed Neural Networks (PINNs), which employ classical Neural Networks (NNs) to represent the solution to the PDE system. DQC extends this concept by incorporating quantum NNs (QNNs). By leveraging QNNs, DQC offers the potential for a spectral basis-set size that can scale exponentially with the number of qubits, enabling accurate fitting of solutions even in higher-dimensional problems, while remaining compatible with near-term quantum processors. Herein we follow a pragmatic approach by analysing different aspects of the DQC algorithm and providing insights regarding its scalability and applicability.

Our study focuses on examining the impact of various feature maps utilized to encode the data into the quantum circuit, along with different Ansaetze choices for the QNN. We put emphasis on digital-analog architectures as they are particularly suitable for near-term quantum devices such as PASQAL's neutral atoms quantum computers. Additionally, we address trainability considerations, building upon previous research on the analysis of the loss function landscape in QNNs [2]. By investigating the loss landscape we aim to gain valuable insights into the well-known barren plateau problem. This problem arises when the gradient of the loss function becomes exponentially small, resulting in gradient-based optimization techniques becoming computationally infeasible. Our analysis of the DQC loss landscape sheds light on strategies to overcome this challenge, including the exploration of initialization techniques [3] that mitigate the effects of the barren plateau problem.

To demonstrate the developments and the applicability of the method we utilize an industrially relevant use case, namely the computational simulation of electrical Li-ion battery devices [4], where systems of PDEs are used to describe the dynamics of the electrical potentials, currents and mass transport within the battery. We show the effect of our techniques in a relatively simple computational battery model and we highlight the expectation for future development.

References

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