Physics-informed neural network (PINN) for solving quantum master equation via Wigner function

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Quantum master equations refer to operator valued equations that describe open quantum systems via the evolution of their density matrix. Standard techniques, usually based on the associated symmetry group of the system, are applied to transform a master equation to a partial differential equation, a Fokker-Planck type equation (FPE), for a quasi-probability function defined on some underlying phase space. Quasi-probability functions, e.g. the Wigner function, the P, Q functions etc, supported by initial, boundary conditions determine the temporal evolution of the quantum system from which statistical predictions are obtained. One the other hand, the so called physics-informed neural networks, PINNs, based on deep learning ideas, is a recent kind of mathematical and computational solution methodology. PINNs are intended for solving various scientific and engineering problems involving ordinary or partial differential equations. The computational part is based on a developed open source machine learning platform, that includes the scientific software Tensorflow and an application programming interface Keras for deep learning applications. In this work both quantum master problems and PINNs are combined to address the solution of typical master equation problem. Specifically the problem of a single boson mode interacting with a nonlinear Kerr medium yields a third order nonlinear FPE. The equation describes the evolution of Wigner function defined in phase plane with symmetry group the Euclidean group ISO(2) and its algebra of generators i.e. plane translations and rotations. An architecture of the computational model provides two inputs: the time τ and the angle φ variables, hidden layers and one output W, the Wigner function. Providing initial and boundary conditions the unique solution of FPE is obtained everywhere on (τ,φ) domain. A learning is performed through training the PINN in order to fit the FPE, the initial condition ($\tau=0$), the boundary conditions and the normalization integral of Wigner function over the circle at collocation points (training samples). An analysis of numerical results, including a loss function, a choice of a number of hidden layers, neurons, training iterations, samples (collocation points), batch sizes is given. Figures illustrating the evolution of model accuracy, model loss (mean squared error), the output of the neural network and predicted approximate solutions in the discretized domain (τ,φ) are provided. Numerical experiments show that the accuracy of computations mostly depends of the number of training epochs and the number of collocation points. Increase of number of hidden layers and neurons improves the convergence rate, at the cost of rapid increase of computation time. Thus, NN parameters should be chosen carefully to reach desired results. These issues confirm an efficiency of the introduced, PINN-in-quantum-master-equation, methodology.