Stiff-PINN: Physics-Informed Neural Network for Stiff Chemical Kinetics

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Abstract

Recently developed physics-informed neural network (PINN) has achieved success in many science and engineering disciplines by encoding physics laws into the loss functions of the neural network, such that the network not only conforms to the measurements, initial and boundary conditions but also satisfies the governing equations. This work first investigates the performance of PINN in solving stiff chemical kinetic problems with governing equations of stiff ordinary differential equations (ODEs). The results elucidate the challenges of utilizing PINN in stiff ODE systems. Consequently, we employ Quasi-Steady-State-Assumptions (QSSA) to reduce the stiffness of the ODE systems, and the PINN then can be successfully applied to the converted non/mild-stiff systems. Therefore, the results suggest that stiffness could be the major reason for the failure of the regular PINN in the studied stiff chemical kinetic systems. The developed Stiff-PINN approach that utilizes QSSA to enable PINN to solve stiff chemical kinetics shall open the possibility of applying PINN to various reaction-diffusion systems involving stiff dynamics.

Introduction

Deep learning has enabled advances in many scientific and engineering disciplines, such as computer visions, natural language processing, and autonomous driving. Depending on the applications, many different neural network architectures have been developed, including Deep Neural Networks (DNN), Convolutional Neural Networks (CNN), Recurrent Neural Networks (RNN), and Graph Neural Network (GNN). Some of them have also been employed for data-driven physics modeling [1–8], including turbulent flow modeling [9] and chemical kinetic modeling [10]. Those different neural network architectures introduce specific regularization to the neural network based on the nature of the task such as the scale and rotation invariant of the convolutional kernel in CNN. Among them, the recently developed Physics-Informed Neural Network approach (PINN) [11–17] enables the construction of the solution space of differential equations using deep neural networks with space and time coordinates as the inputs. The governing equations (mainly differential equations) are enforced by minimizing the residual loss function using automatic differentiation and thus it becomes a physics regularization of the deep neural network. This framework permits solving differential equations (i.e., forward problems) and conducting parameter inference from observations (i.e., inverse problems). PINN has been employed for predicting the solutions for the Burgers' equation, the Navier–Stokes equations, and the Schrodinger equation [12]. To enhance the robustness and generality of PINN, multiple variations of PINN have also been developed, such as Variational PINNs [18], Parareal PINNs [19], and nonlocal PINN [20].

Despite the successful demonstration of PINN in many of the above works, Wang et al. [21] investigated a fundamental mode of failure of PINN that is related to numerical stiffness leading to unbalanced back-propagated gradients between the loss function of initial/boundary conditions and the loss function of residuals of the differential equations during model training. In addition to the numerical stiffness, physical stiffness might also impose new challenges in the training of PINN. While PINN has been applied for solving chemical reaction systems involving a single-step reaction [15], stiffness usually results from the nonlinearity and complexity of the reaction network, where the characteristic time scales for species span a wide range of magnitude. Consequently, the challenges for PINN to accommodate stiff

kinetics can potentially arise from several reasons, including the high dimensionality of the state variables (i.e., the number of species), the high nonlinearity resulted from the interactions among species, the imbalance in the loss functions for different state variables since the species concentrations could span several orders of magnitudes. Nonetheless, stiff chemical kinetics is essential for the modeling of almost every real-world chemical system such as atmospheric chemistry and the environment, energy conversion and storage, materials and chemical engineering, biomedical and pharmaceutical engineering. Enabling PINN for handling stiff kinetics will open the possibilities of using PINN to facilitate the design and optimization of these wide ranges of chemical systems.

In chemical kinetics, the evolution of the species concentrations can be described as ordinary differential equation (ODE) systems with the net production rates of the species as the source terms. If the characteristic time scales for species span a wide range of magnitude, integrating the entire ODE systems becomes computationally intensive. Quasi-Steady-State-Assumptions (QSSA) have been widely adopted to simplify and solve stiff kinetic problems, especially in the 1960s when efficient ODE integrators were unavailable [22]. A canonical example of the utilization of QSSA is the Michaelis–Menten kinetic formula, which is still widely adopted to formulate enzyme reactions in biochemistry. Nowadays, QSSA is still widely employed in numerical simulations of reaction-transport systems to remove chemical stiffness and enable explicit time integration with relatively large time steps [23,24]. Moreover, imposing QSSA also reduces the number of state variables and transport equations by eliminating the fast species such that the computational cost can be greatly reduced. From a physical perspective [22,25], QSSA identifies the species (termed as QSS species) that are usually radicals with relatively low concentrations. Their net production rates are much lower than their consumption and production rates and thus can be assumed zero. From a mathematical perspective [22], the stiffness of the ODEs can be characterized by the largest absolute eigenvalues of the Jacobian matrix, i.e., the Jacobian matrix of the reaction source term to the species concentrations. QSSA identifies the species that correspond to the relatively large eigenvalues of the chemical Jacobian matrix and then approximates the ODEs with differential-algebraic equations to reduce the magnitude of the largest eigenvalue of the Jacobian matrix and thus the stiffness.

In the current work, we evaluate the performance of PINN in solving two classical stiff dynamics problems and compare it with the performance of Stiff-PINN, which incorporates QSSA into PINN to reduce stiffness. While current work focuses on PINN, the mitigation of stiffness via QSSA can also be applied to other data-driven approaches, such as neural ordinary differential equations.

Results

We present the results of regular-PINN and stiff-PINN to solve the classical stiff ROBER problem, i.e.,

$$\frac{dy_1}{dt} = -k_1 y_1 + k_3 y_2 y_3,$$
$$\frac{dy_2}{dt} = k_1 y_1 - k_2 y_2^2 - k_3 y_2 y_3,$$
$$\frac{dy_3}{dt} = k_2 y_2^2.$$

The results are then shown in the figure below. It is found that the regular-PINN failed to capture the dynamics of such a stiff system while stiff-PINN with QSSA can successfully solve it.

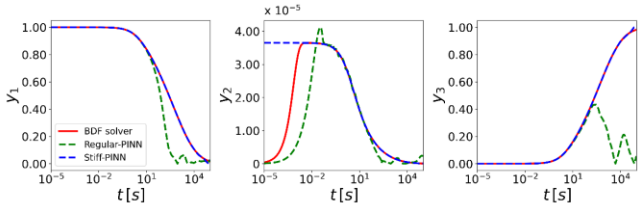

Figure 1. Solutions of the benchmark ROBER problem using the BDF solver (the exact solution), regular-PINN, and Stiff-PINN with QSSA. While the regular-PINN fails to predict the kinetic evolution of the stiff system, Stiff-PINN with QSSA works very well. The associated code can be found at https://github.com/DENG-MIT/Stiff-PINN.

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