

Generalized Lagrangian Neural Networks

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Abstract. Incorporating neural networks for the inverse problem of solution of Ordinary Differential Equations (ODEs) represents a pivotal research direction within computational mathematics. Within neural network architectures, the integration of the intrinsic structure of ODEs offers advantages such as enhanced prediction accuracy and reduced data utilization. Among these structural ODE forms, the Lagrangian representation stands out due to its significant physical underpinnings. Building upon this framework, Bhattoo introduced the concept of Lagrangian Neural Networks (LNNs). Then in this article, we introduce an extension (Generalized Lagrangian Neural Networks) to Lagrangian Neural Networks (LNNs) mainly based on mathematics and physics, innovatively tailoring them for non-conservative systems. By leveraging the foundational importance of the Lagrangian within Lagrange's equations, we formulate the model based on the generalized Lagrange's equation. This modification not only enhances prediction accuracy but also guarantees Lagrangian representation in non-conservative systems. Furthermore, we perform various experiments, encompassing 1-dimensional and 2-dimensional examples, along with an examination of the impact of network parameters, which proved the superiority of Generalized Lagrangian Neural Networks (GLNNs).

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1 Introduction

Machine learning has found significant applications in the field of mathematics, revolutionizing traditional approaches to problem-solving and analysis. With its ability to automatically learn patterns and make predictions from data, machine learning techniques

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have been successfully applied to various mathematical tasks. One significant direction is the utilization of machine learning to address mathematical problems associated with differential equations and dynamical systems [1,5–11,14].

In the existing methods for solving dynamical system problems using machine learning, they can be mainly categorized into two types. One type is unstructured methods [7,11,25,31,33–35], which do not consider the physical or mathematical structure of the equations or dynamical systems. When employing this approach, the focus is typically on minimizing the model error or complexity. For example, symbolic regression [33] is a regression method where the control equation under study is treated as an unknown target, and this unknown target is regarded as a function of the state variable data and its time derivative, using certain sparse approximations; Galerkin-closure methods [35] aim to approximate the unresolved scales of turbulence by using a closure model based on a truncated set of resolved scales; furthermore, unstructured neural networks such as LSTM [34] can be used to directly predict the solutions of differential equations or the phase flow of dynamical systems.

In contrast to unstructured methods, considering the inherent properties of the system and utilizing neural networks with specific structures can significantly enhance the predictive performance on specific systems. By incorporating the knowledge of system properties, such as conservation laws, symmetries, or known mathematical structures, into the design of neural networks, it becomes possible to improve the accuracy and effectiveness of predictions for the targeted system [1,6,8–11,15,16,18]. Hamiltonian Neural Network (HNN) [11], is a typical example of a structured neural network that takes into account the geometric structure of Hamiltonian systems. It utilizes neural networks to approximate the Hamiltonian of the system, thereby achieving improved predictive performance. OnsagerNets [14], as a systematic method that can overcome the aforementioned limitations, are based on a highly general extension of the Onsager principle for dissipative dynamics. Lagrangian Neural Networks (LNN) [1] are a class of neural networks specifically designed to parameterize arbitrary Lagrangians through their network architecture. Unlike traditional approaches, LNNs do not impose restrictions on the functional form of the learned energies, allowing them to produce models that conserve energy.

LNNs have demonstrated exceptional performance in many tasks. However, LNNs are limited to Lagrangian systems that adhere to the principle of energy conservation. However, in practical problems, we often encounter non-conservative systems. In the study of Euler-Lagrange equations [2,3], it is known that non-conservative systems can be formulated in the form of generalized Euler-Lagrange equations [5], which can be expressed as follows:

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}_k} \right) - \frac{\partial \mathcal{L}}{\partial q_k} = F_k.$$

In this article, we extend the scope of LNNs by constructing neural networks specifically designed for non-conservative systems. Our main inspiration stems from the special physical significance of the Lagrangian in Lagrange's equations. Since the Lagrangian