
Data and Modeling Assumptions in Physics-Informed Operator Learning

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Abstract

Operator networks have emerged as promising surrogate models, replacing computationally expensive numerical solvers for differential equations. Beyond achieving competitive accuracy with traditional solvers, the practical viability of this approach greatly depends on its training cost, which is comprised of ground truth data acquisition and network optimization. Physics-informed machine learning seeks to reduce reliance on labeled data by embedding the governing differential equations into the loss function; however, such models are often very challenging to train using physics constraints alone.

In this paper, we study how varying amounts of labeled data and architectural choices affect convergence and final performance in operator learning. Specifically, we compare an architecture developed for operator learning, i.e., Deep Operator Network, with a simpler MLP baseline across three training regimes: purely data-driven, purely physics-informed with no labeled data, and hybrid approaches that leverage *both* data and physics information. Our experiments on the double-mass-spring-damper system indicate that the physics-informed Deep Operator Network converges faster to the same performance if small amounts of labeled data are used. For the MLP architecture, which is not as well-tailored to the underlying dynamics, a purely physics-informed approach fails. In this case, incorporating labeled data mitigates architectural deficiencies and always substantially improves convergence and performance.

1 Introduction

Most processes in science and engineering are governed by differential equations (DEs). These processes are typically solved using state-of-the-art simulation frameworks, such as Runge-Kutta-based solvers, which over the years have been developed to reliably achieve high accuracy. However, depending on the underlying DEs, and investigated system size, obtaining these solutions can be computationally expensive, which is especially detrimental in research and development processes where repeated solver runs are required. To alleviate this limitation, recent research and development have explored the use of neural networks (NNs) as surrogate models for numerical solvers of DEs. Once trained, such networks can infer the solutions at a fraction of the computational cost of traditional numerical solvers. NNs as surrogate models have successfully been applied across a wide range of domains, including aerodynamics [Sun and Wang, 2019], fluid dynamics [Cai et al., 2021], weather forecasting [Bi et al., 2023], chemical engineering [Esche et al., 2022], and the rail-vehicle industry [Zhou et al., 2023, Ye et al.].

Operator learning has recently emerged as a promising approach for surrogate modeling. In this approach, the network aims to learn the underlying solution operator of the DE directly from data

[Boullé and Townsend, 2024], e.g., Deep Operator Networks (DeepONets) [Lu et al.]. Despite their potential, operator networks require labeled data, which can be costly to generate. This shifts computational effort from inference to training; once trained, predictions are fast, but the data-gathering and training process can be resource-intensive. A parallel line of research on physics-informed neural networks (PINNs) [Raissi et al., 2019] can help to alleviate this problem. Indeed, the physics-informed loss used for training PINNs incorporates known DEs directly into the loss function, thus allowing to solve these DEs with little to no labeled data. Wang et al. [2021] suggested using this physics-informed loss for operator learning. While such a physics-based approach reduces the dependence on labeled data, it often leads to optimization difficulties [Hao et al., 2022].

The practical viability of NNs as a surrogate model depends primarily on four major factors: accuracy, training time, generalization ability, and reliability. In scenarios where one cannot gather additional training data, one must rely heavily on the incorporated physics-constraints. Conversely, in scenarios where training data acquisition is cheap, data-driven approaches work well. However, many real-world scenarios (e.g., NNs as surrogates for computationally demanding solvers) lie between these extremes. This raises the question: how valuable is additional labeled data in physics-informed operator learning? In this work, we aim to get a better understanding of how labeled data, network architecture, and inductive biases influence physics-informed machine learning. We use the double-mass-spring damper system with external excitations as a challenging benchmark problem to investigate how varying amounts of labeled data impact the accuracy and training efficiency of DeepONets and traditional MLPs under both purely data-driven, purely physics-informed and hybrid training regimes. Furthermore, we show the importance of inductive bias through the utilization of Fourier features to encode the input time.

2 Related work

The concept of physics-guided NNs dates back to the 1990s. Raissi et al. [2019] introduced PINNs, popularizing the concept by leveraging automatic differentiation and increased computational power to make this approach practically viable. However, training NNs exclusively using a physics-informed loss is often challenging [Wang et al., a, Rohrhofer et al.], particularly for systems involving high-frequency dynamics due to the spectral bias of NNs [Wang et al., b, Steger et al., 2022]. Applying input encodings has proven to be beneficial for learning higher frequencies in both data-driven and physics-informed learning settings, either through Fourier features [Tancik et al., 2020], [Wang et al., 2021] or by modifying the employed activation functions [Sitzmann et al., 2020, Wong et al., 2022, Hofmann-Wellenhof et al., 2024].

Operator learning aims to learn nonlinear mappings between function spaces. Among the most widely adopted architectures in this domain is DeepONet [Lu et al.], motivated by the Universal Approximation Theorem for Operators [Chen and Chen, 1995]. The DeepONet architecture has also been extended to multiple outputs, partitioning the output neurons of the subnetworks and computing multiple dot products [Lu et al., 2022]. Originally introduced as purely data-driven models, DeepONets have since been extended to physics-informed variants [Wang et al., 2021]. Recent studies explored extensions of these architectures to improve adaption to time-dependent inputs [Liu et al., 2023, He et al., 2024].

3 Methodology

In the following experiments, we employ a double mass–spring–damper system with external excitations (the quarter-car model), as it possesses several properties that make it a compelling test case. It is the easiest multibody system that exhibits coupled dynamics, is highly oscillatory, which poses challenges for NN learning, and involves time-varying input excitations, a scenario that has been relatively less explored for (physics-informed) DeepONets. The system is given by:

$$m_1 \ddot{y}_1 = k_1(y_2 - y_1) + c_1(\dot{x}_2 - \dot{x}_1) \quad (1a)$$

$$m_2 \ddot{y}_2 = k_2(u - y_2) + c_2(\dot{u} - \dot{x}_2) - k_1(y_2 - y_1) - c_1(\dot{x}_2 - \dot{x}_1), \quad (1b)$$

where $u(t)$ is the time varying excitation, m_1, m_2 being the weight of the masses, k_1, k_2 being the first and second spring constant, c_1, c_2 are the damping constants, and y_1, y_2 are the displacements of the first and second mass. The task is to train a surrogate model that takes the excitation signal $u(t)$ and time t as input and responds with the displacements $y_1(t)$ and $y_2(t)$, as shown in Figure 1.

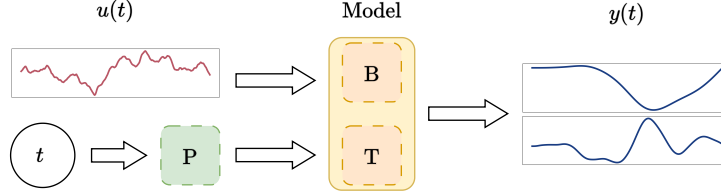


Figure 1: Overview of the learning task. The DeepONet takes the excitation $u(t)$ and projected time t as inputs to its branch and trunk networks, respectively, while the MLP uses their concatenation. Both models output the predicted displacements of the two masses, $y_1(t)$ and $y_2(t)$.

Table 1: Relative L_2 test error for the different architectures with and without input Fourier encoding. The data-driven and hybrid training scheme was trained on 270 data pairs.

	data-driven	hybrid	physics-informed
DeepONet + input proj.	0.072 ± 0.007	0.032 ± 0.004	0.031 ± 0.001
DeepONet	0.112 ± 0.004	0.159 ± 0.056	0.211 ± 0.038
MLP + input proj.	0.048 ± 0.001	0.043 ± 0.003	0.091 ± 0.018
MLP	0.081 ± 0.005	0.101 ± 0.020	0.179 ± 0.017

We compare two model architectures: a baseline MLP and a DeepONet. In most DeepONet applications, an initial condition is provided and propagated forward in time to obtain the solution. Our benchmark problem differs, as it additionally requires time-dependent excitation signals as inputs. DeepONet consists of two sub-networks whose outputs are combined via a dot product. Here, one sub-network, i.e., the trunk net, encodes the coordinates of the solution functions (i.e., the time variable t), while the other, the branch net, encodes the input function (i.e., the excitation signal $u(t)$). For the trunk net, we also analyze the effectiveness of linearly spaced Fourier feature encodings, projecting the input time t to a vector $\mathbf{v}(t)$ consisting of 200 sine and cosine pairs. As the system response can be expected to be an oscillating signal, this introduces an inductive bias. All model variants are trained under three regimes: purely data-driven, purely physics-informed, and a hybrid approach that combines both.

4 Experimental setup and results

Both model types have a depth of four and are optimized using Adam [Kingma and Ba, 2017]. The MLP has a width of 64 (70,274 parameters), and the two subnets of the DeepONet have a width of 106 (in total 70,702 parameters). The used excitations are artificially generated signals developed for modeling rail roughness. This data is then split into training, validation, and test sets. Excitations $u(t)$ are two-second snippets, assuming a sampling rate of 250 Hz. The physics residual of the DE (1) is evaluated at $N = 500$ collocation points. Initial displacement and velocity are set to zero for both masses, enforced through the data loss. During training, early stopping was employed. Our main performance metric was the relative L_2 error calculated snipped-wise,

$$L_{2,r} = \frac{1}{N} \sum_{i=1}^N \frac{\sqrt{\sum_{t=1}^T (y_t^{(i)} - \hat{y}_t^{(i)})^2}}{\sqrt{\sum_{t=1}^T (y_t^{(i)})^2}},$$

which is independent of excitation amplitudes. All reported results are averaged over three runs.

Table 1 highlights the importance of inductive biases, introduced through the Fourier encodings, especially for the hybrid and physics-informed training schemes. Across all models, performance improves noticeably if Fourier encodings are introduced. We see that DeepONet performs approximately $7\times$ better with the encodings in the physics-informed case, and about $1.5\times$ better for the data-driven variant. Consequently, all subsequent experiments were conducted using Fourier encodings.

Figure 2 shows $L_{2,r}$ as a function of the number of training data points, i.e., excitation-solution pairs. In the data-driven regime, more data generally improves accuracy. In contrast, for the hybrid and physics-informed DeepONet models, additional data does not yield further performance gains. This indicates that the physics-informed DeepONet can solve the problem solely using the

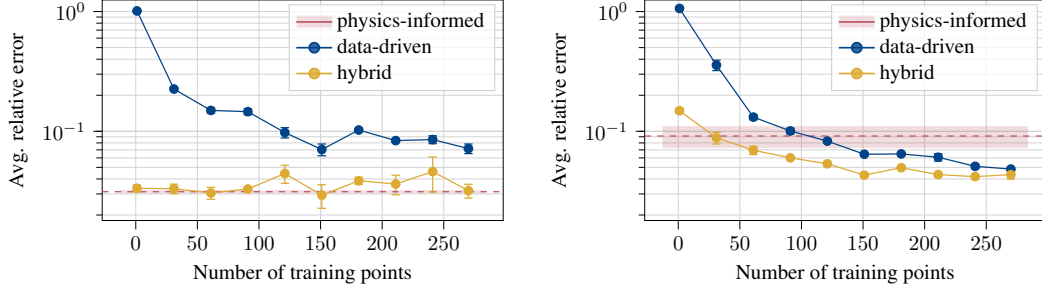


Figure 2: Comparison of data-driven, hybrid, and physics-informed model performance with standard deviation, for the DeepONet (left) and MLP (right) architectures over the number of used training data points (excitation-solution pairs).

physics constraint. Across all dataset sizes, a clear performance gap persists between the data-driven DeepONet and the models incorporating a physics loss. For the MLP, however, the physics-informed variant performs worse than the other paradigms, in all but the very low-data regime. The hybrid MLP outperforms the purely data-driven MLP, although this advantage diminishes as the training set grows. Notably, the MLP performs better than the DeepONet in the purely data-driven setting.

Figure 3 relates $L_{2,r}$ to the number of training epochs, confirming the intuition that the data-driven approach converges fastest, being the easiest to optimize. Additionally, hybrid models converge faster than those relying solely on the physics. Using the physics residual, on the other hand, improves accuracy considerably, albeit at the cost of increased convergence time. One surprising finding is that the amount of data does *not* have a significant impact on convergence speed. Similarly, for the hybrid DeepONet, the amount of used data has little impact on accuracy. For the hybrid MLP, however, accuracy increases with larger datasets, allowing it to surpass the purely physics-informed approach.

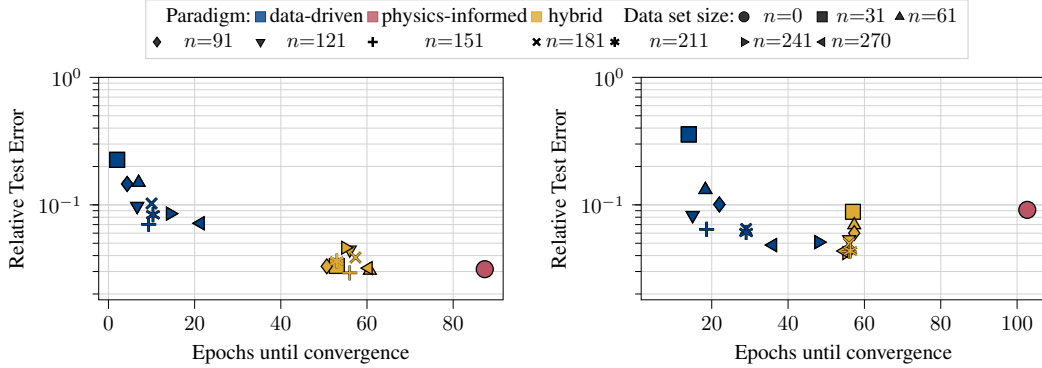


Figure 3: Pareto front comparison of $L_{2,r}$ errors at the early stopping epochs for the DeepONet (left) and MLP (right) architectures. The plots illustrate trade-offs between model training complexity and performance across configurations.

5 Conclusion

In this work, we analyzed how varying amounts of training data and inductive biases influence the convergence behavior and performance of operator networks. Our results show that incorporating training data into a physics-informed training regime can significantly reduce training time. However, this effect does not scale with the amount of data used. Conversely, adding physics-based residuals can substantially enhance performance, if the network architecture is well-suited to exploit the underlying physical behavior. Architectures specifically designed for operator learning, such as DeepONet, combined with suitable inductive biases, such as Fourier feature embeddings, play a crucial role in leveraging the potential of the physics loss. These findings motivate further research into developing tailored modeling approaches for specific differential equations. Otherwise, training data is required to compensate for suboptimal design choices to achieve satisfactory accuracy.

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