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Analysis of Physics Informed Neural Networks (PINNs)

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Abstract:

Modern physics-informed neural networks (PINNs) will be examined and evaluated from many academics' points of view in this study. Through a focused keyword search in the Scopus and Web of Science databases, 120 research publications from the computational sciences and engineering sector were specifically categorized using the PRISMA framework. Through bibliometric analysis, we have determined which journals have the most publications, which authors receive a lot of citations, and which nations have the most articles on PINNs. Some recently developed strategies that aim to improve PINN performance, lower slowness and high training costs, among other drawbacks, have been noted. To get over PINNs' drawbacks, many strategies have been developed. In this review, we categorized the newly proposed PINN methods into Extended PINNs, Hybrid PINNs, and Minimized Loss techniques. Various potential future research directions are outlined based on the limitations of the proposed solutions.

keywords - physics-informed neural networks (PINNs); partial differential equation (PDE); loss function; activation function; deep learning.

I. INTRODUCTION

Physics-informed neural networks (PINNs) [1] are frequently employed to address a variety of scientific computer problems. Due to their superior approximation and generalization capabilities, physics-informed neural networks have gained popularity in solvinghigh-dimensional partial differential equations (PDEs) [2]. As a deep learning method, physics-informed neural networks bridge the gap between machine learning and scientific computing. PINNs have contributed to improvements in many areas of computer science and engineering due to their simplicity [3,4]. In the engineering and scientific literature, PINNs are receiving more attention for solving a variety of differential equations with applications in weather modeling, healthcare, manufacturing, and other fields [5–7]. How-ever, PINNs are not suitable for several real-time applications because of their high training costs. Although various proposals have been made to enhance the training effectiveness of PINNs, only some have considered the effects of initialization [8–10]. Another obstacle to the application of PINNs to a wide range of real-world problems is their poor scalability [5].Due to the sheer number of residual points in time-constrained space, an accurate network, called a physics-informed neural network (PINN), can be trained by minimizing only the residual loss. Moreover, the prediction of the high-fidelity solution for complex nonlinear problems in low-dimensional space is more accurate than the solutions of the reduced-order equations.

The ability of PINNs to learn from sparse input is one of their most well-known features Initial and boundary terms are not systematically given in the context of PINN structure; therefore, they need to be incorporated in the loss function of the network, which must be learned simultaneously with the uncertain functions of the differential equation (DE) [16,17]. While implementing gradient-based approaches, combining multiple targets during the network's training can lead to biased gradients, leading to PINNs failing to appropriately learn the fundamental DE solution [18–20].

According to Raissi et al. [1], Schiassi et al. [21], and Zhang et al. [22], the key draw-back of conventional PINNs is that even the DE limitations are still not mathematically solved, hence they need be learned concurrently with the DE solutions within the do- main. As a result, we cope with competing goals during PINN training: learning the concealed DE solutions well in domains while also learning the hidden DE solutions on the boundary [21,23,24]. This results in imbalanced gradients during

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network training using gradient-based approaches, causing PINNs to fail to learn the basic DE solutions accurately [21,25]. According to Dwivedi et al. [26], despite the numerous benefits that PINNs provide, they have three major drawbacks. The first is their slowness [26,27] when applied to real problems; PINNs use up gradient descent optimization and are quite slowwhen compared to other numerical approaches. For highly deep networks, PINNs are vulnerable to vanishing gradient problems [6,26,28]. There is also the possibility that a solution will become stuck at a minimal point. Finally, the PINN's learning process is fine-tuned by hand. We cannot ascertain exactly how much data or even which framework is sufficient for a particular set of sample instances [1, 29–31].

The weighted least-squares collocation approach utilized in PINNs can be interpreted as a hybrid physics/data loss scheme [32–34]. As a result, PINNs have inherited several drawbacks common to such approaches, including the necessity to evaluate PDE residuals correctly against beginning as well as boundary conditions; a severe regularity demand for solutions remains continuous, as does the inability of natural methods to impose conservation structures [32,35–37].

Although PINNs have been exceptionally beneficial to the scientific community, Colby et al. [18] discovered that they are often incapable of appropriately solving a mathematical model for interfacial problems used for solidification dynamics called "phase field problems". As a result, they found that specific elements of phase field model solutions (both spatially and dynamically) were more difficult to learn than others. These problematic places may alter as you discover the solution.

The goal of this research is to find physics-informed neural network adaptations for solving various problems from the literature and to highlight newly improved PINN methodologies that have been proposed using different techniques. The main objectives of the study were to evaluate the current state of the art in this field of research using numerous bibliometric analyses, identify the full spectrum of eligibility requirements studied in the literature through information synthesis, create a collection of general information abouthow far research on PINNs has changed over time, and identify newly introduced PINN approaches while highlighting some topics for future research. We tried to categorize state- of-the-art PINN techniques into three groups. These are Extended, Hybrid, and Minimized Loss PINN techniques and will be discussed later in Section 4.1. In this literature review, we aimed to answer the following question: What techniques have been introduced to optimize the performance of physics-informed neural networks? Although PINNs are utilized to solve problems in practically all the domains of human endeavor, throughout this review, we focused on computational sciences and engineering.

The rest of the paper is organized as follows: Section 2 presents the background. Section 3 explores the quality assessment and qualitative synthesis used in the literature review for this study. Section 4 discusses the results of the bibliometric analysis, as well as the objectives, methods, and limitations of the newly proposed PINN techniques. Sections 5 and 6 discuss future research directions and conclusions, respectively.

BACKGROUND

Many methods for solving differential equations have been established over the years. Some generate a solution in an array containing the solution's value in a predefined set of locations. Others employ basis-functions to designate the solution in analytic methods and typically translate the genuine problem to a system of algebraic equations. Most pastprojects seeking to solve partial differential equations with neural networks have been limited to the case of solving methods of algebraic equations that come from domain discretization. In 1998, Isaac Lagaris et al. [38] introduced an improved method for solving ordinary DEs and partial differential equations by employing Artificial Neural Networks (ANNs). In their newly introduced method, the differential equation's trial solution was represented by the sum of two parts. There were no adjustable parameters in the first half, which satisfied the initial/boundary conditions. The second component was designed in a way that did not change the initial or boundary conditions. In this section, a feedforwardneural network (NN) with programmable constraints (the weights) was used. Therefore, the network is trained to fit the differential equations together with the initial/boundary conditions that were satisfied by construction [38] methods and can be used for a range of ordinary differential equations (ODEs), coupled ODE systems, and partial differential equations (PDEs).

In 2011, Ladislav Zjavka [39] developed a new technique, known as a Differential Polynomial Neural Network (D-PNN). The proposed D-PNN technique approximates a multi-parametric function by generating and solving unknown partial DEs. A differential equation is substituted to create a system model of dependent variables, leading to the summation of fractional polynomial derivative terms. In contrast to the ANN method, the D-PNN allows each neuron to directly participate in the calculation of the network's overall output. Consequently, in 2013, Ladislav et al. [40] showed that D-PNNs could be applied to solve complex mathematical problems.

In 2015, Ladislav et al. [41] presented a recurrent neural network (RNN) of one layer, which is frequently employed for time series predictions and which was used for comparison. With twenty-four succession samples constantly generated by the benchmark and a continuous step value of 0.1, in the range of 0–2.4, the D-PNN and RNN were trained. Two incredibly different networks were trained with only a relatively narrow range of values, which did not accurately reflect function-specific progress over an entire period. The models were then tested over a longer period. The networks only estimated one benchmark value for the next step x using the calculated accurate function f(x) with three-input sequences, rather than making entire predictions built on prior steps' outputs (approximations).

1.1 Physics-Informed Neural Networks

PDEs with high dimensions are commonly used in a variety of disciplines, including physics, chemistry, engineering, finance, and more [91]. Higher dimensions make numerical PDE computational methods such as finite difference or finite element methods impractical due to the explosion in the number of grid points and the need for smaller time steps.

Physics-informed neural networks (PINNs) are models developed to obey physical laws specified by (nonlinear) partial differential equations (PDEs). They can be used for supervised tasks where the reduction of errors with respect to data and physical laws is required [1,91,92].

The loss function is defined as follows:

 $l = l_{data} + w l_{physics}$

Where l_{data} is the loss with respect to the data, $wl_{physics}$ is a physics law's loss relative to the PDEs, and w is the weight matrix of a physics loss. By using mean-squared error for bothlosses, if f_i is the error of each physical state, we derive:

 $l = \sum_{i} (y_i - y^{\hat{}})^2 - w \sum_{i} f^2$

The input values x, y, and t are used in the architecture of the network, and the output values are u and v. The output variables are used directly to calculate the data loss term. However, we distinguish the variables with respect to the input variables for the physicalloss term to account for the physical loss function, as shown in Figure 1 [91] below. The goal is to minimize deviations from the physics law by monitoring training with measured or generated data (i.e., l_{data}), as well as by training to diminish the departure from the physics law. To further train to minimize deviation from the physical law, by preventing overfitting, the term $l_{physics}$ ensures that such a neural network generalizes better given.



Figure 1. Schematic diagram of a PINN. Adapted with permission from Ref. [91]. Copyright 2021 DeWolff, Carrillo, Martí, and Sanchez-Pi.

2.2 Modeling and Computation

A general nonlinear partial differential equation can be:

$$u_t + N[u; \boldsymbol{\lambda}] = 0, \ x \in \Omega, \ t \in [0, T]$$

U(t, x) denotes the solution, $N[u; \lambda]$ is a nonlinear operator parametrized by λ , and Ω is a Subset of R^{D} .

Numerous problems in mathematical physics, such as conservative laws, diffusion processes, advection–diffusion systems, and kinetic equations, fall under this general category of governing equations.

PINNs can be programmed to solve two major types of PDE problems on the noisy data of a general dynamical system denoted by the above equation [14, 92,93]. These are:

Data-driven solutions.

Data-driven discovery.

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The data-driven solution of PDE findings when calculating the unknown state u(t, x) of the system given noisy measurements z of the state and fixed model parameters λ reads as follows:

 $u_t + N[u] = 0, x \in \Omega, t \in [0, T]$

By defining f(t, x) as

 $F: = u_t + N[u] = 0$

And approximating u(t, x) with a deep neural network, f(t, x) results in a PINN. This network can be differentiated using automatic differentiation.

And f(t, x) can be then learned by minimizing the following loss function L_{tot} .

METHODOLOGY

For reviewing current research, this paper used the PRISMA framework [97–99]. The scoping approach was utilized to retrieve the most relevant papers on physics-informed neural networks. This method aided the control of critical mandatory components and the classification of potential search terms [97,100,101]. To identify relevant scientific papers and articles, multiple databases were searched. A search using a single keyword ("physics- informed neural networks") was conducted to find relevant publications from the most reputable and reliable research resources. Scopus and Web of Science were used, along with the Web of Science core collection, Derwent Innovations Index, MEDLINE, KCI-Korean Journal Database, and SCIELO Citation Index.

The keyword "Physics Informed Neural Network" was solely used in each database search for the relevant literature. Predefined inclusion and exclusion criteria and quality requirements were used to refine the data search. Each filter verified that the quality requirement was met, and the next section discusses the inclusion and exclusion criteria.

Because our search query was put in a double quote, we employed deterministic information retrieval to look for suitable papers, as we described earlier. The literature searches in all the databases listed above retrieved articles from 2019 to 2022. Initially, 530 items were found; however, this was largely made up of a variety of materials, such as research articles, reviews, editorials, and book chapters, among others.

Many researchers use PINNs to solve problems in different areas of human endeavor. We have limited our research to computational sciences and engineering and focused onresearch articles, review papers, and book chapters in our literature search. A total of 288 documents were chosen, as illustrated in Figure 2. Articles from computational sciences and engineering were chosen as the following sequence. This included computer science, engineering, mathematics, and physics. Non-English documents were also excluded. The PRISMA checklist can be found in Supplementary Materials.



Figure 2. PRISMA framework.

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Duplicate articles were also removed from the Scopus and Web of Science metadatafiles. The two files were combined and duplicate journal articles removed. In this review, the PRISMA 2020 flow diagram was used, as shown in Figure 3 below



RESULT OF BIBLIOMETRIC ANALYSES

The main objectives of this research, as mentioned earlier, were to assess the state of the art in this area of study using various bibliometric analyses and to classify the full range of eligibility requirements analyzed in the literature through metadata synthesis to produce a collection of general information on the extent to which the study of PINNs has changed over time.

Figure 4 illustrates physics-informed neural network evolution over the past three and a half years in terms of the number of publication relating to this area of study. Between 2019 and mid-2022, research in this field had been developing steadily, with a current peak in 2021. The trend shows that many researchers are busy finding solutions with PINNs, and some are also trying to optimize performance.





| Correct PDE | $u_t + uu_x + 0.003183u_{xx} = 0$ |
|-----------------------------|---|
| Identified PDE (clean data) | $u_t + 1.000 u u_x + 0.003193 u_{xx} = 0$ |
| Identified PDE (1% noise) | $u_t + 1.000uu_x + 0.003276u_{xx} = 0$ |

Burgers equation: Top: Solution u (t, x) along with the temporal locations of the two training snapshots. Middle: Training data and exact solution corresponding to the two temporal snapshots depicted by the dashed vertical lines in the top panel. Bottom: Correct partial differential equation along with the identified one obtained by learning λ_1, λ_2

Burgers' equation: Percentage error in the identified parameters λ_1 and λ_2 for different gap size Δt Between noise level

| | | | % error in λ_1 | | | <u>% error</u> in λ_2 | | | | | |
|--|------------|---------------------|------------------------|-------|-------|-------------------------------|-------|-------|--------|--------|-----|
| | Δt | Nois <mark>e</mark> | 0% | 1% | 5% | 10% | 0% | 1% | 5% | 10% | |
| | | | | | | | | | | |)) |
| | 0.2 | | 0.002 | 0.435 | 6.073 | 3.273 | 0.151 | 4.982 | 59.314 | 83.969 | |
| | 0.4 | | 0.001 | 0.119 | 1.679 | 2.985 | 0.088 | 2.816 | 8.396 | 8.377 | |
| | 0.6 | | 0.002 | 0.064 | 2.096 | 1.383 | 0.090 | 0.068 | 3.493 | 24.321 | |
| | 0.8 | | 0.010 | 0.221 | 0.097 | 1.233 | 1.918 | 3.215 | 13.479 | 1.621 | |
| | | | | | CR. | | | | 5.0 | | |

Burgers' equation: Percentage error in the identified parameters λ_1 and λ_2 for different number of hidden layers and neurons in each layer

| | | % error | in λ_1 | | <u>% error in</u> | - | |
|--------|---------|---------|----------------|-------|-------------------|---------|---------|
| Layers | Neurons | 10 | 25 | 50 | 10 | 25 | 50 |
| 1 | | 1.868 | 4.868 | 1.960 | 180.373 | 237.463 | 123.539 |
| 2 | | 0.443 | 0.037 | 0.015 | 29.474 | 2.676 | 1.561 |
| 3 | | 0.123 | 0.012 | 0.004 | 7.991 | 1.906 | 0.586 |
| 4 | | 0.012 | 0.020 | 0.011 | 1.125 | 4.448 | 2.014 |

We previously pointed out various limitations of PINNs that were highlighted by different authors and later discussed the newly proposed techniques used to solve most of the mentioned problems. We have also outlined the limitations of the newly proposed PINN methods. The focus of our future research will be more on the limitations of the newly proposed techniques. Since they have addressed most of the PINN limitations, the limitations of some selected articles are discussed because of their significance. One of the main benefits of using the cPINNs introduced by [35] to solve complicated problems is their capacity for parallelization, which effectively lowers training costs; however, they cannot be used for parallel computation. In future research, cPINNs may be extended foruse in parallel computation.

The enhanced PINN technique proposed by [115] improves neural network performance. Through numerous trainable parameters in the activation function, they noted that an important issue for the future was considering how to integrate machine learning using integrable systems theory more fully and construct substantial integrable deeplearning algorithms.

A new approach presented by [21] can also be applied to data-driven discoveries and solutions of parametric differential equations. Future research will focus on extending this method to data-driven problem discovery for solving ODEs using both deterministic and probabilistic methods.

Noting the nature of optimization when training PINNs, the capacity to perform uncertainty quantification (UQ) on physical systems was highlighted by [1]. The PINN framework implemented by [92] could be extended to provide these features.

Despite the numerous desirable features of the hybrid approach proposed by [110], their findings proved that the methodology has a shortcoming that could be considered as a topic of future research. Their research has limitations regarding training results, as they were proven to be very responsive to the initial hyper parameters of the neural network; even if the proposed auxiliary planes are used to initialize the neural network, the poor initialization of these parameters can potentially hinder training. Therefore, optimization with a wide range of initial hyper parameter values is still required.

The recent work of Liu X. et al. [8] has one limitation. As a new reptilian initialization learning task, NRPINN needs prior information, especially higher- and zero-order information. As a result, NRPINN is not suitable for handling problems where previous information is not available. Using transfer learning from related efforts to acquire an initialization may be another technique for improving the performance of PINNs in future studies.

A new hybrid technique proposed by [106] cannot be used to solve the domain decomposition of basic problems with big spatial databases.

CONCLUSIONS

The review and bibliometric analysis of the published literature revealed several limitations of PINNs. We discovered that a significant amount of experimental research in the 120 peer-reviewed articles used conventional PINNs to solve various scientific and engineering problems. In contrast, other studies developed new methods to overcome the limitations of PINNs and achieve higher performance results.

Data evaluation was an essential and significant step in the review. Based on the relative number of PINN-related journals, two reputable databases were chosen: Scopus and Web of Science. The first PINN papers were published in early 2019. For this reason, the papers used in this study are from 2019 to mid-2022.

We discussed the objectives, methodologies, and limitations of the newly proposed PINN techniques. Despite the feedforward nature of PINNs, we have found several articles that combined them with other neural network architectures. While some extended the conventional PINNs, others tried to improve performance by using different techniques for reducing loss. We have also identified several potential research directions for PINNs based on the limitations of proposed solutions to increasing prediction power andoptimizing performance.

As part of our contribution to the literature, we intend to implement a new model that combines PINNs with either a graph neural network or a recurrent neural network using a time series dataset.

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