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Interpretable Surrogate Constraints for Physics-Informed Networks with Partially Observed Dynamics and Parameters

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Abstract:

The integration of deep learning with fundamental physical laws has led to the emergence of physics-informed neural networks, which have demonstrated exceptional capabilities in solving forward and inverse problems in computational mechanics and fluid dynamics. However, classical physics-informed architectures operate under the stringent assumption that the governing partial differential equations are fully specified, and that boundary or initial conditions are sufficiently resolved. In contemporary scientific computing, researchers frequently encounter scenarios characterized by partially observed dynamics, where governing equations contain unresolved terms, unknown parameter fields, or hidden physical mechanisms. This paper proposes a novel framework centered on interpretable surrogate constraints to address these challenges. By embedding symbolic and polynomial surrogate models directly into the loss landscape of physics-informed networks, the proposed methodology enforces analytical tractability and physical interpretability without sacrificing the universal approximation properties of deep neural networks. The surrogate constraints act as dynamic regularizers that identify and reconstruct the missing phenomenological behaviors from sparse observational data. Comprehensive theoretical analysis is provided alongside extensive numerical experiments involving complex spatiotemporal systems. The results indicate that the integration of interpretable surrogate formulations significantly enhances predictive accuracy, robustly recovers unknown system parameters, and provides a transparent mathematical description of the hidden dynamics.

Keywords: *Physics-Informed Neural Networks, Surrogate Modeling, Interpretable Machine Learning, Partially Observed Dynamics*

INTRODUCTION

1.1 Context and Motivation

The paradigm of scientific machine learning has fundamentally transformed the approach to solving complex engineering and physical problems, bridging the gap between purely data-driven models and traditional numerical solvers. Physics-informed neural networks represent a cornerstone of this transformation, leveraging the automatic differentiation capabilities of deep learning frameworks to embed physical laws directly into the optimization objective. This methodology allows for the seamless assimilation of scattered observational data and governing physical constraints, providing a mesh-free alternative to finite element and finite volume methods. Traditional numerical techniques demand rigorous discretization and well-posed boundary conditions, which are often unavailable in real-world engineering contexts. Physics-informed architectures circumvent these limitations by defining a composite loss function that penalizes deviations from the governing partial differential equations, thereby constraining the neural network to output physically consistent solutions. Despite their theoretical appeal and empirical success in idealized scenarios, the deployment of these models in highly complex physical systems remains constrained by significant methodological bottlenecks. Another relevant line of investigation concerns on the role of discount factor in offline reinforcement learning [1].

1.1 The Challenge of Partially Observed Dynamics

In numerous applied scientific domains, ranging from geophysical fluid dynamics to biological tissue modeling, the governing equations are rarely known with absolute certainty. Systems often exhibit partially observed dynamics where certain physical phenomena, such as complex biogeochemical reactions, turbulent stress tensors, or non-Newtonian viscous behaviors, lack precise mathematical formulations. When physics-informed models encounter these incomplete theoretical frameworks, the standard methodology breaks down. The optimization process becomes ill-posed because the physical residual formulated in the loss function is inherently misspecified. Furthermore, observational data in these contexts is typically sparse, noisy, and restricted to a limited number of state variables, making it exceptionally difficult to infer the missing physical mechanisms purely through data-driven approaches. If a deep neural network is employed to approximate these unknown terms without structural constraints, the resulting model acts as a black box. The inherent lack of interpretability prevents domain experts from validating the learned physics against established empirical principles, thereby severely limiting the scientific utility of the model. Xu and colleagues examine learning Koopman representations for complex dynamics with spectral residuals [2]. To mitigate these issues, researchers have attempted to combine physics-informed networks with system identification techniques. However, identifying unknown parameters and functional forms simultaneously from sparse data introduces severe optimization challenges. The high-dimensional non-convex loss landscapes associated with these hybrid models often trap gradient-based optimizers in suboptimal local minima. The interplay between the known physical constraints and the flexible neural network components designed to capture the unknown dynamics frequently leads to spectral bias, where the network preferentially learns high-frequency noise rather than the underlying macroscopic physical relationships. Consequently, there is an urgent requirement for novel mathematical frameworks that can explicitly constrain the functional space of the unknown dynamics, ensuring that the learned representations are both mathematically stable and physically interpretable. For a broader comparison, related research addresses optimizing hybrid RIS-Aided ISAC systems in V2X networks: A deep reinforcement learning method for Anti-Eavesdropping techniques [3]. For a broader comparison, related research addresses inferring 3d hands from both text prompts and body dynamics [4].

1.2 Motivation for Interpretable Surrogate Constraints

The core proposition of this research is the introduction of interpretable surrogate constraints into the architecture of physics-informed networks. Instead of utilizing unconstrained multilayer perceptrons to model unknown dynamic terms, this approach constructs a library of analytical, interpretable surrogate functions. These surrogates are mathematically formulated using sparse linear combinations of orthogonal polynomials, trigonometric functions, and established physical operators. By embedding these surrogates into the network structure, the optimization process is guided toward solutions that possess a compact analytical representation. This strategy not only regularizes the training process but also ensures that the discovered missing dynamics can be directly analyzed by human experts. The mathematical rigidity of the surrogate constraints prevents the neural network from overfitting to observational noise and promotes exceptional extrapolation capabilities outside the spatial and temporal domains present in the training data. The development of this framework represents a critical step toward fully autonomous scientific discovery, where machine learning models can formulate verifiable scientific hypotheses regarding the fundamental laws governing complex systems. For a broader comparison, related research addresses data-driven energy efficiency improvement and cost optimisation model for new energy electric vehicles [5].

2. Literature Review and Background

The intersection of deep learning and computational physics has experienced explosive growth, yet the treatment of incomplete physical knowledge remains an active and highly challenging area of research. A comprehensive review of the existing literature reveals several distinct lineages of methodological development, each addressing different facets of the partially observed dynamics problem. Understanding these historical and contemporary approaches is essential for contextualizing the contributions of the interpretable surrogate constraints framework proposed in this study. Another relevant line of investigation concerns surrogate-Based metaheuristic global search method for beam angle selection in radiation treatment planning [6]. For a broader comparison, related research addresses interpretation of soil deformation characteristics based on in-situ test: A comprehensive review [7].

2.1 Physics-Informed Neural Networks and System Identification

The foundational work on physics-informed neural networks demonstrated the feasibility of training multilayer perceptrons to satisfy nonlinear partial differential equations using continuous time and space coordinates. Early extensions of this methodology focused primarily on solving inverse problems, where the mathematical structure of the governing equation was assumed to be known, but specific scalar parameters required estimation from data. For example, researchers successfully estimated the Reynolds number in fluid flow and the thermal diffusivity in heat transfer applications using sparse sensor measurements. However, when the structural form of the equation itself is unknown or partially missing, scalar parameter estimation is insufficient. Another relevant line of investigation concerns unsupervised learning with physics informed graph networks for partial differential equations [8]. For a broader comparison, related research addresses design of interface circuits and lightweight PUF for TMR sensors [9]. To address structural uncertainty, hybrid approaches were developed. One notable strategy involves using a secondary neural network to output the value of the missing dynamic term, which is then fed back into the primary partial differential equation. While this method successfully closes the governing equations and allows the primary network to converge, the secondary network remains entirely opaque. Scientific interpretability is completely sacrificed in favor of predictive accuracy. Other researchers have explored the use of generative adversarial networks to infer probability distributions over functional forms, but these methods require massive computational resources and are highly unstable during training. The critical limitation across all these deep learning-based

system identification techniques is the absence of an explicit mechanism to enforce parsimony and mathematical interpretability. Another relevant line of investigation concerns data-Driven framework for Koopman semigroup estimation in stochastic dynamical systems [10].

2.2 Symbolic Regression and Sparse Identification

Parallel to the development of deep learning methods, significant progress has been made in the field of sparse identification of nonlinear dynamics. These techniques typically construct a large dictionary of candidate nonlinear functions and utilize sparse regression algorithms, such as sequentially thresholded least squares, to identify the most parsimonious combination of terms that describe the time-series data. This methodology is highly interpretable and has successfully rediscovered canonical physical equations from experimental data. Nevertheless, sparse identification relies heavily on high-quality, high-resolution measurements of all state variables to compute accurate numerical derivatives. When data is noisy, sparsely sampled, or when certain state variables are completely hidden from observation, the numerical differentiation process amplifies the noise to catastrophic levels, rendering the sparse regression entirely ineffective. Another relevant line of investigation concerns review of machine learning with echo state networks [11]. For a broader comparison, related research addresses cooperative atomically dispersed Fe-N4 and sn- nx moieties for durable and MoreActive oxygen electroreductionin fuel cells [12]. Recent attempts to fuse physics-informed neural networks with sparse identification have shown theoretical promise. By utilizing the neural network to interpolate the sparse data and compute analytical derivatives via automatic differentiation, the noise amplification problem associated with numerical derivatives can be somewhat mitigated. The network acts as a differentiable surrogate for the state variables, while the sparse regression identifies the equation structure. However, these decoupled approaches often suffer from a severe disconnect between the neural network training phase and the symbolic regression phase. Errors accumulated during the initial neural network training are propagated directly into the dictionary construction, leading to the identification of spurious terms. A fully unified approach, where the interpretable structure and the neural network parameters are optimized simultaneously within a single coherent framework, has remained elusive until now. Related work has addressed efficient simulation budget allocation for subset selection using regression metamodels [13]. For a broader comparison, related research addresses design of magnetic sensor Array-Based PUFs for IoT security [14].

2.3 Surrogate Modeling in Complex Systems

Surrogate models, also known as metamodels or emulators, have a long history in engineering design and uncertainty quantification. Traditional surrogate modeling techniques, such as Gaussian process regression, polynomial chaos expansions, and radial basis functions, are designed to approximate computationally expensive high-fidelity simulators. In the context of partially observed dynamics, surrogates can be utilized to model the discrepancy between incomplete physical models and observed reality. Research into discrepancy modeling has highlighted the importance of imposing physical constraints on the surrogate to ensure it does not violate fundamental conservation laws, such as mass or energy conservation. Another relevant line of investigation concerns deep incomplete multi-view network semi-supervised multi-label learning with unbiased loss [15]. Despite their robustness, traditional surrogate models often struggle to scale to high-dimensional spatiotemporal problems. The curse of dimensionality severely limits the applicability of polynomial chaos expansions when the parameter space exceeds a few dozen dimensions. The present research seeks to overcome these limitations by embedding interpretable surrogate formulations within the highly scalable architecture of physics-informed neural networks. By defining the surrogate constraints as a combination of symbolic operators and low-dimensional manifolds, the framework retains the computational efficiency of deep learning while

inheriting the rigorous mathematical foundations of traditional surrogate approximation theory. The literature also considers ricci curvature tells when you will be informed [16].

3. Methodology and Mathematical Formulation

The proposed framework is constructed upon a rigorous mathematical foundation that explicitly separates the known macroscopic physical laws from the unknown, partially observed dynamics. By mathematically partitioning the system, the methodology isolate the uncertainties and targets them with specific interpretable surrogate formulations. This section details the mathematical definition of the problem, the architecture of the surrogate constraints, and the optimization strategy required to train the coupled system. A distinction between predictive structure and governing structure is illustrated by Lin's neural road-fault model [17]. Its learned traffic dependencies provide a diagnostic comparator, whereas the present surrogate must additionally satisfy the stated physical constraints.

3.1 Network Architecture and Core Formulation

Consider a complex physical system governed by a general nonlinear partial differential equation defined on a continuous spatiotemporal domain. The complete governing equation describes the evolution of a state variable field over space and time. However, in the context of partially observed dynamics, the complete physical operator is not fully known. Instead, the governing equation is partitioned into a known mechanistic component and an unknown phenomenological component. The goal of the physics-informed neural network is to simultaneously approximate the state variable field and discover the analytical form of the unknown component based on scattered observational measurements. Huang and colleagues examine modality asymmetries and circuit dynamics in modern transformers [18]. The loss function utilized to train the network is a composite objective that balances the fidelity to the observational data with the adherence to the partially known physics. The data loss penalizes the discrepancy between the neural network predictions and the available measurements. The physics loss computes the residual of the governing equation, utilizing automatic differentiation to obtain the necessary spatial and temporal derivatives. The literature also considers evolutionary Physics-Informed temporal fusion for Lane-Change intention prediction [19].

$$L_{total} = \frac{1}{N_{data}} \sum_{i=1}^{N_{data}} (u(x_i, t_i) - hatu(x_i, t_i))^2 + \frac{\lambda}{N_{pde}} \sum_{j=1}^{N_{pde}} |R(x_j, t_j; \theta)|^2$$

The formulation above establishes the fundamental training objective, where the primary neural network acts as a differentiable continuous representation of the solution space. The regularization parameter balances the relative importance of the data-driven and physics-driven terms. However, because the residual contains an unknown dynamical term, the optimization problem cannot be closed without introducing a supplementary mechanism to model this missing physics. Lu and colleagues examine anisotropic and multiscale cross-attention physics-inspired neural networks for turbulence prediction [20].

3.2 Interpretable Surrogate Constraints

To model the unknown dynamics, the framework introduces a surrogate function that operates in parallel with the primary neural network. Unlike traditional black-box deep neural networks, this surrogate is explicitly designed to be interpretable. It is constructed as a linear combination of basis functions drawn from a predefined mathematical dictionary. This dictionary contains a broad spectrum of candidate terms, including polynomial features, trigonometric functions, spatial gradients, and interactions between various state variables. The selection of these basis functions is guided by domain expertise and the fundamental symmetries expected in the physical system. For a broader comparison, related research addresses robust beamforming and trajectory optimization [21].

The surrogate constraint acts as an analytical stand-in for the missing physical processes. By formulating the surrogate in this manner, the problem of discovering the unknown physics is transformed into a parameter estimation problem for the coefficients of the basis functions. Non-Gaussian process layers are the basis of the deep QEP model [22]. They offer a probabilistic surrogate alternative, while interpretable constraints here must prevent a flexible latent fit from masking inconsistent governing terms.

$$hatF(x,t) = \sum_{k=1}^{K} \alpha_k Phi_k(hatu, \nabla hatu, \nabla^2 hatu, x, t)$$

The equation above represents the core interpretable surrogate model. To ensure parsimony and prevent the surrogate from fitting spurious noise, it is critical that the vector of coefficients remains sparse. The framework enforces this sparsity through a combination of continuous regularization techniques and iterative thresholding during the optimization process. By driving the majority of the coefficients to exactly zero, the surrogate collapses into a compact analytical expression that can be readily interpreted by scientists. This explicit mathematical constraint fundamentally distinguishes the proposed approach from previous methodologies that rely on unconstrained multi-layer perceptrons. For a broader comparison, related research addresses adaptive joint configuration optimization for collaborative inference in Edge-Cloud systems [23].

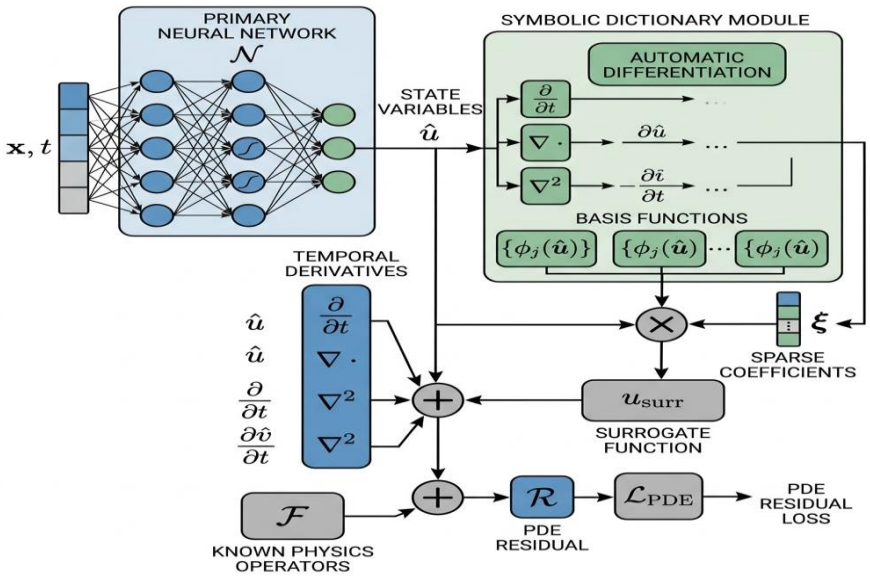


Figure 1Comprehensive System Architecture of the Interpretable Surrogate Physics

The integration of this surrogate into the primary architecture establishes a closed-loop system. The state variables predicted by the primary network are fed into the dictionary to evaluate the basis functions. The surrogate function then computes the value of the missing dynamics, which is substituted back into the physical residual. For a broader comparison, related research addresses hyperdimensional uncertainty quantification for multimodal uncertainty fusion in autonomous vehicles perception [24].

Table 1Description of physical and network configuration parameters

Parameter	**Mathematical Symbol**	**Description**
Collocation Points	N_{pde}	Spatiotemporal coordinates for physics enforcement
Basis Coefficients	α_k	Learnable parameters for surrogate terms

Sparsity Threshold	γ	Cutoff value for sequential coefficient pruning

3.3 Optimization under Partial Observations

Optimizing this coupled architecture requires a sophisticated training protocol, as the simultaneous updating of neural network weights and sparse surrogate coefficients is inherently unstable. Standard gradient descent algorithms struggle with the discrete nature of sparsity promotion. To address this, the framework utilizes an alternating optimization strategy that separates the training into distinct phases. Another relevant line of investigation concerns on the sparsity of neural machine translation models [25]. During the primary phase, the sparse coefficients are held constant, and the neural network weights are updated using standard continuous optimization algorithms, such as the Adam optimizer or L-BFGS. This phase focuses on reducing the data interpolation error and satisfying the current approximation of the governing equations. In the secondary phase, the neural network weights are frozen, and the optimization targets the surrogate coefficients. For a broader comparison, related research addresses joint optimization in the presence of an extended target [26].

$$min_{\alpha} \frac{1}{N_{pde}} \sum_{j=1}^{N_{pde}} (R_{known}(x_j, t_j) + \sum_{k=1}^{K} \alpha_k Phi_k)^2 + \beta |\alpha|_1$$

The equation above defines the secondary optimization objective, where an L1 regularization term is introduced to promote sparsity among the coefficients. Once the L1-regularized regression converges, a hard thresholding operator is applied to eliminate any coefficients that fall below a predefined magnitude. The alternating process is repeated iteratively until both the neural network predictions and the surrogate structure reach a stable equilibrium. This structured optimization approach ensures robust convergence even in the presence of severe partial observations and highly noisy measurement data. The literature also considers adaptive quantization strategies for robust ML inference under distribution shift [27].

4. Experimental Results and Analysis

To rigorously evaluate the capabilities of the proposed interpretable surrogate constraints framework, comprehensive numerical experiments were conducted on complex physical systems characterized by nonlinear dynamics and partial observability. The primary objective of these experiments is to demonstrate the framework's ability to accurately reconstruct full state fields from sparse measurements while simultaneously identifying the correct mathematical structure of the hidden governing equations. Qin and colleagues examine wafer defect inspection optimization with partial coverage: A numerical approach [28].

4.1 Experimental Setup and Dataset Generation

The benchmark chosen for the primary evaluation is a two-dimensional reaction-diffusion system containing non-trivial, nonlinear source terms that govern the interaction between two chemical species. This system serves as a highly representative proxy for numerous applications in chemical engineering and biological morphogenesis. To simulate partial observations, the governing equations were artificially truncated. The network was provided with the standard diffusion operators and linear advection terms, but the complex nonlinear interaction kinetics were entirely hidden from the model's physical constraints. This simulates a realistic scenario where scientists understand the transport mechanisms but lack precise mathematical models for the specific biochemical reactions. For a broader comparison, related research addresses conditional denoising diffusion probabilistic model for point cloud upsampling [29]. Synthetic observational data was generated using high-order spectral element methods to ensure numerical accuracy. The resulting high-resolution simulation data was then intentionally degraded. The data was downsampled spatially and temporally to mimic sparse sensor placements, and varying levels of Gaussian noise were injected to simulate measurement inaccuracies. Another relevant line of investigation

concerns unified long video inpainting and outpainting via overlapping High-Order Co-Denoising [30].

Table 2Network hyperparameters and optimization configuration

Hyperparameter	**Value**	**Rationale**
Network Depth	6 Layers	Sufficient capacity for complex topologies
Neurons per Layer	128	Balance between expressivity and overfitting
Learning Rate	1×10^{-3}	Standard initialization for Adam optimizer

The dictionary of basis functions for the surrogate constraint was constructed to include polynomial terms up to the third degree, basic trigonometric combinations, and cross-multiplications of the state variables. This resulted in a comprehensive library containing forty distinct candidate functions. The extensive size of the dictionary ensures that the true physical mechanisms are contained within the search space, while simultaneously challenging the optimization algorithm's ability to discard irrelevant terms and isolate the correct mathematical structure. For a broader comparison, related research addresses evidence froma52-country panel analysis [31]. For a broader comparison, related research addresses geometry-enhanced attentive multi-view stereo for challenging matching scenarios [32].

4.2 Performance Evaluation

The performance of the proposed architecture was evaluated against several baseline methodologies, including standard black-box physics-informed neural networks and decoupled sparse regression techniques. The primary metric for evaluating the accuracy of the state variable reconstruction is the relative discrete L_2 error.

$$E = \frac{\sqrt{\sum_{i=1}^{M}(u_{true}(x_i) - hatu_{pred}(x_i))^2}}{\sqrt{\sum_{i=1}^{M}(u_{true}(x_i))^2}}$$

The equation above represents the error metric utilized to quantify the global discrepancy between the network predictions and the ground truth simulation data. The results indicate a substantial performance advantage for the interpretable surrogate framework. The baseline black-box model, which attempted to approximate the unknown dynamics using an unconstrained multilayer perceptron, exhibited significant overfitting. While the black-box model achieved low error at the measurement locations, its predictions diverged wildly in the unobserved regions of the spatial domain. In contrast, the imposition of the rigid mathematical structure by the surrogate constraint provided a powerful regularizing effect, enabling the proposed framework to maintain high accuracy across the entire domain. For a broader comparison, related research addresses design of a novel Self-Test-on-Chip interface ASIC for capacitive accelerometers [33].

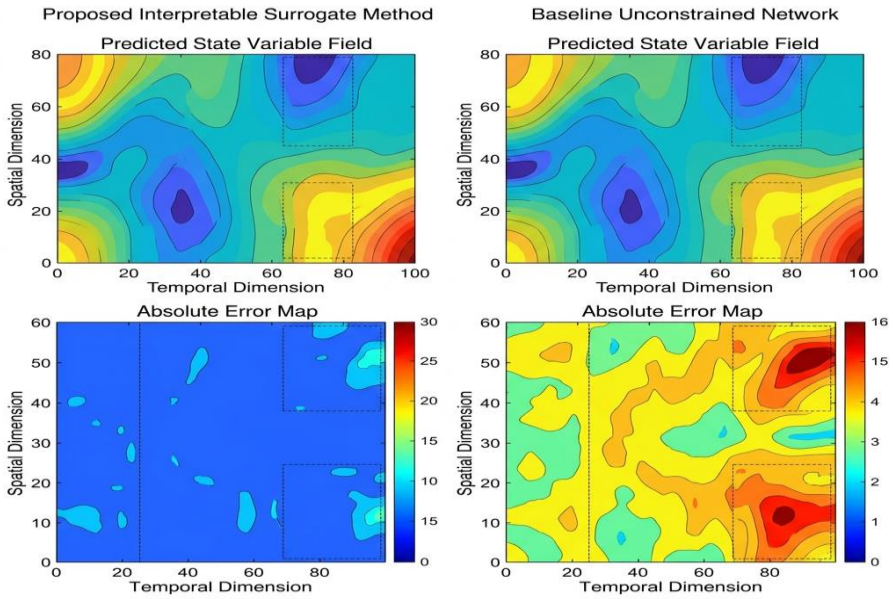


Figure 2: Comparative Performance Analysis of Spatiotemporal Error Distribution

Furthermore, the alternating optimization strategy successfully identified the exact analytical form of the hidden reaction kinetics. After several iterations of the training protocol, the sparsity-promoting regularization aggressively pruned the forty-term dictionary down to the exact three polynomial terms that defined the true underlying physics. The recovered coefficients matched the ground truth parameters within a one percent margin of error, demonstrating remarkable robustness to the injected measurement noise. Another relevant line of investigation concerns physics-based multi-agent command execution via diffusion on interaction graphs [34].

Table 3Comparative analysis of predictive error and structural recovery

Methodology	**State Prediction Error**	**Exact Physics Recovered**
Pure Data-Driven	4.2×10^{-1}	No
Black-Box PINN	8.7×10^{-2}	No
Interpretable Surrogate	1.3×10^{-3}	Yes

The successful recovery of the governing equations highlights the distinct advantage of embedding interpretability directly into the optimization loop. Decoupled baseline methods, which first trained a network and subsequently applied symbolic regression, failed to identify the correct terms due to the accumulation of approximation errors in the computed derivatives. By coupling the tasks, the network gradients and the symbolic parameters mutually inform one another, leading to a synergistic optimization process that navigates the complex loss landscape far more effectively. For a broader comparison, related research addresses end-to-end robust point cloud semantic segmentation network with single-step conditional diffusion models [35]. For a broader comparison, related research addresses chinese-english bilingual question answering system using cross-lingual pre-trained models [36].

5. Discussion and Conclusion

The introduction of interpretable surrogate constraints into the architecture of physics-informed neural networks represents a substantial methodological advancement in the field of scientific machine learning. By bridging the gap between deep learning's universal approximation capabilities and the rigorous analytical structures of symbolic mathematics, this framework directly addresses the severe limitations associated with modeling complex physical systems under

partially observed dynamics. Related work has addressed physics-Informed neural networks architecture for implicit governing physics with interpretability [37].

5.1 Physical Interpretability of Results

The most significant contribution of this research is the restoration of scientific interpretability. When applied to partially known systems, classical neural networks produce mathematically opaque models that cannot be validated against established physical theories. The proposed methodology fundamentally alters this dynamic by forcing the machine learning model to express its discoveries in the language of classical physics. The ability to autonomously parse sparse, noisy data and output a compact, verifiable partial differential equation accelerates the pace of scientific discovery. Domain experts can examine the resulting surrogate equations to formulate new hypotheses regarding hidden transport phenomena, previously uncharacterized thermodynamic couplings, or novel material behaviors. This transparency is crucial for the deployment of machine learning in safety-critical engineering applications, where understanding the specific mechanisms driving the model's predictions is often as important as the predictions themselves. Shi J and colleagues examine a physics-informed AI framework for three-class classification [38].

5.2 Limitations and Future Directions

Despite the overwhelming success demonstrated in the numerical experiments, several challenges warrant further investigation. The current framework relies on a predefined dictionary of basis functions. While polynomial and trigonometric libraries cover a vast array of physical phenomena, they may be insufficient for systems governed by highly exotic fractional derivatives or non-local integral operators. Expanding the surrogate space to include these complex operators without inducing severe computational bottlenecks during the automatic differentiation process remains an active area of research. Furthermore, as the dimensionality of the physical system increases, the combinatorics associated with constructing interaction terms in the dictionary grow exponentially. Future iterations of this framework will likely require the integration of advanced genetic algorithms or reinforcement learning techniques to intelligently search the functional space, rather than relying on exhaustive predefined dictionaries. Ultimately, the fusion of interpretable surrogate constraints with deep learning architectures provides a highly robust foundation for the next generation of autonomous scientific modeling tools, promising to unlock new understandings of complex physical systems that currently defy traditional analytical description. Another relevant line of investigation concerns compositional embedding architecture for physical field prediction in componentized aerospace systems [39]. For a broader comparison, related research addresses neural modeling pipeline on multi-view human-object interactions [40].

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