

Novelty Assessment Report

Paper: Uncertainty-Aware Diagnostics for Physics-Informed Machine Learning

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Abstract

Physics-informed machine learning (PIML) integrates prior physical information, often in the form of differential equation constraints, into the process of fitting ML models to physical data. Popular PIML approaches, including neural operators, physics-informed neural networks, and neural ordinary differential equations, are typically fit to objectives that simultaneously include both data and physical constraints. However, the multi-objective nature of this approach creates ambiguity in the measurement of model quality. This is related to a poor understanding of epistemic uncertainty, and it can lead to surprising failure modes, even when existing metrics suggest strong fits. Working within a Gaussian process regression framework, we introduce the Physics-Informed Log Evidence (PILE) score. Bypassing the ambiguities of test losses, the PILE score is a single, uncertainty-aware metric that provides a selection principle for hyperparameters of a physics-informed model. We show that PILE minimization yields excellent choices for a wide variety of model parameters, including kernel bandwidth, least squares regularization weights, and even kernel function selection. We also show that, prior to data acquisition, a special data-free case of the PILE score identifies a-priori kernel choices that are "well adapted" to a given PDE. Beyond the kernel setting, we anticipate that the PILE score can be extended to PIML at large, and we outline approaches to do so.

Disclaimer

This report is **AI-GENERATED** using Large Language Models and WisPaper (a scholar search engine). It analyzes academic papers' tasks and contributions against retrieved prior work. While this system identifies **POTENTIAL** overlaps and novel directions, **ITS COVERAGE IS NOT EXHAUSTIVE AND JUDGMENTS ARE APPROXIMATE**. These results are intended to assist human reviewers and **SHOULD NOT** be relied upon as a definitive verdict on novelty.

Note that some papers exist in multiple, slightly different versions (e.g., with different titles or URLs). The system may retrieve several versions of the same underlying work. The current automated pipeline does not reliably align or distinguish these cases, so human reviewers will need to disambiguate them manually.

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Core Task Landscape

This paper addresses: **Uncertainty Quantification in Physics-Informed Machine Learning**

A total of **50 papers** were analyzed and organized into a taxonomy with **21 categories**.

Taxonomy Overview

The research landscape has been organized into the following main categories:

- **Methodological Frameworks for Uncertainty Estimation**
- **Domain-Specific Applications of Uncertainty Quantification**
- **Cross-Cutting Methodological Advances and Reviews**

Complete Taxonomy Tree

- Uncertainty Quantification in Physics-Informed Machine Learning Survey Taxonomy
- Methodological Frameworks for Uncertainty Estimation
 - Bayesian and Probabilistic Approaches
 - Bayesian Physics-Informed Neural Networks (5 papers)
 - [2] Uncertainty quantification in Bayesian physics-informed deep learning-based traffic state prediction (Chuan Ding, 2025) [View paper](#)
 - [10] Flow reconstruction with uncertainty quantification from noisy measurements based on Bayesian physics-informed neural networks (Hailong Liu, 2024) [View paper](#)
 - [15] Flow field tomography with uncertainty quantification using a Bayesian physics-informed neural network (Molnar, 2022) [View paper](#)
 - [25] Streamflow simulation in data-scarce basins using Bayesian and physics-informed machine learning models (Dan Lu, 2021) [View paper](#)
 - [43] Predictive Uncertainty Quantification for Bayesian Physics-Informed Neural Network (Pinn) in Hypocentre Estimation Problem (M. Izzatullah, 2022) [View paper](#)
 - Variational and Approximate Inference Methods (2 papers)
 - [41] Physics-guided architecture (pga) of neural networks for quantifying uncertainty in lake temperature modeling (Arka Daw, 2020) [View paper](#)
 - [44] Physics-informed variational inference for uncertainty quantification of stochastic differential equations (Hyomin Shin, 2023) [View paper](#)
 - Distance-Aware and Evidential Uncertainty Methods (3 papers)
 - [9] A principled distance-aware uncertainty quantification approach for enhancing the reliability of physics-informed neural network (Jinwu Li, 2024) [View paper](#)
 - [19] Developing Distance-Aware Uncertainty Quantification Methods in Physics-Guided Neural Networks for Reliable Bearing Health Prediction (Waleed Razzaq, 2025) [View paper](#)
 - [20] Prediction of wind turbines power with physics-informed neural networks and evidential uncertainty quantification (Gijun, 2026) [View paper](#)
 - Ensemble and Generative Adversarial Approaches (4 papers)
 - [7] Uncertainty quantification of car-following behaviors: physics-informed generative adversarial networks (Z Mo, 2022) [View paper](#)
 - [12] Practical uncertainty quantification for space-dependent inverse heat conduction problem via ensemble physics-informed neural networks (Xinchao Jiang, 2023) [View paper](#)

- [18] Wasserstein Generative Adversarial Uncertainty Quantification in Physics-Informed Neural Networks (Gao Yihang, 2022) [View paper](#)
- [50] Probabilistic vehicle weight estimation using physics-constrained generative adversarial network (Yu Yang, 2021) [View paper](#)
- Uncertainty Quantification Under Noisy Inputs and Data (2 papers)
- [5] Uncertainty quantification for noisy inputs-outputs in physics-informed neural networks and neural operators (Zongren Zou, 2023) [View paper](#)
- [35] On the uncertainty analysis of the data-enabled physics-informed neural network for solving neutron diffusion eigenvalue problem (Yang Yu, 2024) [View paper](#)
- Theoretical Foundations and Diagnostic Metrics ★ (2 papers)
- [0] Uncertainty-Aware Diagnostics for Physics-Informed Machine Learning (Anon et al., 2026) [View paper](#)
- [40] Uncertainty quantification of physics-based label-free deep learning and probabilistic prediction of extreme events (Huiru Li, 2022) [View paper](#)
- Domain-Specific Applications of Uncertainty Quantification
 - Fluid Dynamics and Computational Fluid Dynamics
 - Turbulence Modeling and Closure Relations (3 papers)
 - [8] Quantifying Model Uncertainty of Neural Network-based Turbulence Closures (Cody Grogan, 2024) [View paper](#)
 - [13] Uncertainty Quantification in Computational Fluid Dynamics: Physics and Machine Learning Based Approaches (Chu, 2023) [View paper](#)
 - [48] Uncertainty Quantification For Turbulent Flows with Machine Learning (Chu, 2023) [View paper](#)
 - Multiphase and Reactive Flows (2 papers)
 - [28] Uncertainty Quantification for Transport in Porous Media Using Parameterized Physics Informed Neural Networks (Cedric G. Fraces, 2023) [View paper](#)
 - [30] Uncertainty quantification for multiphase computational fluid dynamics closure relations with a physics-informed bayesian approach (Yang Liu, 2023) [View paper](#)
 - Transportation and Traffic Systems (1 papers)
 - [17] Uncertainty Quantification for Physics-Informed Traffic Graph Networks (Tianshu Bao, 2025) [View paper](#)
 - Aerospace and Flight Dynamics (3 papers)
 - [4] Flight dynamic uncertainty quantification modeling using physics-informed neural networks (Piyush Mehta, 2024) [View paper](#)
 - [34] Identification of Uncertain Parameter in Flight Vehicle Using Physics-Informed Deep Learning (Kyung-Mi Na, 2024) [View paper](#)
 - [39] Estimation of aerodynamic uncertainty in missile system using Physics-Informed Neural Network Framework (Kyung-Mi Na, 2022) [View paper](#)
 - Structural Health and Fatigue Prediction (2 papers)
 - [6] Fatigue life prediction and uncertainty quantification of aerospace metals: A Bayesian physics-informed neural network model (Qianling Wang, 2025) [View paper](#)
 - [38] Quantification of uncertainty in a defect-based Physics-Informed Neural Network for fatigue evaluation and insights on influencing factors (Emanuele Avoledo, 2023) [View paper](#)
 - Manufacturing and Materials Science (3 papers)
 - [21] Uncertainty quantification in metallic additive manufacturing through physics-informed data-driven modeling (Zhuo Wang, 2019) [View paper](#)
 - [33] Uncertainty quantification in multivariable regression for material property prediction with Bayesian neural networks (Longze Li, 2024) [View paper](#)
 - [36] Physics-Informed Uncertainty Quantification in Modeling of Machining-Induced Residual Stress (Md. Mehedi Hasan, 2023) [View paper](#)
 - Energy and Nuclear Systems (2 papers)
 - [3] Uncertainty quantification study of the physics-informed machine learning models for critical heat flux prediction (Congshan Mao, 2024) [View paper](#)
 - [37] Fast uncertainty quantification of spent nuclear fuel with neural networks (AlbÃ, 2023) [View paper](#)
 - Geophysics and Earth Systems (2 papers)
 - [31] Experimental Uncertainty Propagation in Neural Network Extraction in Hadronic Physics (Keller, 2025) [View paper](#)
 - [47] Physics-informed deep learning quantifies propagated uncertainty in seismic structure and hypocenter determination (R. Agata, 2025) [View paper](#)
 - Hydrology and Environmental Systems (2 papers)
 - [26] Urban Flood Modeling: Uncertainty Quantification and Physics-Informed Gaussian Processes Regression Forecasting (Amir H. Kohanpur, 2023) [View paper](#)
 - [42] H2MV (v1.0): Global Physically-Constrained Deep Learning Water Cycle Model with Vegetation (Jung Martin, 2024) [View paper](#)
 - Biomedical and Physiological Systems (1 papers)
 - [27] Quantification of total uncertainty in the physics-informed reconstruction of CVSim-6 physiology (De Florio, 2025) [View paper](#)
- Cross-Cutting Methodological Advances and Reviews
 - Survey and Review Studies (5 papers)
 - [1] From PINNs to PIKANs: recent advances in physics-informed machine learning (Juan Diego Toscano, 2025) [View paper](#)
 - [16] Bayesian uncertainty quantification for machine-learned models in physics (Y. Gal, 2022) [View paper](#)
 - [22] Machine Learning With Data Assimilation and Uncertainty Quantification for Dynamical Systems: A Review (Sibo Cheng, 2023) [View paper](#)
 - [23] A survey on machine learning approaches for uncertainty quantification of engineering systems (Yan Shi, 2025) [View paper](#)
 - [45] A survey of Bayesian calibration and physics-informed neural networks in scientific modeling (Felipe Viana, 2021) [View paper](#)
 - Parametric and Multi-Physics Uncertainty Propagation (3 papers)
 - [24] Decomposition-enhanced parameterized physics-informed neural network for uncertainty-aware interior acoustic analysis (Xin Qiang, 2025) [View paper](#)
 - [29] Modeling parametric uncertainty in PDEs models via Physics-Informed Neural Networks (Milad Panahi, 2024) [View paper](#)
 - [32] 3D multi-physics uncertainty quantification using physics-based machine learning (Mauro, 2022) [View paper](#)
 - Spectral and Polynomial Chaos Methods (1 papers)
 - [11] Spectral pinns: Fast uncertainty propagation with physics-informed neural networks (BjÅrn LÃtjens, 2021) [View paper](#)
 - Hybrid and Differentiable Physics-Informed Models (2 papers)

- [46] Physics-informed neural networks with weighted losses by uncertainty evaluation for accurate and stable prediction of manufacturing systems (Jiaqi Hua, 2023) [View paper](#)
- [49] Diffhybrid-uq: uncertainty quantification for differentiable hybrid neural modeling (Deepak Akhare, 2023) [View paper](#)
- Hardware and Edge Computing Implementations (1 papers)
- [14] Bringing uncertainty quantification to the extreme-edge with memristor-based Bayesian neural networks (Djohan Bonnet, 2023) [View paper](#)

Narrative

Core task: uncertainty quantification in physics-informed machine learning. The field organizes around three main branches that reflect complementary perspectives on integrating physical knowledge with data-driven models while rigorously characterizing uncertainty. Methodological Frameworks for Uncertainty Estimation develops foundational techniques—ranging from Bayesian approaches like those in Bayesian Machine Learning[16] and Variational Inference SDEs[44], to ensemble methods and novel diagnostic metrics exemplified by Uncertainty-Aware Diagnostics[0]—that enable practitioners to assess epistemic and aleatoric uncertainties in physics-informed neural networks and related architectures. Domain-Specific Applications of Uncertainty Quantification translates these methods into diverse engineering and scientific contexts, including fluid dynamics (Turbulence Closures Uncertainty[8], Flow Reconstruction[10]), structural health monitoring (Fatigue Life Prediction[6], Bearing Health Prediction[19]), transportation systems (Bayesian Traffic Prediction[2], Car-Following Behaviors[7]), and energy applications (Critical Heat Flux[3], Wind Turbines Power[20]). Cross-Cutting Methodological Advances and Reviews synthesizes insights across domains, offering surveys like Engineering Systems Survey[23] and Bayesian Calibration Survey[45] that distill common challenges and emerging best practices.

Recent work highlights tensions between computational efficiency and rigorous uncertainty bounds, with many studies exploring trade-offs between sampling-based Bayesian inference and faster deterministic approximations. Uncertainty-Aware Diagnostics[0] sits within the Theoretical Foundations and Diagnostic Metrics cluster, emphasizing the development of principled evaluation criteria for uncertainty estimates—a concern shared by Label-Free Deep Learning[40], which addresses uncertainty without extensive labeled data. Compared to application-focused neighbors like Critical Heat Flux[3] or Flight Dynamic Uncertainty[4], Uncertainty-Aware Diagnostics[0] prioritizes methodological rigor in validating uncertainty predictions rather than domain-specific deployment. This positioning reflects ongoing debates about whether general-purpose diagnostics can adequately capture the nuances of physical constraints, or whether each application domain requires tailored uncertainty metrics that respect governing equations and boundary conditions.

Related Works in Same Category

The following **1 sibling papers** share the same taxonomy leaf node with the original paper:

1. Uncertainty quantification of physics-based label-free deep learning and probabilistic prediction of extreme events

Authors: Huiru Li, Jian-Hua Yin, Xiaoping Du, Jianhua Yin, X. Du | **Year/Venue:** 2022 | **URL:** [View paper](#)

Abstract

Surrogate models from machine learning regression have been increasingly used in engineering analysis and design. Since surrogate models are usually built using data from solving expensive physical models, label-free machine learning methodologies have been developed to reduce the computational cost. Understanding and quantifying the model (epistemic) uncertainty of surrogate models is critical for their applications with quantified confidence. It is, however, much more computationally expensi...

Relationship Analysis

Both papers belong to the Theoretical Foundations and Diagnostic Metrics category, focusing on uncertainty quantification frameworks for physics-informed machine learning. They overlap in addressing epistemic uncertainty estimation and developing diagnostic metrics for PIML models. However, the original paper introduces the PILE score for Gaussian process-based PIML with emphasis on model selection and hyperparameter optimization, while the candidate paper focuses on post-hoc uncertainty quantification for neural network-based label-free regression using Gaussian Process error modeling for extreme event prediction.

Contributions Analysis

Overall novelty summary. The paper introduces the Physics-Informed Log Evidence (PILE) score as a unified metric for hyperparameter selection in Gaussian process-based physics-informed models. It resides in the Theoretical Foundations and Diagnostic Metrics leaf, which contains only two papers total. This sparse population suggests the development of principled selection criteria for physics-informed models remains an underexplored area. The leaf sits within the broader Methodological Frameworks branch, which encompasses Bayesian approaches, ensemble methods, and distance-aware techniques, indicating the work contributes to foundational methodology rather than domain-specific applications.

The taxonomy reveals substantial activity in neighboring methodological categories—Bayesian Physics-Informed Neural Networks contains five papers, Variational and Approximate Inference Methods has two, and Distance-Aware and Evidential Uncertainty Methods includes three. These sibling leaves focus on posterior inference, variational approximations, and calibrated predictions respectively. The PILE score diverges by addressing model selection through marginal likelihood rather than posterior sampling or ensemble aggregation. The scope note for Theoretical Foundations explicitly excludes application-specific validation, positioning this work as a general-purpose diagnostic framework applicable across the diverse domain-specific branches visible in the taxonomy.

Among twenty-eight candidates examined, none clearly refute the three core contributions. The PILE score itself was assessed against ten candidates with zero refutable overlaps; the data-free Fredholm determinant formulation examined eight candidates with no prior work identified; empirical validation against ten candidates likewise found no substantial precedent. This limited search scope—roughly half the taxonomy's fifty papers—suggests the analysis captures top semantic matches but cannot claim exhaustive coverage. The absence of refutable candidates across all contributions indicates either genuine novelty within the examined set or that closely related work lies outside the top-K retrieval window.

The analysis reflects a targeted literature search rather than comprehensive field coverage. The sparse Theoretical Foundations leaf and zero refutable pairs across contributions suggest the PILE score addresses a gap in uncertainty-aware model selection for physics-informed Gaussian processes. However, the twenty-eight-candidate scope leaves open the possibility that relevant prior work exists in adjacent methodological areas or domain-specific applications not captured by semantic similarity. The taxonomy structure indicates active development in related Bayesian and variational methods, which may share conceptual overlap not detected by the current search strategy.

This paper presents **3 main contributions**, each analyzed against relevant prior work:

Contribution 1: Physics-Informed Log Evidence (PILE) score

Description: The authors propose the PILE score, a single uncertainty-aware metric derived from the marginal likelihood of a Gaussian process model. This score resolves the multi-objective ambiguity in physics-informed machine learning by providing a principled way to select hyperparameters such as kernel bandwidth, regularization weights, and kernel functions without relying on ambiguous test losses.

This contribution was assessed against **10 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. G-pinns: a Bayesian-optimized gru-enhanced physics-informed neural network for advancing short rate model predictions

URL: [View paper](#)

Brief Assessment

GRU-Enhanced PINNs[56] focuses on combining GRU with PINNs for short rate model predictions using Bayesian optimization for hyperparameter tuning, not on developing uncertainty-aware metrics for hyperparameter selection in physics-informed models.

2. Prediction and Uncertainty Quantification of the Fatigue Life of Corroded Cable Steel Wires Using a Bayesian Physics-Informed Neural Network

URL: [View paper](#)

Brief Assessment

Corroded Cable Fatigue[51] focuses on fatigue life prediction of corroded cable steel wires using Bayesian physics-informed neural networks for structural engineering applications, not on developing uncertainty-aware metrics for hyperparameter selection in physics-informed machine learning models.

3. A novel physical constraint-guided quadratic neural networks for interpretable bearing fault diagnosis under zero-fault sample

URL: [View paper](#)

Brief Assessment

Quadratic Neural Networks[52] focuses on bearing fault diagnosis using quadratic neural networks with physical constraints, not on uncertainty-aware metrics for hyperparameter selection in physics-informed machine learning models.

4. Developing Distance-Aware Uncertainty Quantification Methods in Physics-Guided Neural Networks for Reliable Bearing Health Prediction

URL: [View paper](#)

Brief Assessment

Bearing Health Prediction[19] focuses on uncertainty quantification in physics-constrained neural networks for bearing degradation estimation, not on hyperparameter selection metrics for physics-informed Gaussian process models. The candidate does not address marginal likelihood-based model selection or the PILE score framework.

5. Uncertainty Quantification for Transport in Porous Media Using Parameterized Physics Informed Neural Networks

URL: [View paper](#)

Brief Assessment

Porous Media Transport[28] focuses on parametric uncertainty quantification in reservoir engineering using physics-informed neural networks for stochastic PDEs, not on developing uncertainty-aware metrics for hyperparameter selection in physics-informed machine learning models.

6. Semi-supervised transfer learning preserving spatial homogeneity for gearbox diagnostics in extraneous transient noise

URL: [View paper](#)

Brief Assessment

Gearbox Diagnostics Transfer[55] focuses on semi-supervised transfer learning for gearbox fault diagnostics in mechanical systems, not on uncertainty-aware metrics for hyperparameter selection in physics-informed machine learning models. The candidate addresses a completely different application domain (mechanical diagnostics) rather than PIML model selection.

7. A Framework for Parameter Estimation and Uncertainty Quantification in Systems Biology Using Quantile Regression and Physics-Informed Neural Networks.

URL: [View paper](#)

Brief Assessment

Systems Biology Framework[54] focuses on parameter estimation and uncertainty quantification in systems biology using quantile regression methods, not on hyperparameter selection metrics for physics-informed machine learning models with Gaussian processes.

8. Acceleration of a physics-based machine learning approach for modeling and quantifying model-form uncertainties and performing model updating

URL: [View paper](#)

Brief Assessment

Model-Form Uncertainties[57] focuses on the nonparametric probabilistic method (NPM) for structural dynamics with hyperparameter optimization via stochastic loss functions, not on uncertainty-aware metrics for physics-informed machine learning hyperparameter selection in the context of Gaussian processes and kernel methods.

9. Integrating Physics and Data-Driven Approaches: An Explainable and Uncertainty-Aware Hybrid Model for Wind Turbine Power Prediction

URL: [View paper](#)

Brief Assessment

Wind Turbine Hybrid[53] focuses on wind turbine power prediction using hybrid physics-data models with SHAP explainability and conformalized quantile regression for uncertainty. It does not address hyperparameter selection metrics for physics-informed machine learning or propose uncertainty-aware model selection criteria like PILE.

10. Diffhybrid-ug: uncertainty quantification for differentiable hybrid neural modeling

URL: [View paper](#)

Brief Assessment

Differentiable Hybrid Modeling[49] focuses on uncertainty quantification in hybrid neural models combining physics-based solvers with deep learning, not on hyperparameter selection metrics for physics-informed kernel learning. The candidate addresses aleatoric and

epistemic uncertainty propagation through ensemble methods and unscented transformations, while the original introduces PILE as a marginal likelihood-based metric for model selection in Gaussian process regression frameworks.

Contribution 2: Data-free PILE score via Fredholm determinant

Description: The authors introduce a data-free variant of the PILE score that converges to a Fredholm determinant as the number of quadrature points increases. This metric enables a priori kernel selection before any data is collected, identifying kernels that are inherently suited to solving a given partial differential equation.

This contribution was assessed against **8 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. Nonlinear PDEs for Fredholm determinants arising from string equations

URL: [View paper](#)

Brief Assessment

Nonlinear PDEs Fredholm[69] focuses on Fredholm determinants arising from string equations in 2D gravity and random matrix theory, not on data-free kernel selection methods for solving partial differential equations in physics-informed machine learning contexts.

2. Level-Spacing Distributions and the Bessel Kernel

URL: [View paper](#)

Brief Assessment

Bessel Kernel[72] studies Fredholm determinants in the context of random matrix theory and level-spacing distributions, not for data-free kernel selection in physics-informed machine learning or PDE solving.

3. Enhanced stability and accuracy in solving nonlinear Fredholm integral equations using hybrid radial kernels and particle swarm optimization

URL: [View paper](#)

Brief Assessment

Fredholm Integral Equations[67] focuses on numerical methods for solving nonlinear Fredholm integral equations using hybrid radial kernels and particle swarm optimization, not on data-free kernel selection for PDEs or Fredholm determinants as model selection criteria.

4. A Convex Optimization Approach for Backstepping PDE Design: Volterra and Fredholm Operators

URL: [View paper](#)

Brief Assessment

Backstepping PDE Design[73] focuses on boundary control design for PDEs using Volterra and Fredholm operators in a control theory context, not on data-free kernel selection for physics-informed machine learning or Gaussian process regression frameworks.

5. Fredholm determinants and the Evans function

URL: [View paper](#)

Brief Assessment

Fredholm Evans Function[74] focuses on spectral theory and the Evans function for differential operators, not on data-free kernel selection methods for physics-informed machine learning or Gaussian process regression frameworks.

6. Kernel-based approximation methods using Matlab

URL: [View paper](#)

Brief Assessment

Kernel-Based Approximation[68] is a textbook on kernel methods and reproducing kernel Hilbert spaces. While it discusses Fredholm determinants in the context of Hilbert-Schmidt operators and Mercer series (Section 2.2), it does not address data-free kernel selection for PDEs or propose any metric analogous to the PILE score for a priori model selection before data acquisition.

7. From Bernoulli Numbers to Selector Kernels: Fredholm Determinants, ζ -Regularization, and the Bridge Between Discrete and Continuous Spectra

URL: [View paper](#)

Brief Assessment

Bernoulli to Selector[70] focuses on mathematical connections between Bernoulli numbers, ζ -regularization, and Fredholm determinants in the context of trigonometric selector kernels and random matrix theory. It does not address data-free kernel selection for partial differential equations or physics-informed machine learning, which are the core applications of the original paper's PILE score contribution.

8. The Fredholm determinant method for the KdV equations

URL: [View paper](#)

Brief Assessment

Fredholm KdV Method[71] applies Fredholm determinants to solve KdV equations in mathematical physics, not to data-free kernel selection for physics-informed machine learning or partial differential equation solvers.

Contribution 3: Empirical validation of PILE for hyperparameter optimization

Description: The authors demonstrate through case studies that minimizing the PILE score yields excellent hyperparameter choices across various settings, including kernel bandwidth selection, regularization weight tuning, and kernel function selection. They show that PILE can diagnose model misspecification and identify optimal kernels, leading to vastly improved performance in challenging scenarios such as the wave equation.

This contribution was assessed against **10 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. Integrating data-driven and physics-based approaches for robust wind power prediction: A comprehensive ML-PINN-Simulink framework

URL: [View paper](#)

Brief Assessment

ML-PINN-Simulink Framework[63] focuses on wind power forecasting using machine learning and physics-informed neural networks for wind energy systems, not on hyperparameter optimization methods for physics-informed models or kernel-based Gaussian process regression frameworks.

2. G-pinns: a Bayesian-optimized gru-enhanced physics-informed neural network for advancing short rate model predictions

URL: [View paper](#)

Brief Assessment

GRU-Enhanced PINNs[56] employs Bayesian optimization for hyperparameter tuning in a specific financial modeling context, which differs from the PILE score's approach to hyperparameter optimization through marginal likelihood minimization across various physics-informed settings.

3. Interpretable data-driven ship dynamics model: Enhancing physics-based motion prediction with parameter optimization

URL: [View paper](#)

Brief Assessment

Ship Dynamics Model[64] focuses on ship motion prediction using constrained nonlinear least squares optimization for physics-based model parameters, not on physics-informed machine learning hyperparameter selection via marginal likelihood metrics like PILE.

4. Hyperparameter selection for physics-informed neural networks (PINNs) Application to discontinuous heat conduction problems

URL: [View paper](#)

Brief Assessment

Hyperparameter Selection PINNs[61] focuses on optimizing neural network architecture parameters (hidden layers, learning rate, activation functions) for discontinuous heat conduction problems, not on developing or validating uncertainty-aware metrics like PILE for kernel-based physics-informed models.

5. Importance of hyper-parameter optimization during training of physics-informed deep learning networks

URL: [View paper](#)

Brief Assessment

Hyper-Parameter Optimization[58] focuses on hyperparameter tuning for physics-informed deep learning networks in materials science applications (stress field prediction), not on the PILE score metric or Gaussian process regression framework used in the original paper.

6. Evolutionary Optimization of Physics-Informed Neural Networks: Survey and Prospects

URL: [View paper](#)

Brief Assessment

Evolutionary PINNs Survey[60] focuses on evolutionary algorithms for PINN optimization and does not address Bayesian model selection criteria like PILE. The survey discusses hyperparameter optimization through evolutionary methods (e.g., neural architecture search, transfer learning) rather than uncertainty-aware evidence-based metrics for physics-informed kernel learning.

7. Hybrid physics-based and data-driven models for smart manufacturing: Modelling, simulation, and explainability

URL: [View paper](#)

Brief Assessment

Smart Manufacturing Hybrid[66] discusses physics-based and data-driven models for manufacturing applications, not hyperparameter optimization methods for physics-informed machine learning models or the PILE score framework.

8. Data-driven optimal power flow: A physics-informed machine learning approach

URL: [View paper](#)

Brief Assessment

Optimal Power Flow[62] focuses on power system optimization using stacked extreme learning machines for optimal power flow problems, not on physics-informed machine learning hyperparameter optimization or PILE score validation. The candidate addresses a completely different domain (power systems) with different methods (SELM) and objectives (OPF calculation efficiency).

9. Physically-Consistent Parameter Identification of Robots in Contact

URL: [View paper](#)

Brief Assessment

Robot Parameter Identification[65] focuses on inertial parameter identification for robots in contact using joint torque measurements, not on hyperparameter optimization methods for physics-informed models or kernel selection in Gaussian processes.

10. Evolutionary optimization of physics-informed neural networks: Evo-pinn frontiers and opportunities

URL: [View paper](#)

Brief Assessment

Evolutionary PINNs Frontiers[59] focuses on evolutionary algorithms for PINN optimization and architecture search, not on Gaussian process-based hyperparameter selection methods like PILE.

Appendix: Text Similarity Detection

No high-similarity text segments were detected across any compared papers.

References

- [0] Uncertainty-Aware Diagnostics for Physics-Informed Machine Learning [View paper](#)
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