ABSTRACT

Title of Dissertation: PHYSICS-INFORMED DEEP LEARNING FRAMEWORK FOR PROBABILISTIC MODELING OF ENVIRONMENTALLY INDUCED DEGRADATION

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Evaluating the degradation behavior and estimating the lifetime of engineering systems and structures is crucial to ensure their safe and reliable operation. Deep learning (DL) models, which are in the form of multi-layer neural networks (NN), have been widely used for the prognostics of such systems and structures, primarily by estimating their degradation intensity and remaining useful life (RUL). Although DL prognostic models have shown promising performance, there are limitations with such models that need to be considered. Firstly, they only learn the data patterns without consideration of the governing physics of degradation. Excluding physics, accompanied by the lack of interpretability in DL models, makes them prone to violating physical laws while showing a good fit to the training data. This issue may lead to weak generalization, mainly for predicting situations outside the training dataset. Secondly, they require significant data for

sufficient training, which may not always be available. To estimate degradation and lifetime, NNs are typically trained in a supervised setting using labeled data that ideally have been collected at different levels of degradation up to the failure points. However, collecting that data is usually expensive and time-consuming, particularly for durable systems with long lifetimes, as material degradation (e.g., corrosion, fatigue, wear, or creep) is often slow. Therefore, there is a need for a model that possesses interpretability and follows the underlying physics of degradation that occurs in real-world conditions. Additionally, this model should be trainable with limited data.

This dissertation proposes a novel data-driven framework to address the abovementioned limitations, including disregarding physics, lack of interpretability, and the need for big data in DL prognostics models. The framework comprises two NNs: a physics discovery NN and a predictive NN. The former models the underlying physics of degradation, while the latter makes probabilistic predictions for degradation intensity. The physics discovery NN guides the predictive NN and forces it to follow the underlying physics of degradation, which results in better life estimations. In this way, less data is required for sufficient training as the physics discovery model acts as a constraint and limits the search space for the parameters in the training of the predictive model.

Additionally, integrating the state-of-the-art feature importance measurement methods into the physics discovery model makes it possible to identify the primary environmental factors that significantly impact the degradation process. This work enhances the interpretability by shedding light on the dominant factors influencing the system's degradation. The application of the proposed approach is demonstrated through two case studies based on publicly available datasets for degradation phenomena.

The outcome of this research study can be used to develop a prognostics and health management system that can facilitate a low-cost and high-performance predictive maintenance strategy for systems experiencing environmentally induced degradation. Also, the proposed method can guide data collection from the field by revealing the influential factors that play crucial roles in the degradation of systems. Moreover, the proposed approach offers valuable benefits to designers, enabling them to incorporate appropriate preventive and mitigation strategies into their designs.

PHYSICS-INFORMED DEEP LEARNING FRAMEWORK FOR PROBABILISTIC MODELING OF ENVIRONMENTALLY INDUCED DEGRADATION

by

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Dedication

I dedicate this dissertation to my wonderful wife, Neda, whose continuous support has been a pillar throughout every step of my life. The completion of this dissertation would not have been possible without her encouragement. Additionally, I extend this dedication to my precious baby daughter, Nella, whose presence has illuminated our lives with joy and happiness. I love you both and believe that we did this together.

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List of Abbreviations

DL: Deep Learning

GNN: Guided Neural Network

LR: Linear Regression

MAE: Mean Absolute Error

MAPE: Mean Absolute Percentage Error

ME: Maximum Error

NN: Neural Network

PCA: Principal Components Analysis

PR: Polynomial Regression

ReLU: Rectified Linear Unit

RUL: Remaining Useful Life

SHAP: Shapley additive explanations

SVR: Support Vector Regression

Tanh: Hyperbolic Tangent

Chapter 1: Introduction

This chapter initially provides an overview of the need for degradation modeling and effective degradation maintenance strategies. It includes discussing the potential issues associated with the present models. Then, the expected contributions of the current study are described. Finally, the last section outlines the structure of the dissertation.

1.1. <u>Background</u>

Degradation is an inevitable phenomenon happening to all physical systems with different levels of rate and severity, depending on the material, design, environment, and operating conditions. This usually undesirable process can occur through various degradation phenomena or mechanisms such as corrosion, fatigue, wear, and creep. Regardless of the mechanism, degradation has always been a big concern for organizations with assets exposed to a degrading environment, as it can cause significant losses. For example, corrosion damage costs around 3.4% of the global gross domestic product (GDP) annually, which equals $2.5 trillion [1]. The total annual direct cost of corrosion in the US was estimated at around $276 billion – about 3.1% of the US GDP [2]. Besides the enormous economic loss, many catastrophic failures due to degradation have made the headlines. The Aloha accident [3], the Flixborough explosion [4], and the Silver Bridge collapse [5] are examples of such catastrophic degradation-related events involving fatalities. All these observations and experiences emphasize that systems degradation needs special attention to avoid future economic and life losses.

Degradation can be investigated across various scales, ranging from microscopic level to higher levels involving individual components and entire systems. For instance, corrosion is a failure mechanism that can be investigated at a micro level by examining the movement of electrons and ions between the cathode and anode as a key aspect of the electrochemical reactions. Alternatively, it can be explored at a macro level by assessing the mass loss in a component caused by material oxidation. This study focuses on the assessment of higher-level degradation for evaluating the lifetime of systems, with low-level investigations falling outside the scope of this research.

Corrosion, fatigue, wear, and creep are the prominent degradation mechanisms that researchers have extensively investigated in recent years. Corrosion involves the degradation of a material, particularly metals, as they convert into a more stable state, often in the form of oxides. Various types of corrosion have been identified, including uniform, pitting, crevice, galvanic, stress corrosion cracking, and intergranular corrosion. In 2020, the US Navy identified corrosion as naval aviation's greatest systemic degrader across the fleet [6].

Fatigue, mainly defined by the initiation and propagation of cracks, is a degradation mechanism that occurs under cycling loading when the loads are considerably lower than the strength of the material under static loads. In addition to loading, environmental conditions such as temperature and humidity can affect the rate of fatigue degradation.

Another significant degradation mechanism is wear, which occurs when there is relative motion between surfaces that come into contact. Wear can manifest in various forms, including abrasion, adhesion, erosion, and fatigue-wear.

Finally, creep is another failure mechanism causing plastic deformation under lower loading at high temperatures. Much like fatigue, wear, and corrosion, creep is a critical degradation mechanism that can substantially alter the structural integrity of materials over time. The rate and intensity of such degradation phenomena can vary based on the prevailing environmental conditions and if other degradation mechanisms are concurrently activated. For instance, exposure to aggressive chemicals can accelerate wear and creep mechanisms, ultimately accelerating material degradation.

There have been many research studies on the control of degradation. For example, methods like coatings, cathodic protection, alloying, inhibitors, and passivators were proposed for corrosion prevention [7]. Methods like surface hardening, lubrication, protective coatings, material selection, and wear-resistant alloys were proposed for minimizing wear. However, it is widely accepted that the degradation phenomenon cannot be fully prevented, specifically on large scales. That is why besides the control strategies, many industries invest in maintenance to repair or replace parts after they reach a specific degree of degradation. In addition, sometimes maintenance costs are much lower than prevention, making maintenance a more reasonable solution. Therefore, in many industries, there is a need for an efficient maintenance strategy that can ensure the safe and reliable operation of various systems.

To establish an effective and efficient maintenance strategy, it is imperative to predict degradation behavior. Anticipating how a system or structure will degrade over time is pivotal for planning maintenance interventions that are timely and efficient. This predictive capability enables organizations to proactively address potential faults before they escalate, avoiding unexpected failures and minimizing operational disruptions. A maintenance strategy based on degradation behavior predictions optimizes resource allocation by scheduling maintenance activities when needed, reducing costs and down times. Accurately predicting degradation behavior enables organizations to uphold high operational reliability, safety, and cost-effectiveness in their maintenance operations.

1.2. Motivation

Maintenance is expensive for organizations with physical assets prone to different degradation mechanisms. For example, it was reported that the cost of corrosion maintenance for the US Navy from 2017 to 2020 exceeds $2 billion (just for the F/A-18C-G fleet) [6]. If the high maintenance cost is not managed, it can harm organizations. That is why, to reduce labor and material costs of maintenance and to avoid costly downtime of systems, as well as catastrophic breakdowns, especially for safety critical systems (such as aircraft), more efficient predictive maintenance strategies are replacing traditional costly preventive and corrective maintenance strategies.

In preventive maintenance, regularly scheduled maintenance activities are performed (regardless of the state of health of the system) to avoid any failures in the future. For this reason, the number and severity of failures in such a strategy are so low. However, preventive maintenance is expensive to implement as there can be unnecessary repair activities (i.e., costs) according to the predetermined repair schedules for the healthy systems. This strategy requires much effort to determine the optimum time for maintenance activities. On the other hand, unlike preventive maintenance, corrective maintenance is unplanned and involves corrective actions (i.e., repair) for systems after their breakdown. Therefore, there is no effort for failure prevention in corrective maintenance, and the maintenance cost is mainly for repair activities. This strategy is usually selected for systems whose failures are not costly and do not cause critical situations [8].

Predictive maintenance is a proactive condition monitoring strategy to avoid unnecessary repairs (and their costs) and severe failures by estimating RUL or degradation intensity and determining the best time for repair activities (or replacement). This way, the total maintenance cost (i.e., prevention cost + repair cost) will be minimized (although the repair cost is higher than preventive maintenance and the prevention cost is higher than corrective maintenance), as shown in Figure 1. Thus, the main element of a successful predictive maintenance strategy is the ability to predict failure times based on RUL or degradation intensity, a concept otherwise known as prognostics.

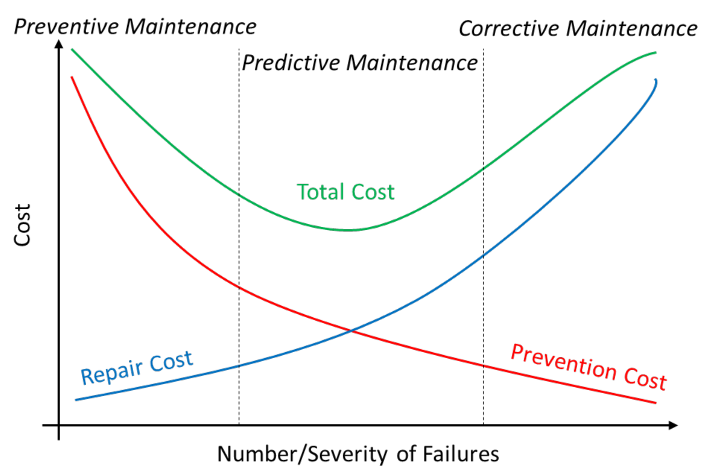

Figure 1. Preventive, corrective, and predictive maintenance comparison

Many prognostics approaches have been broadly investigated in different industries for various equipment [9, 10, 11] to facilitate predictive maintenance by predicting failure times. In the last couple of years, with considerable progress in data-driven approaches, specifically DL methods, as well as the availability of abundant historical data generated by IoT-based devices and sensors, data-driven models have become highly popular in prognostics.

A well-designed data-driven prognostic framework leads to high-performance and cost-effective predictive maintenance. However, some issues, including data scarcity and lack of interpretability in DL models, need to be addressed in the development step and before the implementation of such models in real-world conditions. These issues are discussed in more detail in the next parts of this chapter.

1.3. Problem

Two main approaches in the literature for prognostics and degradation modeling are (1) empirical models based on the physics of failure and (2) data-driven models based on sensor measurements. However, both approaches have their limitations. Empirical models (e.g., Paris law [12]) are obtained experimentally, usually in controlled laboratory environments based on limited accelerated stress variables. While they provide valuable insights, these models do not fully represent the actual degradation process that happens in the field. The reason is that such models have been developed after many simplifications and may exclude specific stresses in the field (e.g., mechanical, temperature, humidity), which can cause considerable estimation errors [13].

On the other hand, data-driven models, particularly DL models in the form of NNs, can incorporate a broad range of stresses and learn the complex interactions between them (since they can fit high dimensional data). However, there are issues associated with

DL models as well. Firstly, such models often disregard the underlying physics of degradation and merely rely on fitting the data. This means if the training dataset does not sufficiently encompass the various conditions in the field, the model may struggle to perform well when confronted with data points outside the training data distribution. The root cause of this issue is that DL models often struggle with extrapolation while they excel at interpolation tasks. Consequently, these models may suffer from poor generalization when faced with unseen data in the field. In DL prognostics models, this deficiency can even lead to the risk of breaking down the underlying physics of degradation while still achieving a good fit for the available data.

Secondly, DL models usually have many parameters, requiring substantial training data. However, collecting data from degradation phenomena, typically slow processes, is time-consuming and expensive. This poses a challenge as obtaining a sufficient dataset becomes difficult, hindering the model's sufficient training.

Finally, a critical limitation of DL models is their lack of interpretability. Their black-box nature makes it challenging to understand how input features and their interactions influence the model's output. As a result, despite being useful for prognostics purposes, DL models do not provide valuable insights into the individual factors' impact on the degradation progression or offer any information about the underlying physics of degradation. While understanding the underlying physics of degradation can help designers to consider mitigation solutions in their designs and allow users to plan for effective maintenance strategies. Additionally, any information about the underlying physics helps develop future data-driven models for prognosis purposes.

In summary, when it comes to prognostic purposes, physics-based models are primarily developed empirically and cannot account for all environmental factors. On the other hand, data-driven models, especially DL models, can incorporate a comprehensive range of environmental factors. However, DL models face challenges related to overlooking the physics of degradation, the requirement for substantial data, and issues of interpretability that must be resolved for successful implementation.

The underlying physics of degradation should be incorporated into developing DL models for prognostics and degradation modeling to address these issues. However, the physics governing degradation processes can be very complex, and the degradation behavior of a system may depend on multiple interacting environmental factors. It means empirically developed models do not represent the physics of degradation since they often fail to account for all environmental factors. Therefore, there is a need for an approach that discovers complex, multi-dimensional physics of degradation and integrates it into predictions of the DL model. In this way, not only the issues of disregarding physics and the lack of interpretability can be addressed, but also the need for vast datasets can be rectified since adding physics imposes a constraint that narrows down the search space for model parameters, allowing for training the model even with limited data.

1.4. Contributions

The main contributions of this study are summarized below:

1. Previously developed physics-informed DL prognostic models incorporated known empirical models or a general understanding of physical principles to enhance predictive capabilities. However, none reflect the governing physics of

degradation in real-world conditions, as explained in the previous section. The introduced approach in this dissertation improves this common practice by integrating a physics discovery model directly into a predictive model. Incorporating a physics discovery model aims to capture the complex underlying physics of degradation that may not be explicitly described by established empirical models or understood through general physical rules.

2. Besides developing a physics-informed predictive model that is cognizant of the complex underlying physics of degradation, another major contribution of this study is introducing a novel approach based on NN theory for discovering the complex underlying physics of degradation in real-world conditions where many stresses act synergically. By having the ability to consider all stresses in the field, the proposed approach provides a comprehensive and accurate representation of the degradation in complex systems.
3. The last major contribution of this study is to integrate the proposed physics discovery model into a feature importance measurement method. Doing so enables identifying the primary stressors that significantly influence degradation. Therefore, the developed approach not only uses the capabilities of NN algorithms for effective prognostics, which is a well-explored topic in the existing literature, but also maintains high interpretability, which is a considerable contribution. Additionally, a recursive feature elimination scheme is implemented to exclude environmental factors without significantly impacting degradation from the discovered physics relationship.

1.5. *Objectives and Outline*

The main objective of this study is to use NN algorithms to develop an integrated framework for discovering the underlying physics of degradation from test and environmental field data. In this study, the term "physics discovery" pertains to the development of a NN model that maps environmental factors to degradation rate values. The objective is to create a surrogate function that accurately represents the physics underlying the degradation process. Since some degradations may also involve chemical, biological or electromagnetic processes, we use the word physics generally to represent all these processes. Importantly, the focus of physics discovery in this study is for identifying the key environmental factors that predominantly influence degradation behavior and exert dominance in the established relationship.

In the next step, the discovered physics guide the predictions of degradation intensity. This framework not only exploits the capability of NNs in fitting high dimensional data, which makes it possible to consider the impacts of all environmental factors on degradation phenomena, but also addresses the issues of disregarding physics, data requirement, and the lack of interpretability in such models. With this aim in mind, this dissertation comprises six chapters, as outlined below:

- Chapter 1 of this dissertation is an introductory section encompassing background information, research motivation, and the addressed problem in this study. It lays the foundation for the subsequent chapters by presenting an overview of the research's context and what it aims to achieve.
- Chapter 2 presents an extensive literature review, focusing on previously developed data-driven models, particularly NNs, utilized in prognostic

applications. The chapter delves into various approaches and applications within the prognostic domain. Additionally, it sheds light on the existing studies on integrating physics into NN models in prognostics, offering a comprehensive understanding of the research landscape.

- Chapter 3 introduces a novel dual NN framework proposed for predicting degradation even with limited training data using the physics discovered from short-term test data. This chapter demonstrates the application of this approach through a detailed case study of atmospheric corrosion in a marine environment.
- Chapter 4 gives a thorough description of how the proposed dual NN framework can be utilized to discover the underlying physics governing degradation. Furthermore, the chapter explores how this framework can identify and analyze the prominent environmental factors influencing degradation behavior. In other words, this chapter focuses more on the interpretability of DL prognostic models.
- Chapter 5 discusses the results obtained from applying the proposed approach and the verification of its effectiveness using a simulated dataset. Additionally, this chapter critically examines the limitations of the proposed framework, providing a balanced view of its capabilities and constraints.
- Finally, Chapter 6 presents conclusions from this research study by summarizing the contributions. It also outlines potential future research directions, suggesting avenues for extending and enhancing the current study.

Notably, all the codes generated for this research study are implemented in Python. They are included in the dissertation as an appendix, ensuring the reproducibility and transparency of the research.

Chapter 2: Literature Review

Using NN models for predicting RUL and degradation intensity has been extensively considered for various systems in the existing literature. However, prior research on DL-based prognostic suffers from three critical challenges: not considering the governing physics of degradation, data requirement, and struggling with interpretability, all of which were discussed in Chapter 1.

The need to bridge the gap between data-driven approaches, specifically DL, and underlying physics has driven the exploration of novel methodologies. However, only a few studies have incorporated physics into NN models to enhance their predictive accuracy and generalizability. This chapter provides a comprehensive overview and synthesis of previous research efforts in this domain, shedding light on the progress made and the existing gaps in the integration of NN and the physics of degradation for effective lifetime prediction.

2.1. Neural Networks for Prognostics

NNs have found broad applications for prognostics based on sensor measurements. Batteries [10], rotating machinery [9], and machining tools [14] are some examples that have been considered in the literature for lifetime predictions by NN models. Prognostic is mainly performed by estimating RUL or damage accumulation (i.e., degradation). This estimation effort is a regression problem that maps the operating conditions to RUL or degradation intensity.

Different NN algorithms have been used for this purpose, such as feedforward NN, convolutional NN, recurrent NN, and autoencoder [15, 16, 17]. Feedforward NNs can learn complex patterns and are relatively straightforward to implement. For example, Kang et al. [18] developed a feedforward NN for estimating RUL for turbofan engines based on sensor measurements. Khumprom et al. [19] evaluated the impact of input features on the performance of a feedforward NN for RUL prediction for the same systems. Elasha et al. [20] used the same type of network for evaluating the RUL of wind turbine gearbox bearing using some extracted features from vibration measurements. Ismail et al. trained a feedforward NN using the extracted features by principal component analysis to estimate RUL for insulated gas bipolar transistors [21]. Convolutional NNs are designed for processing grid-like data to learn hierarchical representations of input data. Liu et al. [22] trained a convolutional NN to model the RUL of bearings after a short-time Fourier transformation of collected vibrations. The same type of NN was used by Modarres et al. [23] for the assessment of structural damages. Aghazadeh et al. [14] used a convolutional NN for tool wear estimation. A convolutional NN was developed by Li et al. [24] for the RUL estimation of turbofan engines.

Recurrent NNs are designed for processing sequential data as they have internal memory to keep information from past inputs for prediction on future inputs. A long short-term memory network, which is a type of recurrent NN, was developed by Hu et al. [25] to predict the degradation of mechanical parts. Zhang et al. [26] used the same type of NN for machine tool wear prediction. Liang et al. [27] developed a recurrent NN for the life assessment of bearings.

Autoencoders can learn meaningful representations of the input data in lower dimensions and are used for feature learning. Verstraete et al. [28] and Ding et al. [29]

used autoencoders for the lifetime prediction of rolling bearings. Wei et al. [30] proposed an RUL prediction framework for Lithium-ion batteries based on an autoencoder. Zhao et al. [31] compared different NN algorithms, such as autoencoder, for the lifetime prediction of machining tools.

Despite significant progress in the NN applications to develop a robust NN model for lifetime and degradation prediction, the issues of data scarcity, potential inconsistencies with physical law, and the lack of interpretability need to be addressed. Certainly, NNs are recognized for their reliance on large amounts of training data, and their optimal performance depends on the accessibility of ample data - a condition rarely met in many scenarios. So far, various strategies have been proposed to address the limited dataset size concerning model generalization and optimization. However, further attention is required to address this persistent challenge [32].

Furthermore, despite the promising outcomes, many companies hesitate to use NNs. This reluctance is primarily related to the inherent black-box nature of such algorithms, which results in a lack of interpretability. The challenge stems from an insufficient comprehension of the model and the rationale behind specific outputs. Notably, recent efforts have addressed this issue, but further investigations are required [16].

Finally, current research studies actively explore ways to integrate physical information into learning algorithms, emphasizing the importance of interpretability in these models. The focus on interpretability arises from the need to make the decision-making processes of complex models transparent, particularly as they incorporate physical principles. This is crucial for building trust and reliability, especially for prognostics of critical systems. The goal is to enhance the accuracy of predictions and provide a clear understanding of how these models utilize data in their decision-making processes [33].

2.2. Incorporating Physics into Neural Networks for Prognostics

The main goals of embedding physics laws in data-driven models are accelerating training (with limited data) and improving the generalization of the models. Researchers have considered different ways of embedding physics in purely data-driven NNs. The developed approaches can be divided into three categories: observational biases, inductive biases, and learning biases [34]. The observational biases approach is the most basic approach using feature engineering and data augmentation based on physics-based models. The inductive biases approach considers designing specialized NN architecture (usually in the form of recurrent NN) by adding physics-based layers that embed the physical laws. The learning biases approach imposes constraints on NN estimations by defining appropriate penalty terms representing physical laws in the cost function. Different research studies use each of these three approaches for the development of physics-informed models [35].

The simplest approach for integrating physics knowledge into an NN is training the model with physics-informed input data. This method generates augmented inputs or extracted features based on domain physical knowledge (e.g., empirical models, simulation, governing equations) for training to incline the NN model to respect physics. For example, Chao et al. [36] used this approach to combine physics-based models with DL algorithms to estimate the RUL of systems. Using a physics-based model, they inferred unobservable features through a Bayesian filter. A combination of them and sensor readings are used as input to an NN, resulting in a DL prognostic model with physics-based features. Ma et al. [37] used features extracted based on domain physical knowledge to model degradation in an electro-hydrostatic actuator system using a long short-term memory network. The observational biases approach has been considered more for diagnostics and fault detection than prognostics. For instance, the same authors showed that a similar approach could be used for fault detection and isolation [38]. In another work, using the idea of physics-informed input data, Wang et al. [39] developed an unsupervised fault diagnosis method for bearings by training a data-driven model on a synthetic fault dataset generated by augmenting real vibration samples for healthy bearings based on expert knowledge. There are more studies in this context [40, 41].

The inductive biases approach adds physics-based layers into NNs [35]. In one of the initial studies in this area, Dourado and Viana [42] developed a physics-informed model by embedding a physics-based model (Paris law [43]) as a layer in a recurrent NN to estimate cumulative damage in Al 2024-T3 alloy material used in fuselage panels of aircraft wings. In their NN model, the adopted Paris law calculates a base crack growth in a separate cell, and then an extra crack growth because of corrosion was obtained by a data-driven cell and added to the base value. A few years later, they implemented the same methodology using the Walker model as the physics-based model for crack growth rather than Paris law [44]. Yucesan and Viana [45, 46] developed a relatively similar physics-informed recurrent NN to estimate cumulative damage in bearing and grease for wind turbines. More research studies use the idea of the physics-informed layer in a recurrent NN [47, 48].

Chen et al. [49] proposed a model for fatigue life prediction by embedding well-known physics-based models (Basquin relation and Walker model) for fatigue in some hidden neurons of the network as the activation function. This way, besides the parameters of the regular neurons (weights and biases), the parameters of the neurons with the physical model activation function were trained during the training. The proposed model showed higher accuracy for fatigue life prediction of Al 2024-T4 and AMS 5707 with a small amount of data compared with other ML models, including random forest and support vector machine (SVM).

The learning biases approach, which was initially proposed by Raissi et al. [50] as a physics-informed neural network (PINN), imposes constraints on NN estimations by defining appropriate penalty terms in the form of a differential equation that represents physical laws in the cost function, as shown in Equation 2-1, where u is the model's output and λ is model's parameters. The network parameters will be learned (estimated) through an optimization effort to minimize the cost function that contains the underlying physics equation as a penalty term (Equation 2-2), as shown in Figure 2. This approach enables the trained model to follow the governing equations and be a surrogate function for the equation solution [51, 52, 53]. Raissi et al. [50] originally proposed PINN for solving challenging partial differential equations (PDE) in fluids, quantum mechanics, reaction-diffusion systems, and the propagation of non-linear shallow-water waves.

$$u_t = f(u, \lambda) \qquad 2\text{-}1$$

$$Physics\ penalty\ term = u_t - f(u, \lambda) \qquad 2\text{-}2$$

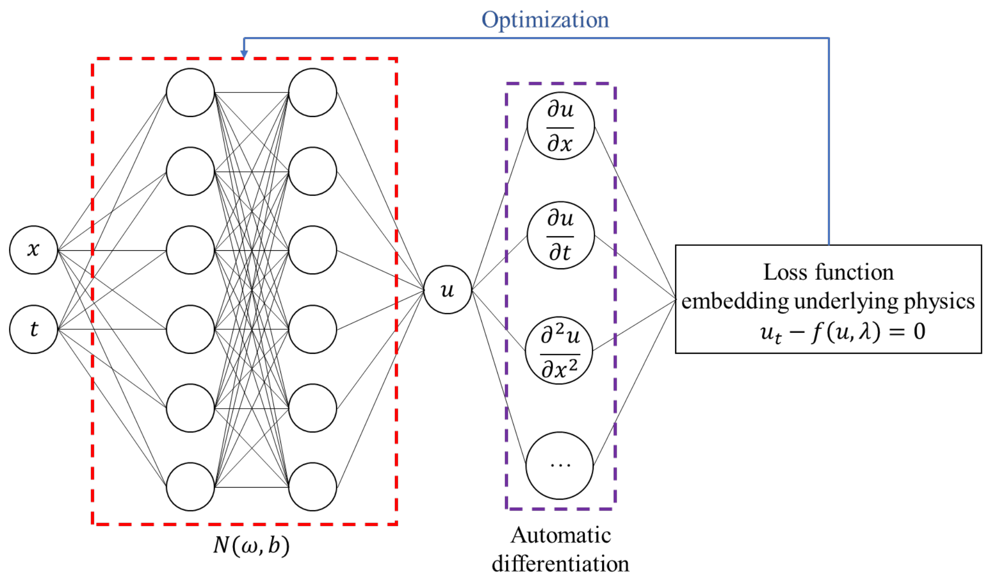

Figure 2. Configuration of PINN *[50]*

The idea of PINN applies to solving challenging differential equations and can be used to develop physics-consistent data-driven models. When the underlying physics of degradation is known, this approach can be used to ensure that the model adheres to the known physics in its estimations. Considering that, PINN was later used in a very limited number of studies to develop NN models for degradation prediction. Zhang et al. [54] used the idea for creep-fatigue lifetime prediction at high temperatures. However, the added physics was just a simple restriction on the estimated lifetimes. They added a penalty term to the network cost function to force the lifetime estimations to be in a specific range (between 0 and 10^5 cycles). Zhou et al. [55] added some simple fundamental rules from fatigue degradation as the underlying physics to an NN model to improve fatigue life predictions. Similarly, Kim et al. [56] considered a few basic understandings, such as the irreversibility of degradation, to guide a NN. Finally, Cofre-Martel et al. [57] used the PINN idea to explain the physics of failure based on latent features.

The major obstacle to using PINN for lifetime estimation purposes is the lack of sufficient knowledge about the underlying physics of degradation. This knowledge is often unavailable for the complex phenomena of degradation in real-world conditions, where multiple stresses act together, affecting the rate and intensity of degradation synergically at different levels. That is why the previous studies mainly considered just some basic understandings of physics to guide NNs. Therefore, for lifetime prediction under degradation, there is a need for a framework to discover the complex underlying physics of degradation and then use the discovered physics to improve the degradation predictions.

2.3. Research Gap

NN models have been widely used for prognostic applications. However, purely data-driven models may overlook physical rules, potentially compromising their generalization and reliability. As discussed before, adding physics to data-driven models and forcing them to follow physical rules can address data scarcity and un-interpretability issues. However, in the research domain of prognostics, only a few studies have tried to make models physics-informed by embedding physical rules in the algorithms. The primary impediment has been the lack of sufficient understanding of the underlying physics of complex systems. That is why previous research studies have mainly relied on some basic understandings of physics or empirically derived equations obtained through experiments to integrate physics into the models.

Although such relatively simple physical equations guide and improve purely data-driven methods to some extent, it cannot be asserted that the resulting models possess enough awareness of the underlying physics. Even empirically derived relationships, which are more sophisticated, have primarily been developed after many simplifications and within highly controlled laboratory environments that do not fully mirror real-world conditions. Consequently, a promising research opportunity lies in merging data-driven models with the complex underlying physics that governs the degradation process in real operating conditions. This underlying physics can be revealed by analyzing patterns in the data associated with the degradation mechanism. To the best of our knowledge, there have been minimal research efforts to integrate a physics discovery model with a physics-informed predictive model for prognostic purposes. In this context, physics pertains to the correlation between degradation rate, which is the first derivative of degradation intensity with respect to time, and various environmental factors. The integration of these two models offers a high level of interpretability. This interpretability is not only in the sense that the predictive model adheres to the complex physics of degradation but also in how it determines the dominant environmental factors influencing the degradation process. These factors should be measured from the field to accurately estimate system degradation under environmentally induced conditions. Additionally, understanding the degradation mechanism can guide designing accelerated life/aging tests within laboratory settings by identifying crucial stress agents that significantly impact degradation.

Chapter 3: Predicting System Degradation with Guided Neural Network

This chapter addresses two major challenges in DL prognostic models: disregarding physics and the need for substantial data for sufficient training. To tackle these issues, a dual NN framework enables physics-informed prediction of long-term degradation intensity using limited data obtained from short-term tests. This chapter is a reproduction of a previously published paper[1].

3.1. Introduction

Evaluating the physical degradation behavior and estimating the lifetime of engineering systems and structures is crucial to ensure their safe and reliable operation. This chapter develops a physics-informed NN-based framework for time-efficient modeling of field degradation using sensor measurements from short-term actual operating conditions degradation tests. The framework comprises two NNs: a physics discovery NN and a predictive NN. The former models the underlying physics of degradation, while the latter makes probabilistic predictions for degradation intensity. The physics discovery NN guides the predictive NN for better life estimations. The proposed framework addresses two main challenges associated with applying NN for degradation estimation: incorporating the underlying physics of degradation and requirements for extensive training data. The effectiveness of the proposed approach is demonstrated through a case study of atmospheric corrosion of steel test samples in a marine

[1] Hamidreza Habibollahi Najaf Abadi and Mohammad Modarres, "Predicting system degradation with a guided neural network approach," Sensors, vol. 23, no. 14, p. 6346, 2023.

environment. Employing the proposed data-driven framework for degradation prediction, systems safety, and reliability can be evaluated efficiently, and maintenance activities can be optimized.

3.2. Approach

The proposed approach in this study leverages the high capacity of NNs to effectively model complex patterns and relationships within the data. By harnessing the power of NNs, the methodology aims to discover and incorporate complex underlying physics of degradation phenomena. The idea is that degradation mechanisms often involve intricate processes deeply embedded within the data. So, NNs provide an avenue to learn about such mechanisms from the data, potentially revealing hidden patterns and fundamental relationships that underlie degradation processes.

What happens in a single hidden layer of an NN is similar to linear regression (LR). However, an activation function $\sigma(.)$ is usually applied on top of the linear transformation to introduce nonlinearity and make the network capable of learning nonlinear patterns in the data. A layer is normally presented mathematically in the form of Equation 3-1.

$$\boldsymbol{h}_i = \sigma(\boldsymbol{W}_i^T \boldsymbol{h}_{i-1} + \boldsymbol{b}_i) \qquad 3\text{-}1$$

where, $\boldsymbol{h}_i$ is the output of hidden layer i, which is obtained after using the activation function σ on the linear transformation of the output of the previous layer (hidden layer i-1). So, $\boldsymbol{W}_i$ and $\boldsymbol{b}_i$, which are the matrix of weights and the vector of biases of the layer, are trainable parameters learned during the network training procedure. For each layer, the bias vector's size equals the number of neurons in the layer. At the same time, the dimensions of the weight matrix depend on the number of neurons in the layer and the layer before, which provided the input for the current layer. In a NN, each layer's output is the next layer's input. Therefore, for an NN with two layers, the final output $\hat{y}$ (e.g., estimation or prediction) can be written as Equation 3-2, where $\boldsymbol{X}$ is the vector of input features of the network.

$$\hat{y} = \sigma(\boldsymbol{W}_2^T(\sigma(\boldsymbol{W}_1^T\boldsymbol{X} + \boldsymbol{b}_1)) + b_2) \qquad 3\text{-}2$$

In a supervised learning setting, the data is labeled, meaning that for each set of input (independent variables), the output (dependent variable) is known. Considering that the loss function is defined as the difference between the estimated output $\hat{y}$ by the network with the actual value (label) y, usually measured in the form of mean square error (i.e., squared L2 norm) (Equation 3-3).

$$Loss_{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2 \qquad 3\text{-}3$$

Figure 3 provides the overview of the training process of the proposed framework for predicting degradation intensity. The framework contains two NNs: 1) physics discovery NN ($N_{\omega,\theta}$) and 2) predictive NN ($M_{\psi,\eta}$). Unlike the traditional PINN, which relies on empirical models for physics, in this approach, the physics discovery NN is responsible for modeling the underlying physics of degradation. Operating conditions impact the degradation rate either linearly or non-linearly, and this linear/non-linear relationship can be captured as a regression model by the physics discovery NN. This network is a feedforward NN with mean squared error (MSE) loss function that maps the operating conditions (x_1, x_2, …, x_n) to the degradation rate ($\frac{\partial D}{\partial t}$). Equation 3-4 shows the MSE function, where N is the number of data points, $\frac{\partial D}{\partial t}$ is the true value of the degradation rate, and $\frac{\widehat{\partial D}}{\partial t}$ is the estimated degradation rate which depends on input features $\boldsymbol{x}$, network weights $\boldsymbol{\omega}$, and bias parameters $\boldsymbol{\theta}$.

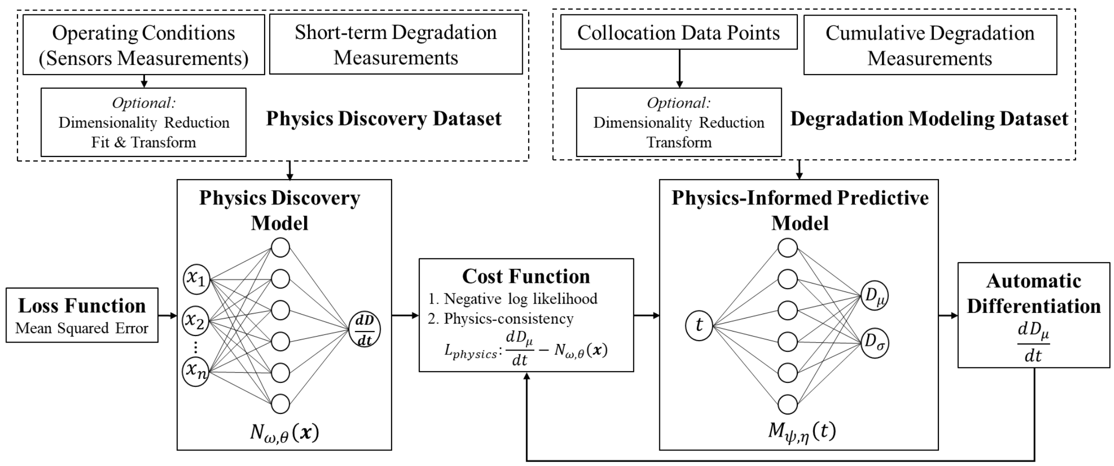

Figure 3. Training of the proposed framework

$$MSE = \frac{1}{N}\sum_{i=1}^{N}\left[\left(\frac{\partial D}{\partial t}\right)_i - \left(\frac{\widehat{\partial D}}{\partial t}(\boldsymbol{x}, \boldsymbol{\omega}, \boldsymbol{\theta})\right)_i\right]^2 \qquad 3\text{-}4$$

Sensor measurements and degradation rates from short-term tests in different operating conditions are used to train the physics discovery NN. The primary goal of the physics discovery model is to capture the impact of operating conditions on the degradation rate rather than temporal patterns in degradation intensity. In this approach, it is assumed that the physics of degradation can be modeled based on the degradation rate (first-order gradient of degradation intensity with respect to time). However, if the degradation behavior undergoes significant changes over time [58], it is important to consider the degradation acceleration (second-order gradient of degradation intensity with respect to time) or higher-order gradients in modeling the underlying physics. This case can be a part of the future extensions of the current study.

The model's ability to discover physics is reflected in its goodness of fit, indicating how effectively it captures the relationship between the variables. Additionally, the model's capacity to discover can be further evidenced by the subsequent enhancements to the predictive model's estimations achieved by incorporating the underlying mechanism.

The predictive NN estimates the degradation intensity probabilistically. The uncertainty in the estimated degradation intensity can be presented by different parametric distributions. Assuming a normal distribution with the mean of D_μ and standard deviation of D_σ, the outer layer of the predictive NN has two neurons for D_μ and D_σ. Since D_σ must be a positive value, the Softplus activation function, which ensures positive output, is used for the corresponding neuron in the outer layer. Softplus is a smooth and non-linear activation function, defined as the logarithm of the exponential function applied to the input [59]. For the other neurons, different activation functions can be used based on the ultimate performance of the model. Hyperbolic Tangent (Tanh) and Rectified Linear Unit (ReLU) are the most common activation functions for regression problems. However, some extensions of ReLU, most commonly Leaky ReLU, were also used before.

Tanh may suffer from the vanishing gradient problem, which can impact training NNs. On the other hand, ReLU avoids the vanishing gradient and is also computationally efficient. However, ReLU can cause, in some instances, some neurons to become permanently inactive. That is why the ReLU extensions were considered before. Leaky ReLU solves the inactive neuron issue, but its hyperparameter needs to be manually set, which requires additional hyperparameter tuning [59].

Equation 3-5 shows the cost function of the predictive NN, which has two terms: 1) L_{data} for fitting the data and 2) $L_{physics}$ for following the underlying physics learned by the physics discovery NN. The model is trained using the labeled data and L_{data} represents the error between the estimates (i.e., the network's output) and the observed (true) values. $L_{physics}$ is a constraint in the optimization process of the network cost function and the scalar parameter λ weights the constraint. The proposed approach aims to achieve consistency of the predictions with the underlying physics, which is discovered by the first NN, by minimizing $L_{physics}$. The output of the predictive NN is a parametric distribution, which is why the negative log-likelihood of the actual values of degradation intensity is used as the loss term for fitting the data. In Equation 3-5, t is time, $\boldsymbol{\psi}$ represents the vector of weights, and $\boldsymbol{\eta}$ is the vector of bias parameters of the network. The automatic differentiation technique [60] is used to calculate $\frac{\partial \widehat{D_\mu}}{\partial t}$ term in $L_{physics}$.

$$Cost = L_{data} + \lambda \times L_{physics} \qquad 3\text{-}5$$

$$L_{data} = \frac{1}{2}\left[\frac{D - \widehat{D_\mu}(t, \boldsymbol{\psi}, \boldsymbol{\eta})}{\widehat{D_\sigma}(t, \boldsymbol{\psi}, \boldsymbol{\eta})}\right]^2 + \frac{1}{2} log\,[\sqrt{2\pi} \times \widehat{D_\sigma}(t, \boldsymbol{\psi}, \boldsymbol{\eta})]^2$$

$$L_{physics} = \frac{\partial \widehat{D_\mu}(t)}{\partial t} - N_{\omega,\theta}(\boldsymbol{x})$$

The physics discovery model guides the predictive model to learn the parameters so that they follow physics besides fitting the data. After training, only time is needed as the input for predicting field degradation intensity, as no sensor measurements are available regarding future operating conditions. It means the sensor measurements from short-term tests are used indirectly to help the predictive NN to find the right parameters for linking degradation intensity to time. So, for the prediction of degradation intensity in the future, the only available feature is use/exposure time, which is required as input.

The proposed approach uses two different datasets to train the two NNs. The first dataset, used to train the physics discovery model, has sensor measurements as input features and degradation rates as labels. However, further feature selection/extraction and data preprocessing methods can be used as required. This dataset can be obtained from short-term tests in various operating conditions. For example, samples of materials from a considered system/structure can be exposed to different environmental factors, such as temperature and humidity, within the range of its actual operating conditions in the field, and the degradation rate for each condition be measured. Using sensors, the environmental factors associated with degradation rates can be measured. The degradation rate can be quantified differently depending on the considered degradation mechanisms. For example, the degradation rate can be expressed as the resulting mass loss rate for the corrosion mechanism.

Duration and specifications of the tests vary case by case and depend on the nature of the systems and the associated failure mechanism. However, it is crucial to include critical variabilities and initial conditions that affect degradation, such as variations in geometry and environmental conditions, in the training dataset, to ensure that the physics discovery model represents and closely mimics the degradation process. To include variability in initial damages in the developed model, samples with different levels of initial degradation can be used in the short-term tests. It is worth noting that these tests are performed under operational conditions rather than accelerated conditions. The primary advantage of conducting short-term tests is the emphasis on obtaining degradation rate labels, which can be promptly collected, as opposed to measuring degradation intensity, which is time-consuming for long-term degradations. The second dataset, which includes the exposure times as input features and associated degradation intensities as labels, is used for training and testing the predictive model. Similar to the first dataset, degradation intensity can be measured differently by considering the degradation mechanism. Two examples include mass loss due to corrosion and crack growth because of fatigue.

3.3. Case Study

The proposed framework is designed to predict the degradation in systems and structures when there is limited knowledge about the complex underlying physics of degradation and the impact of various operating conditions on lifetime. This case study applies the proposed framework to the steel structure of a subsystem within an aircraft, working in marine environments and subject to degradation due to corrosion. However, because of the unavailability of datasets associated with the degradation of such a steel structure, degradation in coupons made from steel is considered for the case study.

Different parts of aircraft under high mechanical stresses during operation, such as landing gears, are made of steel.

In this case study, we use data from the degradation of C1010 steel coupons from a previous study [61]. The C1010 is a low-carbon steel alloy known for its high weldability, ductility, and tensile strength. The coupons used in this study were exposed to atmospheric corrosion in a marine environment at the U.S. Naval Research Laboratory Key West, a testing facility situated on Fleming Key in Florida, within the U.S. Naval Air Station. The exposures were conducted between 28 August 2014 and 28 August 2015. The coupons were $3'' \times 3'' \times 1/6''$ in dimension and were affixed with two 3/16" diameter mounting holes facing south to ensure consistent mounting. Coupons had a glass bead blasted surface. On-site environmental data were collected from a weather station. Two datasets were gathered, one for short-term and another for long-term exposure. The link to the datasets can be found in [62]. Some specific information, such as the test standards used to prepare the coupons and the test conditions and details of the instrumentation used for measurements, are unknown. However, these details do not impact the results of the case study.

In this study, it is assumed that coupons represent simplified forms of a structure and degradation intensity is defined as the mass loss of the coupons resulting from corrosion over time. Mass loss was calculated as the difference between the initial mass of a coupon and its final mass after removing the corroded mass. Thus, the initial and final mass was recorded before exposure and at the designated checkpoints for each coupon.

The first dataset contains operating conditions and degradation measurements for 72 coupons with no initial damage in the field between 24 to 36 days. The operating conditions, including temperature, humidity, and solar radiation, were collected every 30 minutes, as shown in Figure 4, and the mass losses were recorded before removing the coupons (i.e., 72 data points). Figure 5 shows the distribution of the calculated degradation rates using this dataset. The second dataset is similar to the first dataset, except that the coupons were kept in the field for one year and the mass loss measurements were collected cumulatively at the end of each month, as shown in Figure 6.

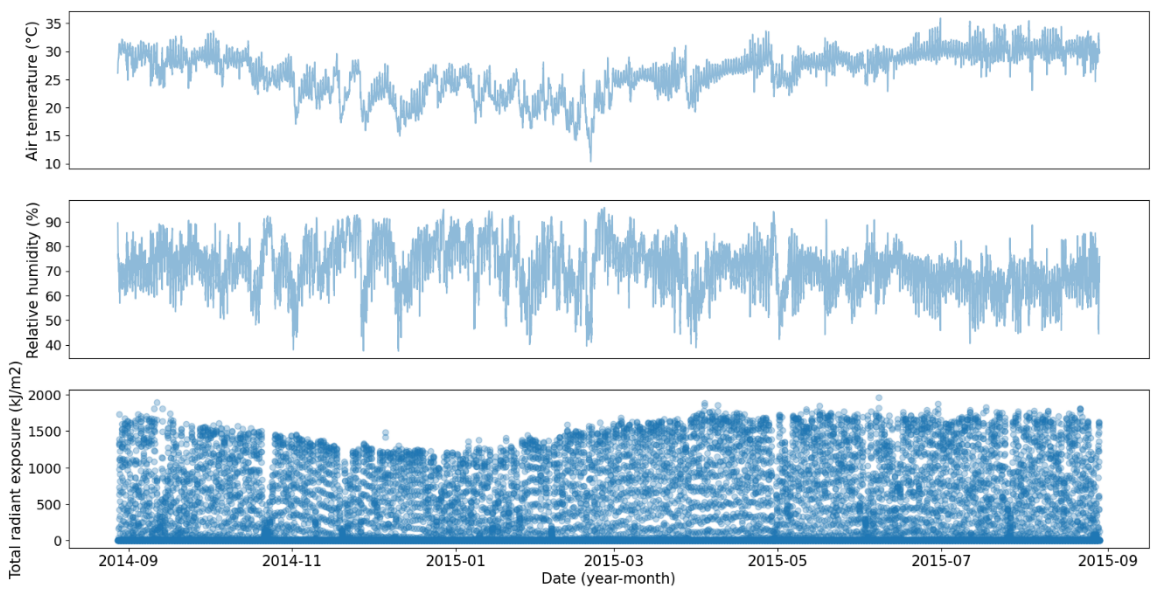

Figure 4. Measured operating conditions

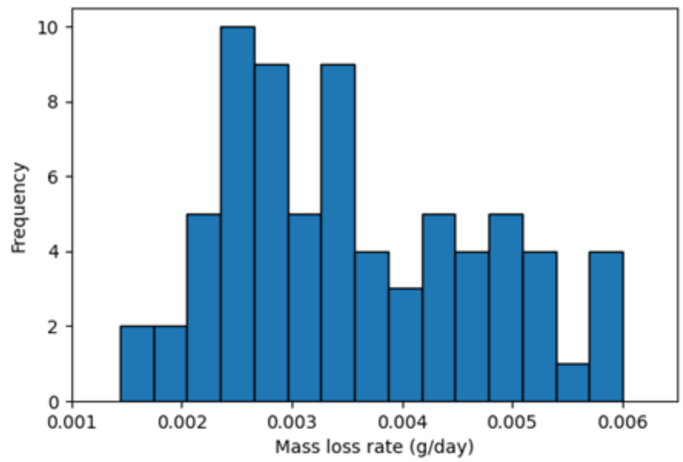

Figure 5. Distribution of mass loss rate (i.e., degradation rate) obtained from monthly removed coupons

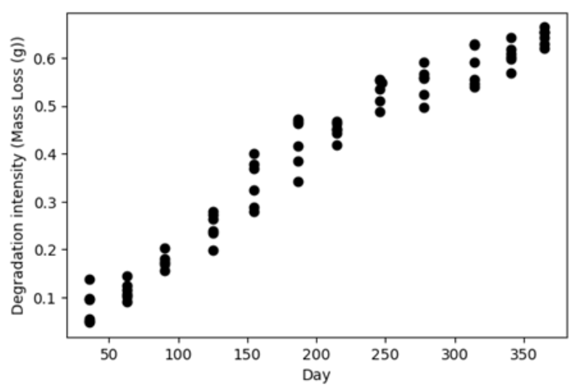

Figure 6. Mass loss (i.e., degradation intensity) of coupons

The first dataset (i.e., short-term degradation data) is used to model the underlying physics by the physics discovery NN. The second dataset (i.e., cumulative degradation data for a whole year) trains and tests the physics-guided predictive NN. Different initial observations of cumulative degradations in the second dataset are used to train the predictive model, while the remaining observations are used to test the predictive model's performance.

Twelve features, including means and standard deviations of air temperature ($°C$), relative humidity (%), and total radiant exposure (KJ/m^2) as well as their gradients with respect to time over the month before each mass loss measurement are used as inputs for the framework. Because of the high dimensionality of the feature space and considering the size of the dataset, a dimension reduction technique is used to extract influential features in a lower dimensional space. There are different methods for data dimension reduction, such as principal components analysis (PCA) [63], t-distributed Stochastic Neighborhood Embedding [64], and autoencoders [65] that can be used. However, to avoid complications of data preprocessing, which is not in the scope of this study, the straightforward linear PCA is considered. Using the PCA as an effective method for reducing the number of input features, the twelve environmental features were reduced into only two to avoid the need for a large network with many parameters. The two extracted features are linear combinations of the twelve original features, representing a significant fraction of the variance. The first two principal components, with a total variance ratio of around 0.8, retain most of the relevant information. It is worth mentioning that the first three principal components reflect a total variance ratio of above 0.9. However, using the three principal components did not improve the model performance, so the first two principal components were considered in the analysis.

An NN with a hidden layer containing four neurons is trained to model the degradation rate (i.e., mass loss rate) based on the first two principal components. The optimal size for the NN is selected based on the size of the dataset and by trial and error [66]. For larger datasets, deeper NNs can be used [67]. The Tanh activation function is used in the NN as it showed desirable model performance in this case study. The goodness of fit is assessed using the mean absolute error (MAE) and the mean absolute percentage error (MAPE) of the estimates. The model produces an MAE of 0.0004 and a MAPE of 0.13, indicating a relatively good fit. The inaccuracies in the estimates may be due to the complexity of the corrosion degradation phenomenon, which depends on many conditions beyond the three conditions considered here. Therefore, it may not be possible to estimate the corrosion rate solely based on these factors accurately. Nevertheless, the model still partially learns the underlying physics relationships between the inputs and the output of the NN. This acquired knowledge can be valuable in guiding the development of a more accurate predictive model in the next step.

To guide the predictive model to achieve physics-consistent estimates and limit the search space for its parameters, the physics discovery model is incorporated into the training process of the predictive model. Figure 7 compares the degradation predictions made by the guided neural network (GNN) with those made by a regular NN for different portions of training data. The dashed lines represent the distance of $2 \times D_{\sigma}$ (the standard deviation of degradation intensity) above and below D_{μ} (the mean degradation intensity), which corresponds to a 95% confidence interval for the estimates. Both networks have the same structure: a one-dimensional input layer (representing time), one hidden layer of six neurons with Tanh activation functions, and two neurons at the output layer for the parameters of the probability density function of the degradation intensity (D_{μ} and D_{σ}) with linear and Softplus activation functions. The only difference between the two NNs is in their cost functions, where the GNN's cost function includes a term that accounts for the physics of degradation ($L_{physics}$ in Equation 2). A weight of 10^5 is considered for the physics term ($\lambda = 10^5$).

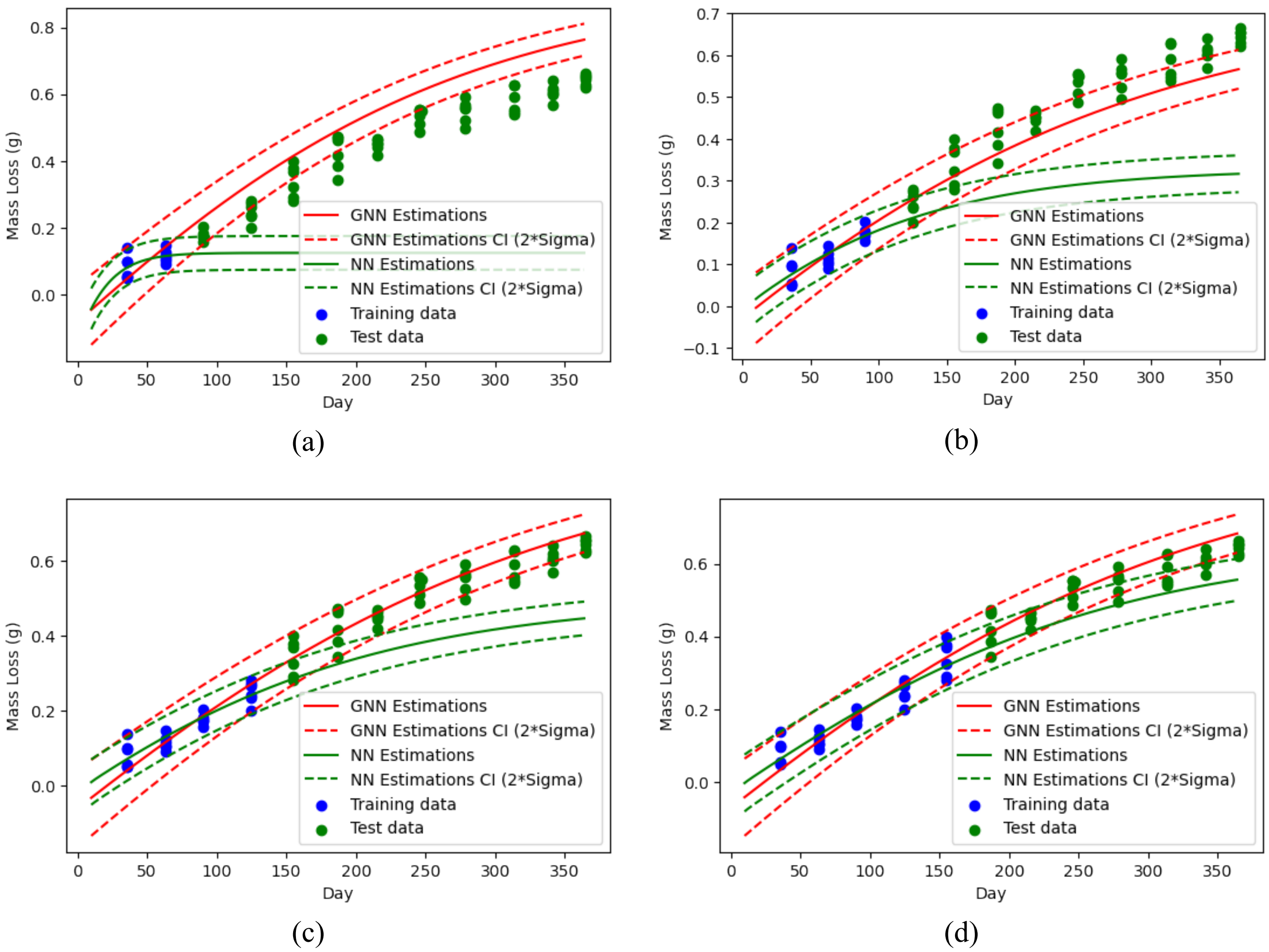

Figure 7. Comparing estimations of GNN with regular NN for different portions of training data: (a) 2 months; (b) 3 months; (c) 4 months; (d) 5 months

The only input for both GNN and regular NN is time. However, the GNN is trained so that the estimated degradation intensities conform to the discovered physics (i.e., $N_{\omega,\theta}$) during the training. For this purpose, 200 random data points (collocation points) are generated from uniform distributions within the sensor measurements range in the first dataset. These data points are then fed into the network to adjust the network parameters by forcing the model to make the automatic differentiation of the mean of the estimated distribution for degradation intensity (i.e., $\frac{\partial \widehat{D_\mu}}{\partial t}$) close to the expected value determined by the physics discovery model (i.e., $\frac{\widehat{\partial D}}{\partial t}$) for each of the collocation data points. This is achieved by minimizing the penalty term for the physics in the cost function (i.e., $L_{physics}$).

Comparing the predictions of the two NNs for the test data (i.e., the green data points in Figure 7) reveals that guiding the NN significantly improves its performance. In the case with limited training data (Figure 7a and b), the regular NN overfits the training data points and fails to learn the underlying pattern. However, the GNN provides relatively acceptable estimates for long-term degradations.

Increasing the initial observation time (i.e., the portion of training data shown by blue dots in Figure 7) results in more accurate estimations. Observing the initial degradation intensities for the first four months, the predictions of the GNN are excellent, while the regular NN shows significant errors and requires at least 5 months of training data to generate close estimations of the actual values, as demonstrated in Figure 7c and Figure 7d, respectively.

To further evaluate the performance of the proposed method, its prediction accuracy is compared to other machine learning (ML) techniques, including support vector regression (SVR), LR, and polynomial regression (PR) (See Table 1). Non-linear models of PR and SVR with polynomial kernel function show the worst performances, as shown in Figure 8. Although they represent a good fit for the training data, their estimates for the test data points are considerably inaccurate.

Table 1. Considered models for comparison with the GNN.

#	Model	Specifications
1	SVR	Linear kernel, C=0.1, ε=0.05
2	SVR	Polynomial kernel, degree 2, C=0.1, ε=0.05
3	LR	Least squares method
4	PR	Degree 2, Least squares method

Linear models, including LR and SVR with linear kernel, perform better than the non-linear models. However, they cannot consistently predict the degradation intensities with accuracy. This is because the degradation phenomena have a highly non-linear nature, which makes the linear models perform well only on certain parts of the period (e.g., the middle portion in Figure 8d). In addition, when the training data is limited, their estimates differ significantly from the actual values, as shown in Figure 8a.

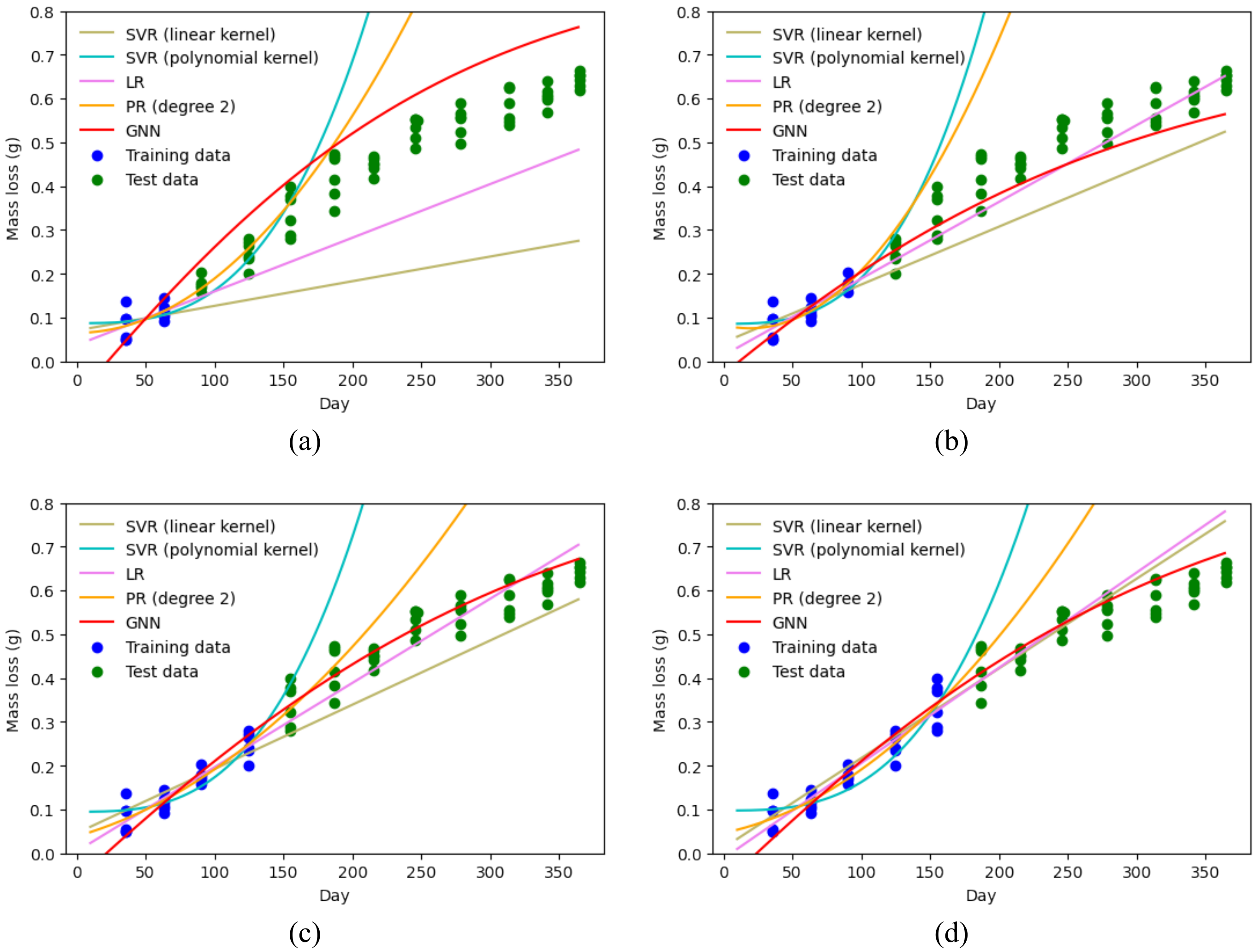

Figure 8. Comparing degradation prediction by different machine learning models for different portions of training data: (a) 2 months; (b) 3 months; (c) 4 months; (d) 5 months

Table 2 presents the goodness of fit to the test data for the considered models with different observation times (i.e., training data), allowing for a comparison of their performance in predicting the degradation intensity. Four evaluation metrics are used: MAE, maximum error (ME), MAPE, and R^2, which are calculated using Equations 3-6 to 3-9, where D is actual degradation intensity, $\widehat{D}$ is estimated degradation intensity,

N is the number of data points, $\overline{D}$ is the mean of the actual values of degradation intensity, and ν is a small positive number to avoid undefined function when D is zero.

Table 2. Metrics for quantifying the quality of degradation predictions (test data)

Training data	Model	MAE	ME	MAPE	R^2 score
2 months	SVR (linear)	0.257	0.387	0.535	-2.450
	SVR (poly)	0.995	3.100	1.725	-93.357
	LR	0.135	0.215	0.285	0.030
	PR	0.383	1.094	0.681	-11.801
	Regular NN	0.335	0.539	0.683	-5.042
	GNN	**0.095**	**0.170**	**0.227**	**0.520**
3 months	SVR (linear)	0.115	0.185	0.236	0.05
	SVR (poly)	1.667	4.553	2.902	-315.067
	LR	**0.047**	0.130	**0.102**	**0.776**
	PR	0.767	1.871	1.372	-58.94
	Regular NN	0.206	0.347	0.394	-2.157
	GNN	0.059	**0.109**	0.119	0.723
4 months	SVR (linear)	`0.084	0.152	0.166	0.163
	SVR (poly)	1.303	3.287	2.242	-284.497
	LR	0.048	0.108	0.095	0.697
	PR	0.238	0.589	0.417	-8.231
	Regular NN	0.134	0.217	0.249	-1.042
	GNN	**0.032**	**0.075**	**0.068**	**0.849**
5 months	SVR (linear)	0.060	0.142	0.107	0.136
	SVR (poly)	1.149	2.626	1.958	-324.905
	LR	0.069	0.162	0.123	-0.166
	PR	0.335	0.726	0.578	-25.327
	Regular NN	0.064	0.108	0.116	0.199
	GNN	**0.036**	**0.088**	**0.068**	**0.704**

$$MAE(D,\widehat{D}) = \frac{1}{N}\sum_{i=1}^{N}\left|D_i - \widehat{D}_i\right| \qquad 3\text{-}6$$

$$ME(D,\widehat{D}) = max\ (\left|D_i - \widehat{D}_i\right|) \qquad 3\text{-}7$$

$$MAPE(D,\widehat{D}) = \frac{1}{N}\sum_{i=1}^{N}\frac{|D_i - \widehat{D}_i|}{max\ (\nu, |D_i|)} \qquad 3\text{-}8$$

$$R^2(D,\widehat{D}) = 1 - \frac{\sum_{i=1}^{N}(D_i - \widehat{D}_i)^2}{\sum_{i=1}^{N}(D_i - \overline{D}_i)^2} \qquad 3\text{-}9$$

Among the considered models, GNN exhibits the best performance, although for one of the cases (3 months of observation) LR shows a slightly better fit based on three of the parameters (MAE, MAPE, and R^2). However, the ME of the GNN is still lower than the LR model, which means even for this specific case LR estimations are worse than GNN for some parts of the period. It should be noted that LR is a linear model and not suitable for modeling physical degradation progress due to its disability to capture non-linearity. The good performance of LR observed for some cases (e.g., 3 months and 4 months of observation cases in Table 2) is likely due to the low level of non-linearity of the cases considered for the specific period (1 year). However, collecting degradation data over a longer time (more than a year) would likely result in a higher non-linearity and can underline the weakness of LR more clearly. On the other hand, GNN's ability to learn non-linear patterns in the data is evident from Figure 8.

The models considered in this study exhibit good fits to the training data for all cases, except for the 2-month observation data, as shown in Table 3. This indicates the potential for overfitting for the models with low performance on the test data. GNN exhibits the worst fit for the training data yet performs the best on the test data. This suggests that the GNN model does not overfit the training data. In contrast, the other models exhibit lower performance on the test data than on the training data, indicating overfitting.

Table 3. Metrics for quantifying the quality of fitting degradation data (training data)

Training data	Model	MAE	ME	MAPE	R^2 score
2 months	SVR (linear)	**0.022**	**0.047**	0.291	0.200
	SVR (poly)	**0.022**	**0.047**	0.291	0.200
	LR	**0.022**	0.057	0.270	**0.283**
	PR	**0.022**	0.057	0.270	**0.283**
	Regular NN	**0.022**	0.057	**0.269**	**0.283**
	GNN	0.0307	0.089	0.289	-0.655
3 months	SVR (linear)	0.022	**0.047**	0.252	0.657
	SVR (poly)	0.020	**0.047**	0.233	0.681
	LR	0.020	0.061	0.213	0.705
	PR	**0.018**	0.057	0.210	**0.729**
	Regular NN	0.020	0.062	0.220	0.688
	GNN	0.021	0.076	**0.195**	0.632
4 months	SVR (linear)	0.025	**0.050**	0.244	0.808
	SVR (poly)	0.023	**0.050**	0.221	0.831
	LR	0.021	0.064	**0.181**	0.864
	PR	**0.020**	0.059	0.183	**0.871**
	Regular NN	0.021	0.067	0.185	0.853
	GNN	0.024	0.098	0.191	0.757
5 months	SVR (linear)	0.029	0.070	0.219	0.875
	SVR (poly)	0.030	**0.061**	0.219	0.871
	LR	**0.025**	0.074	**0.166**	0.893
	PR	**0.025**	**0.061**	0.172	**0.907**
	Regular NN	0.027	0.081	0.172	0.881
	GNN	0.029	0.103	0.195	0.849

Finally, although in this case study the performance of the GNN on test and training data is evaluated to demonstrate the proposed approach's capability for predicting degradation intensity, there are other approaches, such as the formal methods described in [68, 69] that can be employed to validate the model. Considering these approaches can benefit the future extensions of this study.

3.4. Conclusions

NN models used for degradation prediction are purely data-driven approaches and may not accurately predict degradation when insufficient data exists. Furthermore, they do not consider the underlying physics of degradation. This chapter proposes a GNN framework for incorporating complex physics to facilitate physics-consistent prediction of field degradation with limited data. The proposed method is a dual NN framework consisting of two NNs for discovering the underlying physics and predicting degradation intensity. The physics discovery NN relies on environmental factors such as temperature and humidity affecting the degradation rate. Therefore, the underlying physics can be discovered by modeling the degradation rate based on the data obtained from short-term tests and be added as a penalty term to the cost function of the predictive NN for estimating degradation intensity. The predictive model can be trained with limited data by respecting the discovered physics as a constraint that limits the search space for the model parameters. Further, fitting the data and following the physics simultaneously makes the model generalize well for unseen field data.

The performance of the proposed framework is evaluated through a case study of the atmospheric corrosion of steel coupons as simplified forms of a structure. The results indicate the potential of the proposed GNN for predicting long-term degradations based on limited observations of the initial degradation intensities. At the same time, other ML models may overfit the data. The proposed approach enables the efficient evaluation of the lifetime of systems and structures, thereby ensuring their safety and reliability as well as minimizing their maintenance costs. Accurate lifetime estimation allows for appropriate risk management measures to prevent accidents and ensure reliable functionality. Additionally, optimized predictive maintenance can be implemented to avoid unnecessary repairs and unexpected downtimes.

Finally, it is important to acknowledge the limitations of the proposed framework. Firstly, the framework requires degradation data for training purposes, albeit less data than a regular NN. However, collecting such data can be time-consuming and expensive as degradation is often a slow process. Also, the framework primarily focuses on degradation. However, potential failures may occur in the field due to discrete over-stress conditions rather than gradual and temporal degradation. Lastly, systems may involve high variations and uncertainties in their degradation behaviors in real-world situations, depending on their operating conditions. These variations may exist even in identical systems. This approach has not considered these variations and the resulting uncertainties in the degradation predictions. Such assessments can be viewed as future extensions of this work.

Chapter 4: Discovering the Underlying Physics of Degradation

The configuration of the proposed dual NN framework can be adapted based on the objectives and available data characteristics. Considering that two distinct scenarios can be explored:

- Scenario 1: The main objective is to add physics to predictions to improve the accuracy and generalization of the model and enable sufficient training with limited data.

- Scenario 2: The main objective is to discover the underlying physics of degradation and identify dominant environmental factors with significant effects on degradation.

The first scenario considers the two issues of disregarding physics and data requirements, while the second scenario is related to providing interpretability in DL prognostics models.

The first scenario was explored in Chapter 3 where degradation rate labels were collected from short-term tests and then were used for the separate training of a physics discovery NN. This NN model was later used to guide predictions of a predictive NN. It is worth mentioning although the physics discovery NN guides the predictive NN for more accurate estimations, it does not provide any information regarding the dominant environmental factors and their effect on the progress of degradation (because of lack of interpretability). This issue is considered in the current chapter. So, this chapter focuses on the second scenario and adapts the framework for discovering the underlying physics of degradation and identifying dominant environmental factors by integrating the dual NN framework with a feature importance measurement method. This chapter is a reproduction of a previously published paper[2].

4.1. Introduction

Although DL models have shown promising performances on RUL estimation, their black-box nature hinders understanding the effects of inter- and intra-environmental factors and their interactions on the degradation process (i.e., physics of degradation). Understanding these effects, specifically for complex systems where many factors may act synergically, is essential during the design and operation stages.

This chapter proposes a DL-based approach to discover the complex interacting phenomena that underlie the physics of degradation from the observed field data and shows how the discovered physics can be added to data-driven prognostics models for better estimations. The proposed approach consists of two NNs: the predictive and physics discovery networks. These NNs are trained simultaneously in a supervised setting using a customized cost function. The former network models the intensity of the complex interactive degradation phenomena, while the latter discovers the underlying physics from the observed reliability tests and environmental field data. The discovered physics is a nonlinear relationship between many environmental factors that affect the degradation rate. This relationship can be further simplified using a recursive

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[2] Hamidreza Habibollahi Najaf Abadi and Mohammad Modarres, "A deep learning approach for discovering the underlying physics of degradation for data-driven prognostics," in 70th Annual Reliability and Maintainability Symposium, Albuquerque, New Mexico, USA, 2024.

feature elimination strategy. This way, the dominant environmental factors are identified. Finally, the application of the proposed approach is shown through a case study.

4.2. Approach

The proposed approach assumes the physics of degradation can be represented by the relationship between degradation rate (i.e., the first-order gradient of degradation with respect to time) and effective environmental factors. The basis for this assumption is that the applied stresses to a system affect its degradation rate rather than degradation intensity. For instance, environmental factors such as temperature and relative humidity directly impact the pit growth rate in pitting corrosion. Therefore, determining the dimensions of the pits solely based on instantaneous environmental factors is not feasible. Based on this assumption, discovering the underlying physics of degradation involves determining a function that links the degradation rate to influential environmental factors. Considering that system RUL represents degradation intensity in systems, Equation 4-1 shows the relationship for the underlying physics of degradation, where S_n is the environmental factor measurement collected by the sensor n, and f is the function that links the degradation rate to sensor measurements.

$$\frac{\partial RUL}{\partial t} = f(S_1, S_2, \dots, S_n) \quad \text{4-1}$$

Figure 9 illustrates the proposed approach for discovering the underlying physics of degradation. This approach has two main parts: (1) a dual NN framework that models the underlying physics of degradation and (2) a feature importance measurement method that evaluates and ranks environmental factors according to their significance in influencing the degradation process. In addition to identifying the impactful factors, a recursive feature elimination is employed to remove the factors with negligible effects on the degradation. The rest of this section describes the two main parts of the proposed approach in more detail.

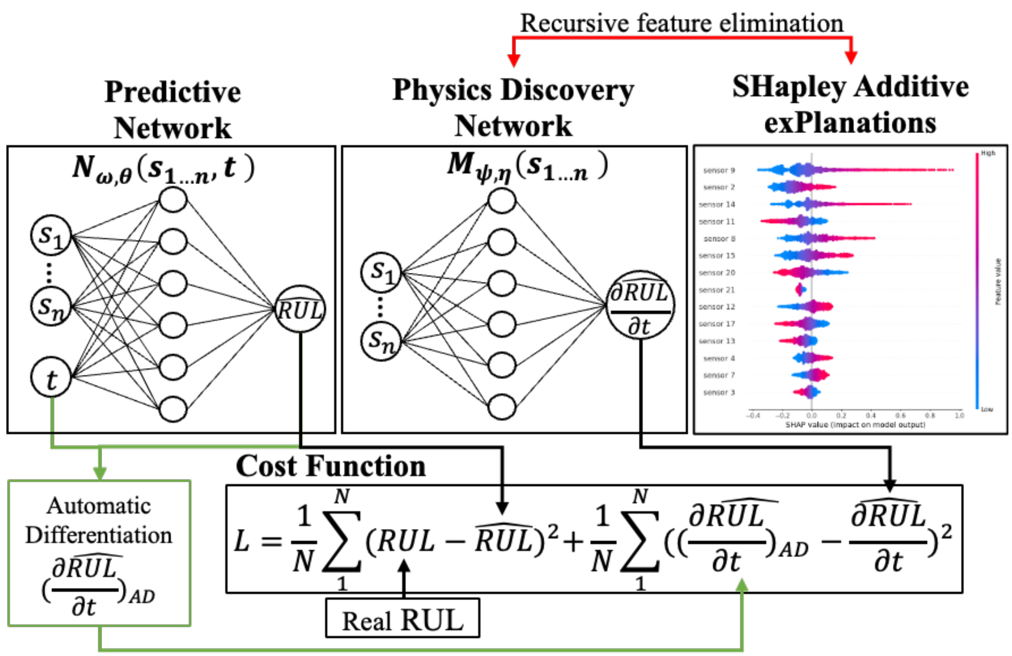


Figure 9. Proposed approach for discovering the underlying physics of degradation

4.2.1. Dual neural network framework

The dual NN framework consists of two interconnected NNs working together to discover the physics of degradation based on the environmental factors measured by sensors: (1) predictive network $N_{\omega,\theta}$ and (2) physics discovery network $M_{\psi,\eta}$. The predictive network maps time and sensor measurements to RUL, making it possible to calculate the first-order gradient of RUL with respect to time (i.e., degradation rate) through automatic differentiation [70]. The calculated degradation rate for each data point (i.e., sensor measurements) is considered a label for the same data point to train the second network (physics discovery network). Both networks are trained simultaneously in supervised settings by minimizing a custom-designed cost function, shown by Equation 4-2, where RUL and $\widehat{RUL}$ are actual and estimated RULs by the predictive network, respectively. $(\frac{\partial \widehat{RUL}}{\partial t})_{AD}$ is the calculated gradient of $\widehat{RUL}$ using automatic differentiation of the predictive network and $\left(\widehat{\frac{\partial RUL}{\partial t}}\right)$ is the estimated gradient of RUL by the physics discovery network. λ represents a weight coefficient. Finally, N is the number of data points in the training dataset.

$$L = \frac{1}{N}\sum_1^N (RUL - \widehat{RUL})^2 + \frac{\lambda}{N}\sum_1^N ((\frac{\partial \widehat{RUL}}{\partial t})_{AD} - \widehat{\frac{\partial RUL}{\partial t}})^2 \qquad 4\text{-}2$$

After sufficient training of the framework, the physics discovery model $M_{\psi,\eta}$ describes the underlying physics of degradation f based on our assumption that physics can be represented by the relationship between the system's internal and external environmental factors and degradation rate. In other words, the physics discovery model is a regression model that represents how environmental factors impact the degradation rate. This model is in the form of an NN. More details about the mathematical form of NNs can be found in the literature [71].

Minimizing the first term of the cost function leads to a close estimation of RUL by the predictive model. Minimizing the second term makes the physics discovery model output close to the gradient of the estimates obtained from the predictive model. It means the correctness of the labels of the training dataset for the physics discovery model depends on the accuracy of the estimations made by the predictive model. Thus, to ensure the discovered physics by the second network is accurate, both cost function terms should be minimized effectively.

4.2.2. Feature importance measurement

Although the physics discovery model represents the underlying physics of degradation, it does not clarify which environmental factors cause dominant stresses and significantly impact degradation behavior. In other words, the physics discovery model maps all provided input features (i.e., environmental factors measured by sensors) to the degradation rate, even though certain input features may have minimal effects on this rate. Therefore, an advanced feature importance measurement mechanism is required to quantify the significance of each environmental factor's effect precisely.

SHapley Additive exPlanations (SHAP) [72] is a powerful method for explaining the contribution of each feature to a model’s final output. This method is inspired by cooperative game theory, where the SHAP value determines each player’s contribution to a game outcome by dividing the rewards among all players [73]. In ML, this idea is applied by treating each feature as a player, and the SHAP value is utilized to quantify the influence of each input feature on the output. The SHAP method assesses the model’s output for all possible feature combinations and determines each feature's effect when used in conjunction with others. Consequently, a SHAP value is computed as the average contribution of the feature across all possible feature combinations minus the average contribution when the feature is absent. This value is assigned to each feature, representing its importance.

4.3. Case Study

In this case study, the FD001 sub-dataset from the benchmark dataset C-MAPSS [74] is used to showcase the practical application of our proposed approach. This dataset has been widely considered for evaluating DL models for RUL estimation [24]. FD001 consists of measurements of 27 different sensors from simulated run-to-failures of 100 aircraft engines. The simulation assumes different levels of initial degradation for the engines. Readers are referred to the explanations provided in [75, 76] to understand the dataset's creation and simulation process. Previous studies have demonstrated that out of the 27 sensors, only 14 yield statistically significant measurements for RUL prediction, while the remaining sensors seem to lack relevance [76]. Accordingly, these 14 sensors were exclusively used for the present case study.

Figure 10 shows the data allocations and how the dataset was used to train and test the developed models. The collected sensor measurements for 50% of the engines (50 engines out of 100 engines), which were selected randomly, were used to discover the underlying physics of degradation. The collected measurements from the remaining engines were used for validation to show how incorporating the discovered physics into a purely data-driven NN can improve its generalization and performance.

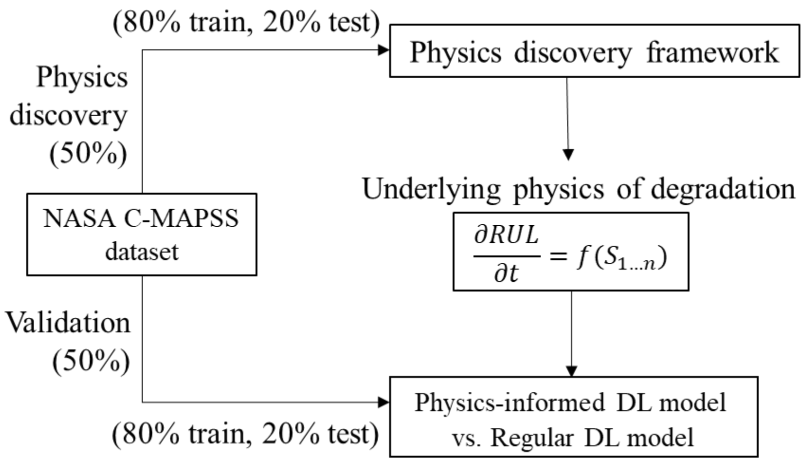


Figure 10. Data allocations for the case study

Both NNs of the physics discovery framework were designed with a common structure, comprising four layers, each with 10 neurons and utilizing the Tanh activation function. The optimal structures and activation functions for the NNs in this study were selected by trial and error to achieve the highest performance. The dual network framework was trained for 5000 epochs with a learning rate of 10^{-3}. Goodness-of-fit results for both networks on the training and test datasets are presented in Table 4. Three metrics of MSE, MAPE, and R^2 were used for quantifying the goodness-of-fit. Based on the relatively good fit observed from the calculated metrics, it can be inferred that the physics discovery model effectively captures the relationship between environmental factors and degradation rate, reflecting the underlying physics of degradation.

Table 4. Goodness-of-fit of the dual NN framework on training and test datasets with the measurements of 14 sensors.

Model	Dataset	MSE	MAPE	R^2
Predictive model	Training	9.82	0.17	0.90
	Test	13.62	0.21	0.82
Physics discovery model	Training	0.04	0.12	0.99
	Test	0.07	0.15	0.99

To validate the ability of the physics discovery model to represent the underlying physics of degradation, we evaluated the improvement achieved by incorporating the discovered physics into a purely data-driven model trained on the validation portion of the dataset. For this purpose, an NN with four layers, each consisting of ten neurons with Tanh activation function, was considered for RUL estimation. The NN was trained for 5000 epochs with a learning rate of 10^{-3}.

Figure 11 compares actual RULs versus estimated RULs for both models before and after incorporating the discovered physics. The purely data-driven model demonstrated a better fit to the training dataset than the physics-informed model. However, for the test dataset, the performance of the purely data-driven model decreased considerably, while the physics-informed model maintained its effectiveness. This shows how incorporating physics allows the model to generalize better and avoid overfitting the training dataset. Additionally, the two models were compared quantitatively using three metrics: MSE, MAPE, and R^2. Table 5 presents the results, showing that adding physics to the model enhances its robustness across all metrics.

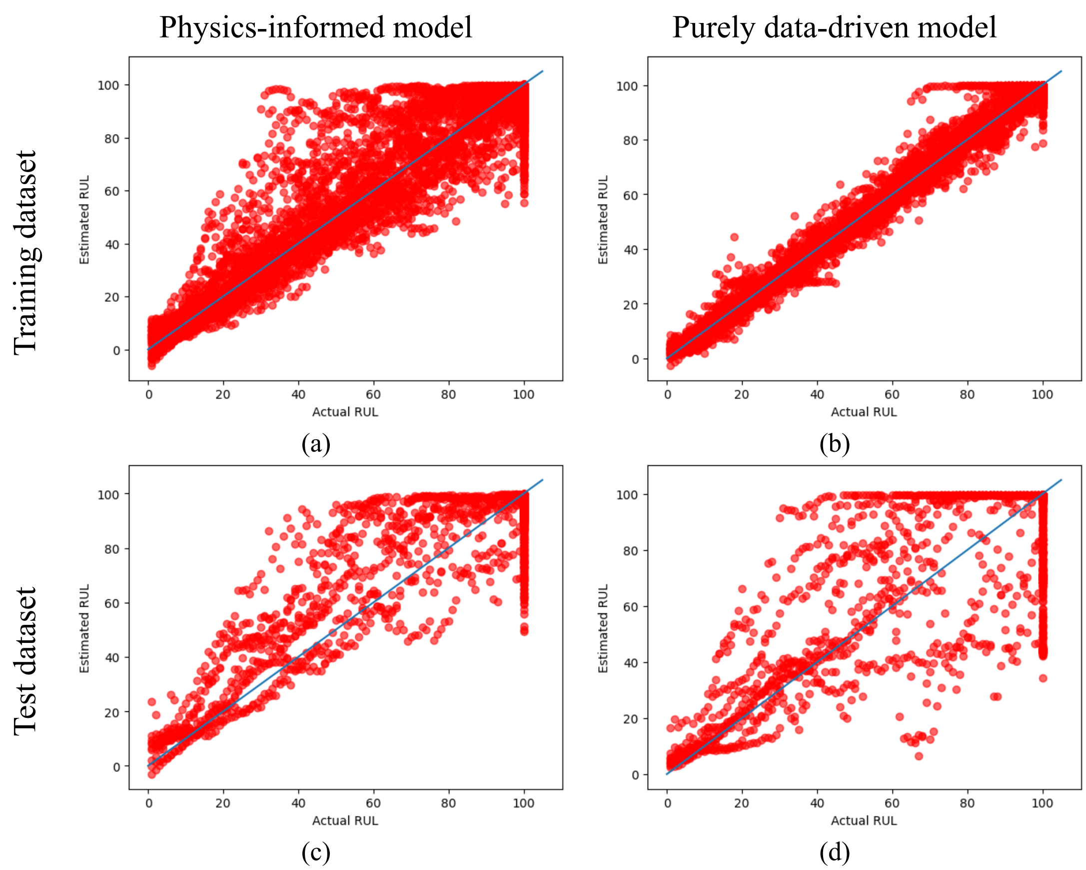


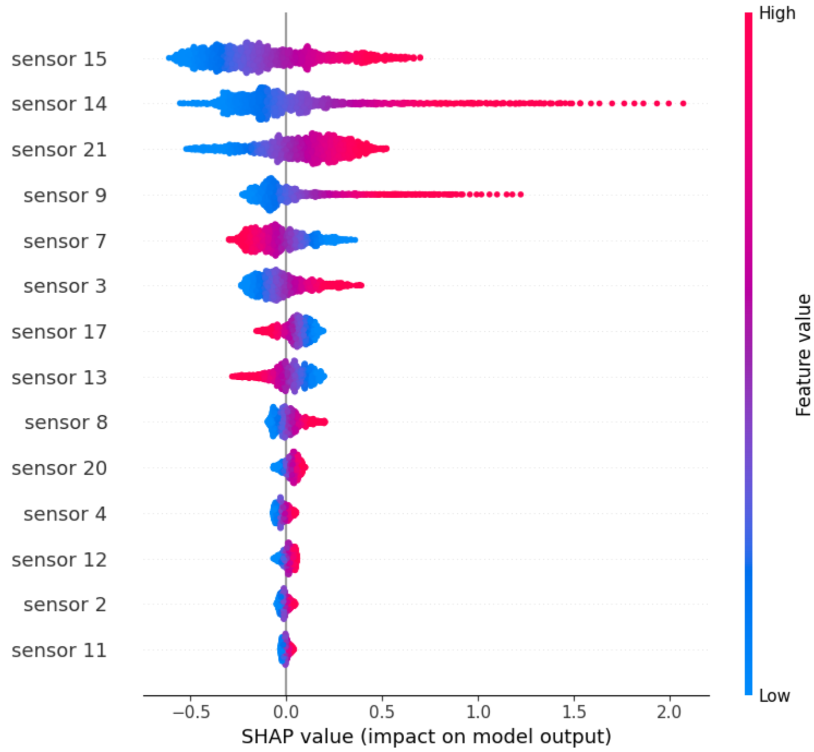
Figure 11. Comparing actual RUL with estimated RUL by physics-informed and purely data-driven model for training and test datasets

Table 5. Comparing goodness-of-fit by physics-informed and purely data-driven models for training and test datasets (using 14 sensor measurements)

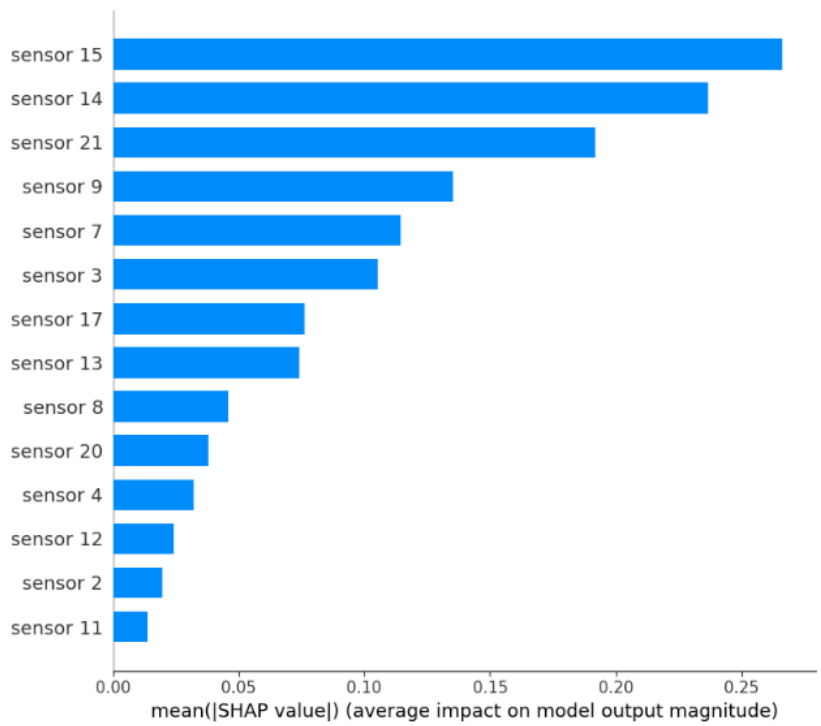
Model	Dataset	MSE	MAPE	R^2
Physics-informed model	Training	10.30	0.17	0.89
	Test	14.72	0.27	0.79
Purely data-driven model	Training	3.54	0.06	0.98
	Test	20.18	0.28	0.61

The accuracy of the physics discovery model and its impact on improving estimations of a purely data-driven model trained on the validation dataset determines its ability to discover and represent physics. However, the physics discovery model lacks the ability to identify which environmental factors predominantly influence degradation behavior. To address this ambiguity, the SHAP method is employed, which ranks the environmental factors based on their significance in influencing the degradation rate.

Figure 12 illustrates the results of applying the SHAP method to the physics discovery model. Figure 12a shows SHAP values for sensor measurements (i.e., model feature values). It explains which sensor measurements push the RUL prediction higher (positive SHAP values) and which pull it down (negative SHAP values). Moreover, the magnitude of the SHAP value indicates the strength of the measured environmental factor's impact on the prediction. Figure 12b shows the average of the SHAP values for all measurements for each sensor separately. These results highlight certain environmental factors, such as those measured by sensors 15, 14, and 21, have considerable effects on the progression of degradation. On the other hand, some other factors, like the one measured by sensors 11, 2, and 12, have minimal impacts.



(a)



(b)

Figure 12. SHAP results, including (a) the SHAP value for each data point and (b) the average of the SHAP values

By leveraging the impact significance obtained from SHAP, it becomes possible to identify and eliminate irrelevant environmental factors to the degradation mechanism. These factors have a low impact on the model's output. The elimination process was performed recursively, assessing the drop in the performance of the physics-informed model after each factor was removed. The results revealed that considering only the first 6 important factors, the model's performance remains nearly unchanged compared to all 14 factors, as demonstrated in Table 6 (i.e., eliminating 8 less important factors does not impact the model’s performance considerably). However, reducing the analysis to consider the first 5 important factors leads to a poor fit, and the model fails to capture the nonlinear patterns in the data. These results show how SHAP can be instrumental in understanding the impact of environmental factors and simplifying the underlying physics relationship. A more precise and effective model can be developed by focusing on the dominant stresses and disregarding irrelevant factors.

Table 6. Effect of the number of considered factors on the performance of the physics-informed model

Number of considered factors	Dataset	MSE	MAPE	R^2
14	Training	10.30	0.17	0.89
	Test	14.72	0.27	0.79
10	Training	10.67	0.17	0.88
	Test	15.07	0.26	0.78
8	Training	10.57	0.17	0.89
	Test	14.65	0.27	0.79
6	Training	11.05	0.18	0.88
	Test	14.40	0.25	0.80
5	Training	32.03	1.60	0
	Test	32.55	1.71	0

4.4. Conclusions

DL prognostic models for RUL prediction fit the data as a black-box regression model. Although they may perform highly in degradation modeling and RUL prediction, they do not provide any information about the underlying physics of degradation and the dominant stresses that have crucial roles in degradation progression. Therefore, there is a need for an approach that can reveal the underlying physics of degradation by considering the impact of all environmental factors and their interactions. Assuming the relationship between the influential environmental factors and degradation rate can represent the physics of degradation, this chapter proposed an approach utilizing a dual NN framework and a feature importance measurement tool to discover the underlying physics of degradation. The method was applied to a benchmark dataset as a case study to showcase the effectiveness of this approach. The results demonstrated that integrating the discovered physics into a DL prognostic model significantly improved its performance.

The proposed approach offers valuable benefits to designers, enabling them to incorporate appropriate preventive and mitigation strategies into their designs. By integrating these strategies, designers can ensure enhanced reliability and longevity of their products or systems, reducing the risk of failures and downtime. Furthermore, this approach gives users insights into the underlying physics of degradation. Armed with this understanding, users can devise optimized maintenance strategies and minimize the need for costly repairs or replacements. Moreover, the discovery of fundamental physics through this approach holds immense promise for improving the efficiency and robustness of future DL prognostic models. By leveraging the knowledge gained from understanding the physics of the system, prognostic models can make more accurate predictions, enabling timely interventions and preemptive measures to avoid or mitigate potential failures.

Chapter 5: Discussion, Verification, and Limitations

In this chapter, the proposed approaches are verified using a simulated dataset with known underlying physics (unlike the previous chapters, in which the underlying physics in the used datasets was unknown). Also, the limitations of the proposed approach are critically discussed.

5.1. Verification

Verifying the proposed approaches involves demonstrating their ability to discover known underlying physics of degradation. It seeks to answer whether the proposed approaches can explain which environmental factors have a major impact on the degradation behavior of the system. Previously, it was shown the discovered physics improves the prediction of degradation intensity. Chapters 3 and 4 present evidence that integrating the discovered physics into the predictive model enhances accuracy and generalizability.

However, two datasets with unknown underlying physics of degradation were used in previous chapters (i.e., corrosion degradation in steel coupons and degradation in aircraft engines). So, to verify and demonstrate the approaches' ability to discover the physics of degradation, a dataset is generated from a hypothetical physical rule to evaluate the approaches' performance in discovering physics for the scenarios described in Chapters 3 and 4 (i.e., scenario 1- degradation rate labels are available and scenario 2- degradation rate labels are not available). For more clarifications on the two considered scenarios, see the beginning of Chapter 4 of this dissertation.

Figure *13* shows the considered procedure for generating the verification dataset. Initially, a set of random points $S_1, S_2, \dots, S_n$, representing different environmental factors measured by sensors, is generated from known parametric distributions $p_1(\theta), p_2(\theta), \dots, p_n(\theta)$. Then, the degradation rate associated with the generated data point is calculated using the assumed relationship for the underlying physics of degradation (Equation 4-1). Alternatively, the degradation rate can also be derived from a known distribution, and one of the environmental factors can be calculated using the considered underlying physics of degradation. Finally, the environmental factors serve as features and the degradation rate is the corresponding label for the generated data point. This procedure can be iterated until the desired data points are attained.

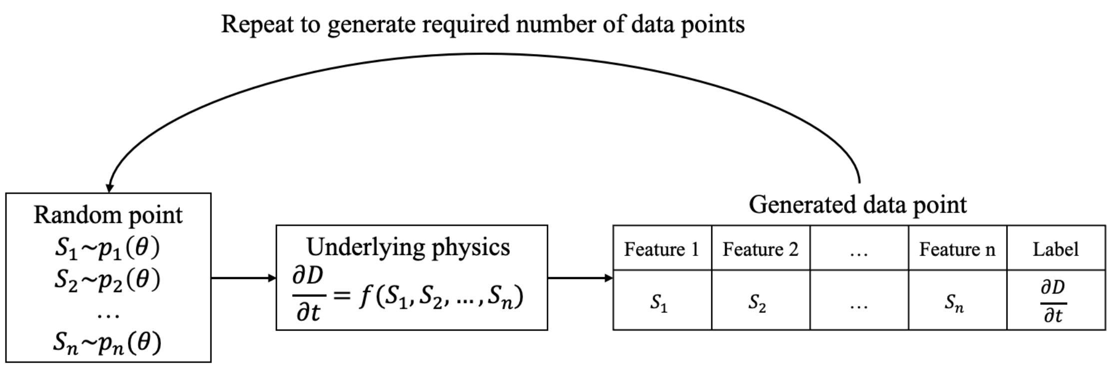


Figure 13. Dataset generation procedure

For the verification of the proposed approaches, it is assumed that seven environmental factors are collected by seven sensors (i.e., $S_1, S_2, \dots, S_7$). However, any number of environmental factors can be considered as NNs could fit high-dimensional data, as discussed before. For each set of sensor measurements, degradation rates can be calculated based on the assumed relationship for the underlying physics of degradation.

Equation 5-1 represents the considered hypothetical relationship for the underlying physics of degradation. It is assumed that the degradation rate is mainly influenced by S_1 and S_7, and other environmental factors have a minor impact. Parameters a, b, and c are constants set to 0.5, 2, and 0.001, respectively.

$$\frac{\partial D}{\partial t} = \mathrm{a} \times \mathrm{Ln}(S_1^2) + b \times S_1 \times S_7 + c \times (S_2 + S_3 + S_4 + S_5 + S_6) \qquad \text{5-1}$$

To have more control over the range of degradation rates, an alternative procedure was followed by sampling the degradation rate from a known distribution and then calculating the last environmental factor S_7 from the underlying physics of degradation. Degradation rates were randomly drawn from a uniform distribution with a minimum value of 0 and a maximum value of 10.

Table 7 provides an overview of the distributions for generating data points for each environmental factor. Also, it needs to be mentioned S_1 and S_6 are generated from a multivariate normal distribution with a covariance of 150. This was done to evaluate the performance of the proposed approaches in dealing with correlated features. Finally, it is worth mentioning these distributions are inspired mainly by real-world environmental factors.

Table 7. Assumed sensor measurements for validation dataset

Sensor	**Distribution**	**Inspiration factor**
S_1	$\mathcal{N}(\mu = 25, \sigma = 10)$	Temperature
S_2	$\mathcal{N}(\mu = 70, \sigma = 15)$	Relative humidity
S_3	$\mathcal{N}(\mu = 7, \sigma = 2)$	pH
S_4	$\mathcal{N}(\mu = 10, \sigma = 2)$	Wind speed
S_5	$\mathcal{U}(\mu = 0, \sigma = 360)$	Wind direction
S_6	$\mathcal{N}(\mu = 100, \sigma = 10)$	Solar radiation

5.1.1. Scenario 1: Degradation rate labels are available.

The proposed approach discussed in Chapter 3 of this dissertation focuses on enhancing the prediction of degradation intensity by leveraging the underlying physics of degradation. This chapter presents an approach that involves training an NN (referred to as the physics discovery model) separately using available data with degradation rate labels. The physics discovery model aims to establish a relationship between environmental factors and degradation rates. This physics discovery model is later incorporated into the predictive model to enhance predictions based on physics-informed insights. The verification goal is to assess the capability of the physics discovery model to capture the relationship between environmental factors and degradation rates.

An NN model with two hidden layers of eight neurons and the ReLU activation function was trained to map the sensor measurements to degradation rates, aiming to serve as a surrogate model for the underlying physics, as described in Equation 5-1. MSE of 0.042 and MAPE of 0.091 on the test dataset represents acceptable fit of the model. It is noteworthy that evaluating the performance of different NN architecture falls outside the scope of this dissertation. While alternative structures may perform better, the employed architecture demonstrates reasonable accuracy.

Chapter 3 used an NN model as a physics discovery model and integrated it into a predictive model for more accurate physics-informed predictions. To show the model has effectively captured the underlying physics of degradation, it should represent the impact of environmental factors on the degradation process (the substantial impact of S_1 and S_7 for the current dataset).

Upon measuring feature importance through the SHAP method, it becomes evident that the model has successfully grasped the dominance of S_1 and S_7 in the degradation process. Refer to Figure 14 for a visual representation of this observation.

SHAP values quantify the individual contribution of each feature to the prediction of a specific data point compared to the average prediction. Figure 14 illustrates the SHAP values corresponding to each feature across all data points in the dataset. This serves as a metric, summarizing the average influence of that feature on model predictions throughout the entire dataset. A high mean of SHAP values for a specific feature suggests a substantial impact on the model's output, while a low mean of SHAP values indicates a comparatively smaller influence.

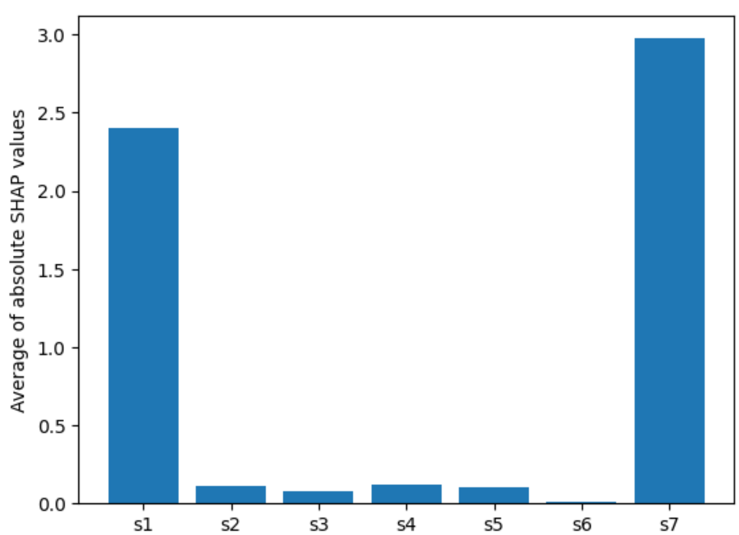


Figure 14. Average of SHAP values for the validation dataset based on separately trained model (scenario 1)

5.1.2. Scenario 2: Degradation rate labels are not available.

The approach proposed in Chapter 4 of this dissertation is designed to discover the physics of degradation by determining the relationship between environmental factors and degradation rates in cases where explicit degradation rate data is lacking in the dataset. The approach involves training two NNs: a physics discovery NN and a predictive NN, simultaneously minimizing a custom-designed cost function.

To demonstrate the ability of this approach to discover the physics of degradation, the validation dataset without degradation rate labels is used. Two NNs with the same structures (two hidden layers with eight neurons and ReLU activation functions) are trained simultaneously. The first NN, called the physics discovery NN, is responsible for mapping environmental factors to degradation rates. Given the absence of degradation rate labels, automatic differentiation of the output of the second NN (the predictive model), which links time and environmental factors to degradation intensity, is used as labels for training the first NN, as shown in Figure *15*. Both models fitted the data relatively good considering the MSE of 421 and MAPE of 0.031 for the predictive model and MSE of 0.801 and MAPE of 0.188 for the physics discovery model on the test dataset.

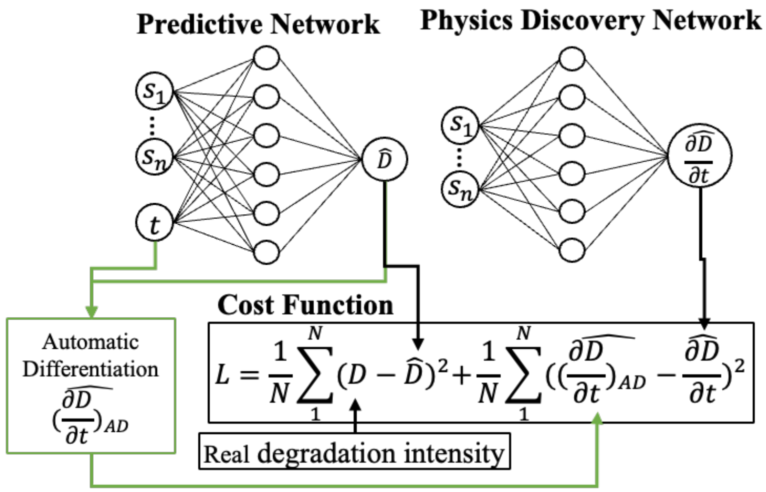


Figure 15. Training of the proposed dual NN framework when degradation rate labels are not available

To evaluate the physics discovery model's ability to grasp the underlying physics, the SHAP method is applied to quantify the influence of environmental factors on the degradation process. A SHAP value for a feature is calculated by considering all possible combinations of features and measuring the average change in the model's output when a specific feature is included, compared to when it is excluded. Therefore, the mean of SHAP values for each feature summarizes the expected influence of that feature on model predictions throughout the entire dataset. Considering this metric, S_1 and S_7 measurements were correctly identified as the most influential features, as shown in Figure 16. The errors pertaining to the relative importance of other factors stem from the challenge of assessing the influence of the factors on degradation rate without access to degradation rate labels, relying solely on degradation intensity labels. While the proposed approach makes it possible, it is important to note that some errors may still be inevitable.

Finally, the values shown in Figure 16 represent the relative importance of features, enabling the comparison of their respective impacts on the degradation rate. However, it cannot identify the main influential factors in one shot. That is why multi-step recursive feature elimination was proposed in Chapter 4. Using a recursive feature elimination scheme helps remove unimportant factors one by one to achieve a model based on influential factors.

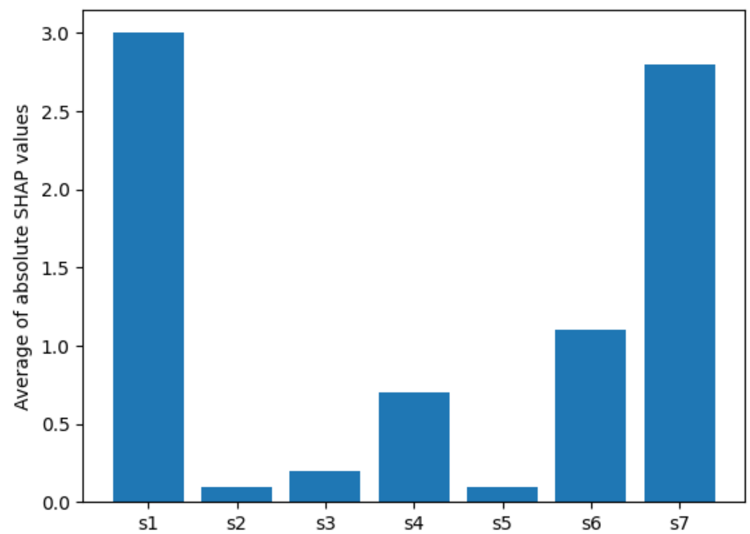


Figure 16. Average of SHAP values for the validation dataset based on models trained together (scenario 2).

5.1.3. Discussion

Verification of the proposed approaches through the utilization of a simulated dataset, generated based on a predetermined hypothetical physics of degradation, showed the efficacy of the proposed approaches for both considered scenarios (i.e., scenario 1- degradation rate labels are available and scenario 2- degradation rate labels are not available).

The analysis carried out during this verification process illustrates the ability of these approaches to identify and pinpoint the predominant environmental factors with a substantial influence on the progression of degradation. This verification not only underscores the reliability of the proposed approaches but also underscores their proficiency in extracting meaningful insights regarding the key drivers behind degradation phenomena.

Additionally, integrating the SHAP feature importance method into the physics discovery NN allows for identifying important environmental factors. It enables the identification and recursive elimination of environmental factors with negligible effects on degradation. This process can be executed without significantly compromising the predictive model's performance, as discussed in Chapter 4 of this dissertation.

5.2. Limitations

It is important to acknowledge the limitations of the proposed framework. Firstly, the framework still requires degradation data for training purposes, albeit less data than a regular NN. Collecting such data can be time-consuming and expensive as degradation is often a slow process. Obtaining a useful dataset that adequately represents different stages and types of degradation can take a considerable amount of time. Researchers and practitioners may need to monitor and record the degradation of systems, materials, or structures over extended periods. This process necessitates careful planning, consistent monitoring, and dedicated resources to ensure the availability of an error-free and meaningful degradation dataset.

Furthermore, the expense of collecting degradation data can be a significant barrier. Acquiring and maintaining equipment to monitor degradation processes can incur substantial costs. Additionally, the expertise required to interpret accurately and record degradation data is a valuable resource that may not always be readily available or affordable.

Another limitation of the proposed framework is that it primarily focuses on degradation. However, potential failures may occur in the field due to discrete over-stress conditions rather than gradual and temporal degradation. In the real world, failures may not always follow a smooth degradation curve. Instead, they can result from failure caused by over-stress conditions, pushing the system or components beyond their intended operational capacity. These conditions might be characterized by sudden spikes in stress, unforeseen environmental factors, extreme operational demands, or unforeseen events that subject the system to intense loading. Unlike cumulative degradation, these overstress conditions can lead to immediate failures. Understanding and addressing these discrete over-stress conditions is crucial for enhancing the system's resilience and ensuring its reliability in diverse operational scenarios.

5.3. Conclusions

Using NNs allows for more accurate degradation predictions by identifying complex and highly nonlinear patterns and relationships in the data that may not be apparent with conventional statistical methods. This has been widely investigated in previous research studies on DL-based prognostic approaches. The key component of better degradation predictions in the proposed approach in this research study is accurate physics discovery. The proposed approach enables accurate degradation prediction by discovering the governing physics of degradation and incorporating it into predictions.

By employing a simulated dataset based on a hypothetical physics of degradation, the proposed approach effectively demonstrates its ability to discover the underlying physics of governing degradation mechanisms. Through this analysis, it was possible to pinpoint the prominent environmental factors that significantly impact degradation progression. The subsequent integration of this discovered physics into the predictions yields substantial improvements, as it facilitates physics informed predictions.

Accurate discovery of the physics of degradation enables efficient prediction of systems degradation behavior, thereby avoiding the repercussions of incorrect lifetime estimations, such as economic losses and potentially life-threatening incidents, particularly for safety-critical systems.

Chapter 6: Conclusions

This chapter provides conclusions, an overview of the contributions made by this research study, a list of papers resulting from the research, and recommendations for future works to build upon the current efforts.

6.1. Conclusions

This research study improves prognostic for systems under environmentally induced degradation through an integrated and adaptable framework. The proposed approach, grounded in NN theory, goes beyond physics-based models to overcome their inherent limitations by considering the impact of all environmental factors on degradation behavior. In addition, this approach improves conventional data-driven models by discovering and incorporating the underlying physics of degradation in the form of a relationship between environmental factors and degradation rate.

The core of the research study's contribution is the innovative dual NN framework, an innovative setup that simultaneously discovers and incorporates the underlying physics of degradation. The proposed approach surpasses conventional data-driven methods by integrating insights from the effects of environmental factors into predictive models. The collaboration of two NNs, each with a unique role, fosters a synergy that enables accurate, physics-informed predictions even in scenarios with limited data.

Another important aspect of the approach is its ability to address the lack of interpretability in prevalent DL prognostic models, often known for being black boxes. The proposed approach goes beyond prediction, discovering the underlying physics of degradation through the dual NN framework and pinpointing influential environmental factors using a feature importance measurement tool. This approach not only enhances prediction accuracy but also empowers designers with valuable insights, allowing them to integrate preventive and mitigation strategies into their designs.

The importance of accurate physics discovery is highlighted throughout this research, impacting the efficient prediction of degradation behaviors. Through a detailed case study on atmospheric corrosion, the framework demonstrates its effectiveness in predicting long-term degradation, even with limited initial observations. This capability is crucial, especially in safety-critical systems, as it prevents the consequences of inaccurate lifetime estimations, such as economic losses and potential safety incidents.

While recognizing the approach's advantages, it is essential to acknowledge its limitations. Though reduced compared to conventional NNs, the need for degradation data poses practical challenges due to the time and cost involved in data collection for slow degradation processes. Additionally, the current focus is on gradual degradation excluding discrete over-stress conditions that can lead to sudden failures. Finally, uncertainties in real-world situations remain to be fully addressed in future studies.

In summary, this research study demonstrated advancement in the prognostic of systems under environmentally induced degradation. The proposed integrated framework enhances the accuracy of degradation predictions and discovers the intricate physics governing degradation mechanisms. This framework holds promise of enhancing the efficiency and robustness of prognostic models, contributing to the reliability and durability assessments of systems exposed to environmental degradation.

6.2. Contributions

The contributions of this research study can be summarized as follows:

1- This dissertation introduces a novel dual NN framework by defining a custom designed cost function for discovering the complex underlying physics of degradation in real-world conditions in the form of a relationship between degradation rate and all measured environmental factors. By having the ability to consider all environmental factors in the field, the proposed approach provides a comprehensive and accurate representation of the degradation in complex systems.

2- Previously developed physics-informed DL prognostics models incorporated known empirical models or a general understanding of physical principles to enhance predictive capabilities. However, the introduced approach in this dissertation improves this common practice by integrating a physics discovery model directly into the predictive model. By incorporating a physics discovery model, it aims to capture underlying physical principles and mechanisms that may not be explicitly described by established empirical models or understood through general physical rules.

3- In this dissertation, the proposed approach is further enhanced by integrating the physics discovery model, a feature importance measurement method, and a recursive feature elimination scheme to exclude environmental factors without considerable impact on degradation from the identified physics relationship. Doing so enables pinpointing the primary stressors that significantly influence degradation. Therefore, the developed approach not only uses the capabilities of NN algorithms for effective prognostics, which is a common practice, but also maintains high interpretability, which is a major contribution.

4- The proposed approach uses NN algorithms for discovering physics and predicting degradation intensity, making it possible to consider the impacts of indirect environmental factors on degradation phenomena. Empirical methods (i.e., physic-based models) have often been confined to a limited number of stresses, hindering applicability to real-world scenarios where multiple stressors simultaneously influence the degradation process.

6.3. <u>Publications</u>

The following peer-reviewed papers were published as an outcome of the PhD research work that resulted in this dissertation.

1. H. Habibollahi Najaf Abadi and M. Modarres, "Predicting system degradation with a guided neural network approach," Sensors, vol. 23, no. 14, p. 6346, 2023 [77].
2. H. Habibollahi Najaf Abadi, J. W. Herrmann and M. Modarres, "Measuring and indexing the durability of electrical and electronic equipment," *Sustainability,* vol. 15, no. 19, p. 14386, 2023 [78].
3. H. Habibollahi Najaf Abadi and M. Modarres, "A deep learning approach for discovering the underlying physics of degradation for data-driven prognostics,"

in 70th Annual Reliability and Maintainability Symposium, Albuquerque, New Mexico, USA, 2024 [79].

4. H. Habibollahi Najaf Abadi, "Physics-informed deep learning-based approach for probabilistic modeling of degradation," in PHM Society Doctoral Symposium, Salt Lake City, Utah, USA, 2023 [80].
5. H. Habibollahi Najaf Abadi, M. Nikiforov, A. Krive, J. W. Herrmann and M. Modarres, "The need for a durability index framework for electrical and electronic equipment to support a circular economy," in *European Conference On Safety And Reliability*, Southampton, United Kingdom, 2023 [81].

6.4. Future works

In the following, some areas for future research have been recommended.

- In this dissertation, there is a fundamental assumption that the complex physics governing degradation processes can be captured and represented by the effect of environmental factors on the degradation rate, which is the first derivative of degradation intensity with respect to time. However, to achieve a deeper and more precise understanding of degradation behavior within a system, it is important to consider effects of environmental factors on higher degrees of gradient of degradation. While the first gradient offers valuable insights to capture the interactions between environmental factors and degradation accurately, the study should be extended to consider the second and subsequent gradient of degradation with respect to time or frequency. These higher-order gradients may be essential for identifying the complex and nonlinear degradation behavior. This expanded perspective enables a more comprehensive modeling approach, facilitating a more accurate prediction of the degradation behavior.

- This research study acknowledges that degradation intensity in a system does not solely depend on time; it can also vary across different frequencies or spatial coordinates within a system. For example, when examining pitting corrosion degradation based on the depth of damage, it's important to recognize that this depth is not uniform across a system and shows variability in different spatial coordinates. In other words, the extent of corrosion in localized pitting can differ significantly based on spatial factors within the system. Understanding and accounting for these spatial variations in degradation intensity is crucial for developing accurate predictive models. Therefore, to obtain a more accurate understanding of degradation behavior, effects of environmental factors on different degrees of gradient of degradation over both space and time should be considered. This implies that the proposed form of relationship for the underlying physics of degradation should incorporate partial derivatives of degradation with respect to space as well.
- The case studies data used in this study contain no data anomalies, and all have the same numerical values. However, challenges such as unlabeled data, anomalies (like missing data and erroneous sensor measurements), and the presence of non-structured, multi-modal, and heterogeneous data are common when dealing with real-world datasets. Therefore, to make maximum use of the available data and effectively apply the proposed approach outlined in this

dissertation, it is necessary to establish a robust data preprocessing framework capable of addressing issues with imperfect data gathered from the field (e.g., identifying and removing outlier data points, addressing missing sensor measurements) and integrating heterogeneous data from various sources (e.g., fusing inspection reports in text format with sensor measurements). Moreover, leveraging data generated by large-scale generative models, such as generative language models, can enhance datasets and contribute to more effective training of prognostic models, including the proposed one.

- Effect of NN configuration, including number of layers, number of nodes in each layer, and activation functions, on the performance of the proposed method for accurate physics discovery and degradation intensity prediction is not investigated in this study. Future research can optimize the NN configuration for better performance.
- This dissertation focuses only on prognostics applications (i.e., estimation of RUL or degradation intensity). However, it is also essential to consider diagnostics to develop a highly effective proactive maintenance strategy. This involves pinpointing the exact faulty component within the target system instead of solely evaluating the overall system’s degradation. Therefore, a future extension of the current research can consider diagnostic aspects. This will ensure a comprehensive approach that integrates both prognostics and diagnostics, fostering a holistic and robust maintenance strategy for optimal system performance and reliability.

Appendices

Appendix A

This section contains all the Python codes used for the developed framework in Chapter 3.

```
# Normalizing data
# using sklearn library for scaling
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
# read and transform dataset
Data = scaler.fit_transform(massloss_df_M[['average radiance', 'std radiance', 'average radiance gra',
    'std radiance gra', 'average tem', 'std tem', 'average tem gra',
    'std tem gra', 'average hum', 'std hum', 'average hum gra',
    'std hum gra']])

Data = pd.DataFrame(Data, columns = ['average radiance', 'std radiance', 'average radiance gra',
    'std radiance gra', 'average tem', 'std tem', 'average tem gra',
    'std tem gra', 'average hum', 'std hum', 'average hum gra',
    'std hum gra'])

# PCA
# using numpy library for PCA
import numpy as np
cov_mat = np.cov(Data.T)
# calculating eigen values
eigen_vals, eigen_vecs = np.linalg.eig(cov_mat)
print('\nEigenvalues \n%s' % eigen_vals)
tot = sum(eigen_vals)
var_exp = [(i / tot) for i in sorted(eigen_vals, reverse=True)]
cum_var_exp = np.cumsum(var_exp)
import matplotlib.pyplot as plt
# plotting using matplotlib library
plt.figure(dpi=100)
plt.bar(range(1,13), var_exp, alpha=1, align='center', label='Individual explained variance')
plt.step(range(1,13), cum_var_exp, where='mid', label='Cumulative explained variance',c='red')
plt.ylabel('Explained variance ratio')
plt.xlabel('Principal components')
plt.legend(loc='best')
plt.show()
print(var_exp)
from sklearn.decomposition import PCA
# selecting number of principle components
pca = PCA(n_components=2)
```

```
Data_pca = pca.fit_transform(Data)
Data_pca_df = pd.DataFrame(Data_pca, columns = ['x1', 'x2'])
```

 # Physics discovery model

```
# setting configuration of the network (size and activation functions)
class Net_physics(nn.Module):
  def __init__(self):
    super(Net_physics, self).__init__()
    self.hidden_layer1 = nn.Linear(2,8)

    self.output_layer=nn.Linear(8,1)

  def forward(self,x1,x2):#,x3,x4,x5):
    inputs = torch.cat([x1,x2],axis=1)
    layer1_out = torch.tanh(self.hidden_layer1(inputs))
    output = self.output_layer(layer1_out)
    return output

net_physics = Net_physics()
net_physics = net_physics.to(device)
mse_cost_function1 = torch.nn.MSELoss(reduction = "mean")
print(net_physics)

# selecting type of optimizer
optimizer1 = torch.optim.Adam(net_physics.parameters(),lr=10e-6)

data_loss1=[]
total_loss1=[]

# determining number of iteration
iterations1=100000
previous_validation_loss1 = 99999999.0

# beginning of the learning loop
for epoch in range(iterations1):
    optimizer1.zero_grad()
# formatting data for pytorch (converting data to variable)
    # Loss based on available data
    x1_data = np.array([Data_pca_df['x1']]).reshape(Data_pca_df.shape[0],1)
    x2_data = np.array([Data_pca_df['x2']]).reshape(Data_pca_df.shape[0],1)
    dm_data=np.array([massloss_df_M['mass loss rate']]).reshape(massloss_df_M.shape[0],1)

    pt_x1_data = Variable(torch.from_numpy(x1_data).float(), requires_grad=False).to(device)
    pt_x2_data = Variable(torch.from_numpy(x2_data).float(), requires_grad=False).to(device)
    pt_dm_data = Variable(torch.from_numpy(dm_data).float(),
requires_grad=False).to(device)
# calculating output of the network
    net_physics_out =
net_physics(pt_x1_data,pt_x2_data)#,pt_x3_data,pt_x4_data,pt_x5_data) # output of u(x,t)
    mse_d = mse_cost_function1(net_physics_out, pt_dm_data)
```

```
    loss = mse_d
# computing gradients using backward propagation
    loss.backward()
    optimizer1.step() # This is equivalent to : theta_new = theta_old - alpha * derivative of J
w.r.t theta
# recording loss values at each learning iteration
    with torch.autograd.no_grad():
        if epoch%50==0:
          print(epoch,"Total Training Loss:",loss.data)
        total_loss1.append(loss.item())
# plotting loss values
plt.plot(total_loss1,label='total_loss')
plt.ylabel('Total loss')
plt.xlabel('Epoch')
plt.show()
```

```
# Automatic differentiation
def f(t,x1,x2):
  prediction = deepnormalmodel(t)
  prediction_t = torch.autograd.grad(prediction.loc.sum(),t,create_graph=True)[0]
  physics=net_physics(x1, x2)
  inc = prediction_t-physics
  return inc
```

 # Predictive model

```
# importing needed libraries
import os
from os.path import join
def warn(*args, **kwargs):
    pass
import warnings
warnings.warn = warn
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import torch
import torch.nn.functional as F
from sklearn.metrics import r2_score
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
from scipy.stats import binned_statistic
import statsmodels.api as sm

# setting configuration of the network (size and activation functions)
torch.manual_seed(47)
class DeepNormalModel(torch.nn.Module):
    def __init__(self):
        super().__init__()
```

```
        self.hidden_layer1 = nn.Linear(1,6)
        self.mean_linear = torch.nn.Linear(6, 1)
        self.std_linear = torch.nn.Linear(6, 1)

    def forward(self, t):
      inputs = torch.cat([t])
      layer1_out=torch.tanh(self.hidden_layer1(inputs))
      mean = self.mean_linear(layer1_out)
      std = torch.nn.functional.softplus(self.std_linear(layer1_out))

      return torch.distributions.Normal(mean, std)

deepnormalmodel = DeepNormalModel()
deepnormalmodel = deepnormalmodel.to(device)

# cost function
mse_cost_function = torch.nn.MSELoss(reduction = "mean")
total_loss1=[]
f_loss1=[]
data_loss1=[]

# selecting optimizer
optimizer = torch.optim.Adam(deepnormalmodel.parameters(),lr=10e-6)
Ass=[]
nss=[]

# beginning of the learning loop
for epoch in range(50000):
  optimizer.zero_grad()
#converting data to variable format (it is needed in pytorch)
  t_data = np.array([x_train['Total Days of Exposure']]).reshape(x_train.shape[0],1)
  y_data=np.array([x_train['Mass Loss (Init-FinalB)']]).reshape(x_train.shape[0],1)
  pt_t_data = Variable(torch.from_numpy(t_data).float(), requires_grad=True).to(device)
  pt_y_data = Variable(torch.from_numpy(y_data).float(), requires_grad=False).to(device)

  net_out = deepnormalmodel(pt_t_data)
  loss_data=torch.mean(-net_out.log_prob(pt_y_data))
# normalizing data
  x_train_stan=scaler.transform(x_train[['average radiance', 'std radiance', 'average radiance
gra',
      'std radiance gra', 'average tem', 'std tem', 'average tem gra',
      'std tem gra', 'average hum', 'std hum', 'average hum gra',
      'std hum gra']])
  x_train_stan_pca=pca.transform(x_train_stan)
  x_train_stan_pca_df=pd.DataFrame(x_train_stan_pca, columns = ['x1','x2'])

  x1_data_col = np.random.uniform(low=x_train_stan_pca_df['x1'].min(),
high=x_train_stan_pca_df['x1'].max(), size=(200,1))
  x2_data_col = np.random.uniform(low=x_train_stan_pca_df['x2'].min(),
high=x_train_stan_pca_df['x2'].max(), size=(200,1))
```

```
  t_data_col = np.random.uniform(low=1, high=365, size=(200,1))
  all_zeros = np.zeros((200,1))

  pt_x1_data_col = Variable(torch.from_numpy(x1_data_col).float(),
requires_grad=False).to(device)
  pt_x2_data_col = Variable(torch.from_numpy(x2_data_col).float(),
requires_grad=False).to(device)
  pt_t_data_col = Variable(torch.from_numpy(t_data_col).float(),
requires_grad=True).to(device)
  pt_all_zeros = Variable(torch.from_numpy(all_zeros).float(),
requires_grad=False).to(device)

  f_out=f(pt_t_data_col,pt_x1_data_col,pt_x2_data_col)
  loss_f = 1.05*10**5*mse_cost_function(f_out, pt_all_zeros)

  loss=loss_data+loss_f

  loss.backward()
  optimizer.step()
```

Appendix B

This section contains all the Python codes used for the developed framework in Chapter 4.

```
# Dual NN for physics discovery
torch.manual_seed(83)
# setting configuration of the predictive model
class DeepNormalModel(torch.nn.Module):
    def __init__(self):
        super(DeepNormalModel,self).__init__()
        self.hidden_layer1 = nn.Linear(15,10)
        self.hidden_layer2 = nn.Linear(10,10)
        self.hidden_layer3 = nn.Linear(10,10)
        self.hidden_layer4 = nn.Linear(10,10)
        self.hidden_layer5 = nn.Linear(10,1)

    def forward(self,t, x1,x2,x3,x4,x5,x6,x7,x8,x9,x10,x11,x12,x13,x14):
      inputs = torch.cat([t,x1,x2,x3,x4,x5,x6,x7,x8,x9,x10,x11,x12,x13,x14],axis=1)
      layer1_out=torch.tanh(self.hidden_layer1(inputs))
      layer2_out=torch.tanh(self.hidden_layer2(layer1_out))
      layer3_out=torch.tanh(self.hidden_layer3(layer2_out))
      layer4_out=torch.tanh(self.hidden_layer4(layer3_out))
      layer5_out=self.hidden_layer5(layer4_out)
      return layer5_out

# setting configuration of the physics discovery model
class DeepPhysicsModel(torch.nn.Module):
```

```
    def __init__(self):
        super(DeepPhysicsModel,self).__init__()
        self.hidden_layer1 = nn.Linear(14,10)
        self.hidden_layer2 = nn.Linear(10,10)
        self.hidden_layer3 = nn.Linear(10,10)
        self.hidden_layer4 = nn.Linear(10,10)
        self.output_layer = nn.Linear(10, 1)

    def forward(self, x1,x2,x3,x4,x5,x6,x7,x8,x9,x10,x11,x12,x13,x14):
      inputs = torch.cat([x1,x2,x3,x4,x5,x6,x7,x8,x9,x10,x11,x12,x13,x14],axis=1)
      layer1_out=torch.tanh(self.hidden_layer1(inputs))
      layer2_out=torch.tanh(self.hidden_layer2(layer1_out))
      layer3_out=torch.tanh(self.hidden_layer3(layer2_out))
      layer4_out=torch.tanh(self.hidden_layer4(layer3_out))
      output=self.output_layer(layer4_out)
      return output

deepnormalmodel = DeepNormalModel()
deepnormalmodel = deepnormalmodel.to(device)

deepphysicsmodel = DeepPhysicsModel()
deepphysicsmodel= deepphysicsmodel.to(device)
params = list(deepnormalmodel.parameters()) + list(deepphysicsmodel.parameters())

# selecting optimizer
optimizer = torch.optim.Adam(params,lr=10e-3)
mse_cost_function = torch.nn.MSELoss(reduction = "mean")

total_loss1=[]
physics_loss1=[]
data_loss1=[]
extra_loss1=[]

# beginning of learning loop
for epoch in range(5000):
  optimizer.zero_grad()

# converting data to right format for pytorch
  t_data =
np.array([df_phydis_train_scaled_smooth_RUL['cycle']]).reshape(df_phydis_train_scaled_s
mooth_RUL.shape[0],1)
  x1_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
2']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x2_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
3']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x3_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
4']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x4_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
7']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
```

```
  x5_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
8']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x6_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
9']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x7_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
11']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x8_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
12']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x9_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
13']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x10_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
14']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x11_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
15']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x12_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
17']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x13_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
20']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  x14_data = np.array([df_phydis_train_scaled_smooth_RUL['sensor
21']]).reshape(df_phydis_train_scaled_smooth_RUL.shape[0],1)
  y_data=np.array([df_phydis_train_scaled_smooth_RUL['RUL']]).reshape(df_phydis_train_s
caled_smooth_RUL.shape[0],1)

  pt_t_data = Variable(torch.from_numpy(t_data).float(), requires_grad=True).to(device)
  pt_x1_data = Variable(torch.from_numpy(x1_data).float(), requires_grad=False).to(device)
  pt_x2_data = Variable(torch.from_numpy(x2_data).float(), requires_grad=False).to(device)
  pt_x3_data = Variable(torch.from_numpy(x3_data).float(), requires_grad=False).to(device)
  pt_x4_data = Variable(torch.from_numpy(x4_data).float(), requires_grad=False).to(device)
  pt_x5_data = Variable(torch.from_numpy(x5_data).float(), requires_grad=False).to(device)
  pt_x6_data = Variable(torch.from_numpy(x6_data).float(), requires_grad=False).to(device)
  pt_x7_data = Variable(torch.from_numpy(x7_data).float(), requires_grad=False).to(device)
  pt_x8_data = Variable(torch.from_numpy(x8_data).float(), requires_grad=False).to(device)
  pt_x9_data = Variable(torch.from_numpy(x9_data).float(), requires_grad=False).to(device)
  pt_x10_data = Variable(torch.from_numpy(x10_data).float(),
requires_grad=False).to(device)
  pt_x11_data = Variable(torch.from_numpy(x11_data).float(),
requires_grad=False).to(device)
  pt_x12_data = Variable(torch.from_numpy(x12_data).float(),
requires_grad=False).to(device)
  pt_x13_data = Variable(torch.from_numpy(x13_data).float(),
requires_grad=False).to(device)
  pt_x14_data = Variable(torch.from_numpy(x14_data).float(),
requires_grad=False).to(device)
  pt_y_data = Variable(torch.from_numpy(y_data).float(), requires_grad=False).to(device)

  net_out =
deepnormalmodel(pt_t_data,pt_x1_data,pt_x2_data,pt_x3_data,pt_x4_data,pt_x5_data,pt_x6
_data,pt_x7_data,pt_x8_data,pt_x9_data,pt_x10_data,pt_x11_data,pt_x12_data,pt_x13_data,
pt_x14_data)
```

```
  loss_data=mse_cost_function(net_out,pt_y_data)

# automatic differentiation
  pt_t_prime=torch.autograd.grad(net_out.sum(),pt_t_data,create_graph=True)[0]
  pt_t_prime=(pt_t_prime-pt_t_prime.mean())/pt_t_prime.std()

  physicsnet_out =
deepphysicsmodel(pt_x1_data,pt_x2_data,pt_x3_data,pt_x4_data,pt_x5_data,pt_x6_data,pt_
x7_data,pt_x8_data,pt_x9_data,pt_x10_data,pt_x11_data,pt_x12_data,pt_x13_data,pt_x14_d
ata)

  loss_physics=1000*mse_cost_function(physicsnet_out,pt_t_prime)

# forming total loss which is loss of predictive model + loss of physics discovery model
  loss=loss_data+loss_physics

  loss.backward()
  optimizer.step()

# recording loss values at each learning iteration
  with torch.autograd.no_grad():
      if epoch%50==0:
        print(epoch,"Total Training Loss:",loss.data)
        total_loss1.append(loss.item())
        data_loss1.append(loss_data.item())
        physics_loss1.append(loss_physics.item())
```

 # Feature importance measurement

```
# using SHAP library for feature importance measurement
import shap
from torch.autograd import Variable
# removing unnecessary columns in the data
data = df_phydis_test_scaled_smooth_RUL.drop(['unit number','cycle','RUL','est. RUL'],
axis=1).values
# converting data to tensor
data_tensor = torch.tensor(data, dtype=torch.float32)
e = shap.DeepExplainer(target_model, Variable( data_tensor ) )
shap_values = e.shap_values( Variable( data_tensor ) )
shap.summary_plot(shap_values, data, df_phydis_train_scaled_smooth_RUL.drop(['unit
number','cycle','RUL','est. RUL'], axis=1).columns)
```

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