Digital Twin for Risk and Uncertainty Analysis in Complex Industrial Control and Automation Systems Using Artificial Intelligence and Machine Learning

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Submitted in total fulfilment of the requirement for

Masters of Engineering Science (Research)

Federation University Australia

July 2023

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Abstract

Industrial control systems play a crucial role in enabling advanced manufacturing operations. However, these systems are inherently susceptible to failure. Detecting faults at an early stage is of paramount importance, as it can prevent the occurrence of fatal and catastrophic consequences resulting from equipment failures. Moreover, timely detection and resolution of faults can save significant costs and time for organizations. The failure of these systems not only poses risks to operators but can also lead to substantial delays in the advanced manufacturing process, imposing substantial financial burdens on organizations.

Therefore, a methodology is needed that can be used to avoid the adverse effects of equipment failure of industrial control systems to achieve smooth advanced manufacturing operations. To achieve this, the methodology should be able to detect the abnormal behaviour of the system at very early stages for predictive maintenance. This methodology can be designed using an extremely popular concept known as the Digital Twin, which has gained significant importance in the era of Industry 4.0.

In this research, artificial intelligence techniques will be employed to develop a highly accurate and detailed digital twin model. This model will serve as a valuable tool for predictive maintenance in complex industrial control systems, facilitating the achievement of smooth and uninterrupted advanced manufacturing processes. Also, the performance of the proposed Digital Twin model will be compared with state-of-the-art anomaly detection approaches.

The digital twin, utilizing the proposed algorithms, will not only be able to detect anomalies but also quantify their severity, classifying them into different levels such as minor, severe, and faulty operations. Furthermore, the research addresses the generalization challenges faced by state-of-the-art approaches, showcasing the digital twin's ability to effectively classify unseen data as healthy or anomalous.

The results obtained from the analysis and comparison of state-of-the-art approaches with the proposed algorithms clearly demonstrate the methodology's capability to detect anomalies, quantify their level, and classify them accurately and effectively in real-world data. This validation underscores the robustness and reliability of the developed methodology, further solidifying its potential as a valuable tool for predictive maintenance in complex industrial control systems.

Acknowledgment

I am deeply grateful to my esteemed principal supervisor, Dr Gayan Kahandawa, and my assistant supervisors, Dr Linh and Dr Hasitha, for their invaluable guidance and unwavering support throughout this research project. Their expertise, dedication, and mentorship have been instrumental in shaping the success of this endeavour.

Dr Gayan, in particular, has been an exceptional mentor, providing unwavering support and guidance throughout the entirety of this research journey. His expertise, depth of knowledge, and dedication to the field have been instrumental in shaping the outcomes of this project. Dr Gayan's ability to challenge and motivate me to push the boundaries of my research has been invaluable, and his insightful feedback and constructive criticism have greatly enhanced the quality of my work.

Furthermore, I am deeply grateful for the genuine care and concern that Dr Gayan has shown towards my academic and personal well-being. His open-door policy, willingness to listen, and willingness to go above and beyond have created a supportive and nurturing environment in which I have thrived as a researcher. Dr Gayan's mentorship has not only enhanced my research skills but has also instilled in me a sense of confidence and resilience that will benefit me in my future endeavours.

I would also like to express my sincere gratitude to Dr Muftooh from Aston University, UK, who served as an external supervisor for this project. Dr Muftooh's invaluable contributions, guidance, and support have been instrumental in shaping the direction of my research and nurturing my passion for this project.

Additionally, I would like to extend my thanks to Dr Majid Hussain from Heriot-Watt University, UK, for his invaluable support and motivation throughout this research journey. Dr Hussain's unwavering belief in my abilities, coupled with his encouragement, has been instrumental in keeping me motivated during challenging times.

Declaration

I hereby declare that the project titled "Digital Twin for Risk and Uncertainty Analysis in Complex Industrial Control and Automation Systems Using Artificial Intelligence and Machine Learning" is my own work submitted for the completion of my Master' (Research) degree. All the information, data, and findings presented in this project are the result of my independent research efforts. I have appropriately acknowledged and cited all the sources and references used in this work. No part of this project has been previously submitted for any other academic qualification or degree. I take full responsibility for the authenticity and originality of this work.

Muhammad Ghulam Mustafa Siddiqui
Date: 10th July 2023

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Chapter 1 – Introduction

This chapter serves as an introduction to the research project, which focuses on the utilization of digital twin technology for predictive maintenance in industrial control systems. The chapter begins by exploring the significance of industrial control systems in the context of advanced manufacturing and Industry 4.0, highlighting their pivotal role in ensuring efficient and reliable operations. Following this, the potential risks associated with industrial control system failures and their catastrophic and detrimental effects are examined, emphasizing the criticality of implementing effective maintenance strategies. Subsequently, various maintenance strategies employed in the industry to mitigate the risks and ensure optimal performance are discussed, providing a foundation for the subsequent investigation. Additionally, the chapter delves into the concept of digital twins—a powerful technology enabling virtual representations of physical systems—and its potential applications in the realm of industrial control systems maintenance. Lastly, the research objectives guiding this study are presented, outlining the specific aims and areas of focus that address research gaps and contribute to the advancement of industrial control systems maintenance practices.

Industry 4.0, also known as the Fourth Industrial Revolution (IR 4.0), represents a paradigm shift in manufacturing, driven by the integration of digital technologies into industrial processes [1]. IR 4.0 refers to the integration of physical components (such as machinery, devices, and sensors) and cyber components (including advanced software) through networks. This integration is driven by technology categories specific to Industry 4.0, which are utilized for prediction, control, maintenance, and process integration in the manufacturing [2]. IR 4.0 places a strong emphasis on the digitalization of the manufacturing process, aiming to leverage technological advancements and digitization to enhance and transform industrial operations [3].

Industrial control system devices play a crucial role in promoting the digitalization of manufacturing in IR 4.0[4]. These systems, with their ability to enhance flexibility and productivity, serve as a fundamental component in advanced manufacturing processes, thereby maintaining their essential role in the industrial operations [5]. The industrial control systems employed encompass various devices such as programmable logic controllers and other control devices. These instrumental devices play a critical role in ensuring the seamless operation of manufacturing processes and finding extensive applications in assembly lines, production lines, and robotics. They are adept at minimizing the disparity between desired and measured outcomes, contributing to efficient and accurate manufacturing operations [6]. Also, automation systems are extensively employed across a range of industries such as smart manufacturing, smart homes, automobile, aerospace, robotics, and healthcare. Some of these industries, for example, healthcare is highly sensitive.

It is essential to acknowledge that while these systems bring numerous benefits, they are not immune to errors. Faults in the automation system used in sensitive industries can have severe consequences, including potentially fatal and catastrophic effects. These implications highlight the critical importance of ensuring the reliability and robustness of the system [7]. Academic experts and industry practitioners believe that in order to meet the future demand in the manufacturing process, automation systems should be improved [8]. Therefore, it is vital to have an approach that can be used to avoid failures of control and automation systems to avoid catastrophic effects.

Effective condition monitoring plays a pivotal role in ensuring seamless advanced manufacturing operations. Maintenance costs, which can account for a substantial portion ranging from 15% to 60% of total manufacturing expenses, underscore the importance of well-planned maintenance strategies [9]. Inefficient maintenance practices can result in a significant reduction of up to 20% in an organization's manufacturing capability [10]. Moreover, inadequate condition monitoring of equipment poses substantial risks to manufacturing workers, with more than 30% of reported fatalities in manufacturing environments linked to maintenance-related activities [11].

Fig. 2. Different maintenance approaches [Ref: MATLAB-https://au.mathworks.com/discovery/predictive-maintenance-matlab.html]

Conventional condition monitoring methods offer reactive and preventative maintenance approaches but come with their own limitations, including higher maintenance costs, increased downtime, and the need for larger spare parts inventory and assets as can be seen in Fig. 2. Predictive maintenance, on the other hand, overcomes these challenges by providing continuous predictions regarding asset failure, thus offering a more proactive and efficient maintenance approach. Predictive maintenance has gained significant importance within the context of IR 4.0. It involves the analysis of data to identify and detect anomalies within a system [12]. Anomaly detection pertains to the task of identifying patterns within data that deviate from the anticipated or normal behaviour [13]. By proactively identifying these irregularities, organizations can take timely action to prevent asset failure and optimize maintenance operations [12]. By detecting machine failures in advance, pre-emptive maintenance and repairs can be carried out more efficiently, leading to a reduction in production costs [14]. These anomalies can be timely detected by using the Digital Twin technology [13].

The concept, known as Digital Twin (DT) has also gained significant importance in the context of IR 4.0 due to the increasing significance of digitalization in the manufacturing process [15]. DT, as a digital replica of a physical system, effectively reflects the status and behaviour of the physical system within the cyber/digital domain [16]. The development of DT technology has generated substantial interest from industry and academia alike in recent years [17]. The growing trend across various industries is the adoption of DT, driven by the wave of digital transformation, as it proves instrumental not only during the phases of conceptualization, prototyping, testing, design, and optimization but also throughout the entire asset lifecycle [18]. DT surpasses traditional computer-based analysis and simulation by faithfully replicating the processes and dynamics of the physical domain within the virtual realm [19]. The adoption of DT technology by NASA has enabled the emulation of its flying vehicles' behaviour, leading to an unprecedented level of safety that would have been unattainable with conventional approaches[20]. The concept of DT has gained widespread acceptance across diverse industries, including manufacturing, aerospace, electric grids, healthcare, petroleum, and more[21]. As a powerful tool, DT holds immense potential in various industrial contexts, serving as a catalyst for prognostic analysis, health management [22], predictive maintenance [13] and other critical applications.

This research presents a comprehensive methodology for predictive maintenance in complex industrial control systems using Digital Twin (DT) technology. In the introduction, an overview of the significance and context of the study has been provided, highlighting the challenges and opportunities in the realm of predictive maintenance for industrial control systems. Building upon this foundation, Section 1.1 delves into the specific research objectives that guide this investigation. These research objectives have been formulated based on a thorough analysis of the existing literature, industry needs, and the potential impact of digital twin technology in the field of predictive maintenance. By aligning the research objectives with the identified gaps and the practical demands of the industry, this study aims to address the pressing issues and contribute valuable insights to the advancement of industrial control systems maintenance practices.

1.1 Research Objectives

The objectives of this research are to develop a robust predictive maintenance algorithm specifically tailored for industrial automation and control systems. The utilization of DT technology was proposed to enable early detection of anomalies, thereby preventing the potentially catastrophic consequences of equipment failure. However, it was recognized that the mere detection of anomalies is insufficient. Therefore, a methodology was also sought to quantify the severity of an anomaly, facilitating appropriate actions to be taken. For instance, in cases where minor anomalies are identified in system performance, repairs or maintenance services can be initiated to mitigate the risk of equipment failure. Conversely, a significant number of anomalies might indicate that a fault has already occurred, necessitating the replacement of the entire system.

However, the initial and fundamental step in this research was to thoroughly investigate and develop a methodology specifically designed for constructing a robust DT model of an industrial control system. This entailed addressing the challenges associated with modelling and understanding the internal workings of the system, which often lack transparency. By focusing on this crucial aspect, the aim was to establish a comprehensive and reliable framework for creating a DT model that accurately represents the behaviour and dynamics of the industrial control system.

The objectives of this research are detailed below.

Research Objective 1: Undertake a comprehensive investigation and devise an advanced methodology for constructing a highly robust and reliable DT model specifically tailored to the unique characteristics and complexities of an industrial control system.
This objective involves analysing existing approaches and techniques for DT modelling, addressing challenges related to limited access to internal algorithms and potential data limitations, and exploring advanced modelling techniques such as physics-based and data-

driven approaches. The ultimate goal is to establish a methodology that ensures an accurate and effective representation of the system in the DT for enhanced predictive maintenance capabilities.

Research Objective 2: Develop and implement a predictive maintenance algorithm utilizing DT technology for industrial automation and control systems. This algorithm will enable the early detection and identification of anomalies, facilitating timely interventions and maintenance actions to ensure the performance and reliability of the systems.
By analysing data from the DT, the algorithm will enable proactive identification of potential issues or deviations from normal behaviour, allowing for timely interventions and maintenance actions. The algorithm aims to optimize the maintenance strategy, minimize downtime, and enhance the overall performance and reliability of the industrial automation and control systems.

Research Objective 3: Examine and validate the proposed methodology in Research Objective 2 to quantify anomaly severity and enhance false positive mitigation in industrial automation and control systems.
To thoroughly examine and validate the proposed methodology outlined in Research Objective 2, focusing on its ability not only to detect anomalies but also to quantify the severity of anomalies and effectively address the challenge of false positive mitigation within industrial automation and control systems. This examination aims to ensure the robustness and reliability of the methodology in providing comprehensive anomaly detection, severity assessment, and false positive mitigation capabilities.

Research Objective 4: Investigate state-of-the-art machine learning, deep learning, and statistical approaches to assess their ability to detect anomalies in unseen data patterns, distinct from the data on which these approaches were trained and evaluate their performance in terms of mitigating false positives.

This objective aims to explore state-of-the-art techniques in machine learning, deep learning, and statistical analysis to assess their capability to mitigate false positives in anomaly detection algorithms. The objective involves a comprehensive examination of advanced architectures, novel algorithms, and established methodologies, all aimed at improving the algorithms' capacity to mitigate false positives and accurately differentiate between healthy and faulty operations under various operating conditions.

The research objectives defined earlier establish a clear focus on leveraging digital twin technology for predictive maintenance in industrial control systems. To accomplish these objectives, it is imperative to examine the existing body of literature in this domain. The subsequent chapter will further explore the existing literature, providing a comprehensive theoretical framework to support and inform the achievement of these research objectives.

The remainder of the thesis structure is as follows. Chapter 2 provides a detailed exploration of the methods employed in the industry for both digital twin implementation and predictive maintenance. It examines the current practices, techniques, and challenges associated with these areas, offering a comprehensive overview of the existing landscape. In Chapter 3, state-of-the-Art anomaly detection approaches are used to detect anomalies in real-time sensor data. Chapter 4 introduces the methodology for developing a robust DT model and predictive maintenance algorithm, leveraging Artificial Intelligence techniques. The effectiveness of the proposed methodology is then validated through a detailed case study in Chapter 5, which involves the application of the methodology on a real industrial control system. Chapter 6 presents the results and discussions derived from the case study, providing insights into the performance and capabilities of the methodology. Finally, Chapter 7 offers a conclusion summarizing the key findings, contributions, and implications of the study. Future directions are discussed in Chapter 8.

Chapter 2: Literature Review

The literature review presented in this chapter offers a broad exploration of the current state of research and practices in the field of digital twin technology for predictive maintenance in control systems. The review encompasses several crucial areas of investigation, including the challenges, research gaps, and related work associated with digital twin implementation. Additionally, it delves into various modelling approaches utilized in digital twin development, with a specific focus on pattern recognition state-of-the-art approaches. Furthermore, the review encompasses an analysis of maintenance strategies employed in industry settings to address maintenance-related challenges. By synthesizing the wealth of existing knowledge, this literature review serves as a foundation for identifying areas where further research is warranted. Finally, in alignment with the review findings, the chapter concludes with a presentation of the research questions that will guide the subsequent investigation.

2.1 Related Work, Challenges and Contribution

Creating a high-fidelity DT model of a physical system within a cyber-domain can present challenges [23]. However, robust DT modelling can be achieved through the application of physics-based and data-driven approaches. The physics-based approach, widely employed by the engineering community across various industries, is the predominant method for DT modelling [24]. Software tools such as MATLAB, ADAMS, and COMSOL are commonly utilized for physics-based approaches [25]. It is important to have enough reliable data for the effective implementation of the physics-based approach, as corrupt data can lead to the underperformance of the DT model [17].

2.1.1: Digital Twin for Industrial Control System (ICBBS)

While researchers have extensively explored the concept of digital twins for multiple control applications, it is noteworthy that the predominant emphasis has been on a physics-based approach. For instance, in [25], a comprehensive architecture for feedback infrared temperature uniformity control was proposed, while [26] presented a DT framework for distributed control systems. [27] discussed the analytical design of optimal fractional order PID control for industrial robots based on DT. Additionally, [28] introduced a self-optimizing control approach that combines DT, intelligence, and derivative-free optimization. The virtual modelling of physical systems within the cyber domain has been accomplished using software tools like MATLAB, Unity 3D, and others in these studies. However, employing a traditional physics-based approach for virtual modelling of industrial control systems used in advanced manufacturing poses significant challenges, as the internal algorithms may be unknown, and data sets may be unavailable, rendering these systems as black boxes.

A 'black box' refers to a system or device whose internal workings and processes are not readily accessible or understood. Instead, the system's behaviour and functionality are assessed solely by examining the inputs it receives and the outputs it generates. In essence, it operates as an opaque entity where the inner mechanisms, algorithms, and processes remain concealed. For example, an industrial control system in a manufacturing facility. This system may regulate various processes, such as temperature control, production line speed, or material handling. While the system's inputs, such as sensor data, control signals, and operator commands, are well-documented, the intricate details of how these inputs are processed and translated into actions are not visible or easily decipherable. Therefore, a 'black box' system is characterized by the necessity to infer its behaviour solely from the observable inputs and outputs, without access to the underlying internal processes. This concept is essential in scenarios where understanding the inner workings of the system is not the primary focus, but rather assessing its performance and functionality in practical applications.

In this work, black-box systems applied to industrial control are referred to as Industrial Control Black Box System (ICBBS). These ICBBS represent a unique and critical component within industrial control systems due to their inherent complexity. While there are existing black box systems based on machine learning in research, this study has identified a notable gap in the development of a framework specifically for constructing a DT model of the ICBBS. For example, in [29], a DT architecture was presented for a power electronic converter, treating the simulation model as a black box. However, this research relied on simulation data for validation and focused on a different application domain than industrial control systems. Consequently, formulating a comprehensive and systematic methodology for constructing a digital twin model of an ICBBS that addresses the specific requirements of industrial control systems remains a challenging task.

2.1.2 Digital Twin Based Anomaly Detection

In [30], the authors introduce an innovative approach termed 'end-to-end anomaly detection' designed to identify real-time anomalies using Digital Twin (DT) technology. This method relies on attention mechanisms and multidimensional deconvolutional networks to discern crucial features during the anomaly detection process. Nevertheless, it's worth noting that the study lacks an in-depth exploration of the specific hardware configurations within the Industrial Control Systems (ICS) utilized for their case study. Such details hold significant importance in research since the complexity of the hardware environment can substantially impact the efficacy of the proposed methodology. Furthermore, the validation of the methodology's effectiveness appears to lack transparency regarding the data patterns used for evaluation.

In [13], researchers present an approach for detecting anomalies in real-world scenarios employing DT technology. This study introduces two distinct methodologies: a clustering-based method referred to as 'cluster centres' (CC) and a neural architecture based on the Siamese Autoencoder (SAE). To construct the Digital Twin, a physics-based approach was employed, integrating tools like the Greencity library and Simulation X for simulation purposes. However, it's essential to recognize that these approaches may face considerable challenges when applied to complex systems like Industrial Control Systems (ICS), where internal system details are often limited, resulting in 'black-box' characteristics. Additionally, the reliance on physics-based information necessitates an abundance of data sheets for the virtual modelling of the DT, which may not always be readily accessible for ICS within manufacturing environments.

2.1.3 Anomaly Detection Using Conventional Approaches

In the study conducted by [31], the authors introduced the fault-attention generative probabilistic adversarial autoencoder (FGPAA) approach for anomaly detection. FGPAA is designed to automatically identify low-dimensional structures within high-dimensional signal data, effectively reducing information loss during feature extraction. Additionally, in the research outlined in [32], a hybrid Nonlinear Multimode Framework was employed. This strategy combines techniques such as the Dirichlet process Gaussian mixed model (DPGMM) for mode classification and support vector data description (SVDD) to construct monitoring statistics for fault detection without prior knowledge. In [33] , the proposed Optimal Window-Symbolic Time Series Analysis (OW-STSA) methodology aims to optimize feature extraction and pattern classification in industrial processes. The focus is on distinguishing between normal and anomalous operations by segmenting time series into optimized windows, computing stationary state probability vectors for anomaly prediction, and determining locally optimal accuracy for detection. Subsequently, [34] introduced the one-class support Tucker machine (OCSTuM) and the OCSTuM based on tensor tucker factorization and a genetic algorithm (GA-OCSTuM). These novel methods were developed for unsupervised anomaly detection in large-scale Internet of Things (IoT) sensor data. Leveraging tensor representations, these approaches retain structural information within the data, leading to improved accuracy and efficiency in outlier detection compared to traditional vector-based methods. Furthermore, in [35], the authors presented the smoothness-inducing sequential variational auto-encoder (SISVAE) model, designed for robust estimation and anomaly detection in multidimensional time series. This model utilizes flexible neural networks to capture temporal structures and applies a smoothness-inducing prior.

However, it's important to note a common limitation in these approaches, including Variational Autoencoders (VAE) and Generative Adversarial Networks (GAN). They often exhibit suboptimal decision criteria as their primary objective functions are designed for tasks other than anomaly detection, such as generic summarization, data synthesis, or sequence prediction [36].

Finally, [37] proposes an integrated deep generative model known as AMBi-GAN for industrial time-series anomaly detection. This approach utilizes bidirectional LSTM networks with an attention mechanism to capture time-series dependencies and features. However, based on the information available in the paper, it remains unclear whether the data used in the study is specifically derived from an industrial system. The paper mentions three datasets, including Yahoo, social media time-series plus (SMTP), and an activity recognition system based on multi-sensor data fusion (AReM). While the AReM dataset appears to involve sensor data related to various human activities, such as standing, sitting, bending, cycling, etc., there is no explicit mention of industrial system data. Therefore, the effectiveness of this approach on real-time industrial time-series data, especially data with noise, remains uncertain.

It is clear from the existing review that the proposed approaches have limitations. Therefore, a novel approach is needed that can be used to not only detect anomalies but it can also quantify the level of anomalies and mitigate false positives for the smooth operation and condition monitoring of industrial control systems.

2.2: Data-Driven Model

After extensive research and investigation, it has been determined that artificial neural networks (ANNs), drawing inspiration from the biological neural network in the human brain, offer a promising data-driven approach. ANNs have emerged as a powerful tool for modelling black box systems due to their ability to learn intricate relationships between inputs and outputs, capture non-linear dependencies, and exhibit robustness to noise. As a result, ANNs have gained significant traction in the industry for addressing pattern recognition challenges [38].

2.2.1 ANN

ANNs have become increasingly appealing, effective, efficient, and successful in achieving pattern recognition (PR) in numerous problem domains[39]. Unlike conventional pattern approaches, artificial neural networks (ANNs) have the inherent capability to effectively model complex or multi-complex tasks with relative ease [40]. The preceding conventional methodologies employed for addressing PR issues can be categorized into structural, statistical, and hybrid methodologies[38]. However, both the statistical and structural approaches may not provide satisfactory results when applied as solutions to complex PR problems alone. For example, the structural method may be weak in handling noise patterns and ineffective in addressing challenges related to the numerical semantic information [38]. Similarly, the statistical method lacks the capability to utilize information pertaining to pattern structures. Consequently, the integration of both approaches has garnered research interest, leading to the development of a hybrid approach. However, in contemporary times, Artificial Neural Network (ANN) models are increasingly employed due to their ability to yield superior outcomes in PR problems, including those involving multiple complex tasks [38].

2.2.2ANN Pattern Recognition

A pattern can be defined as a collection of items, objects, images, events, cases, situations, features, or abstractions in which elements within the set share common characteristics in a distinct manner. Whereas Norbert Wiener provided a definition of a pattern as an arrangement based on the sequence of its constituent features, Watanabe offered an alternate perspective by defining a pattern as "an entity" [41]. ANNs in pattern recognition (PR) leverage insights from human brain processing. They are well-suited for identifying patterns and employ large networks of nonlinear and straightforward units known as neural nets. PR tasks are accomplished using feedforward networks (FFNNs) that process data in a forward direction [42, 43].

2.2.3 Types of ANN

There are various types of ANNs. Among them, the two major networks are Convolutional Neural Networks(CNNs), Feedforward Neural Networks and Recurrent Neural Networks [RNNs] [44]. CNNs are a specialized type of neural network architecture designed to effectively process and analyse visual data, making them highly suitable for tasks such as image classification, and image recognition [45]. A feedforward neural network is a type of artificial neural network where information flows in a single direction, from the input layer to the output layer. It consists of multiple layers of interconnected nodes, or neurons, where each neuron in a given layer is connected to every neuron in the subsequent layer [46]. For regression, RNNs are highly efficient [47].

2.2.3.1 Recurrent Neural Network (RNN)

Most of the sensor data are in time series. RNN-based models have shown significant progress in various time series forecasting tasks, which are essential in industrial and business decision processes [48]. Also, the majority of the real-world systems utilized in industry exhibit dynamic characteristics [49].

It is important to note that to model the dynamic behaviour of the physical system in the virtual world, the neural network should also be dynamic in the nature [29]. One suitable option for modelling dynamic systems is a recurrent neural network (RNN) [50]. RNNs are particularly well-suited for sequential and time series data [49] and have demonstrated state-of-the-art performance in these domains [51].

The NARX (nonlinear autoregressive network with exogenous inputs) is a type of recurrent dynamic network that incorporates feedback connections and multiple layers. This neural network, known as NARX, is well-suited for forecasting nonlinear time series data [52, 53].

Unlike feedforward neural networks (FNN), NARX incorporates internal states and can perform backpropagation, enabling them to effectively model dynamic systems. In contrast, FNNs lack the backpropagation option and can only predict output based on the present input value, making them unsuitable for dynamic system modelling [29].

2.2.3.2 NARX Basics

The NARX model, as a discrete-time nonlinear system, can be represented mathematically as [54]:

$$y(n + 1) = f[y(n); u(n)] \quad (1)$$

In this representation, y(n) and u(n) denote the output and input regressors, respectively. The mapping function f(·) is typically unknown and requires approximation.

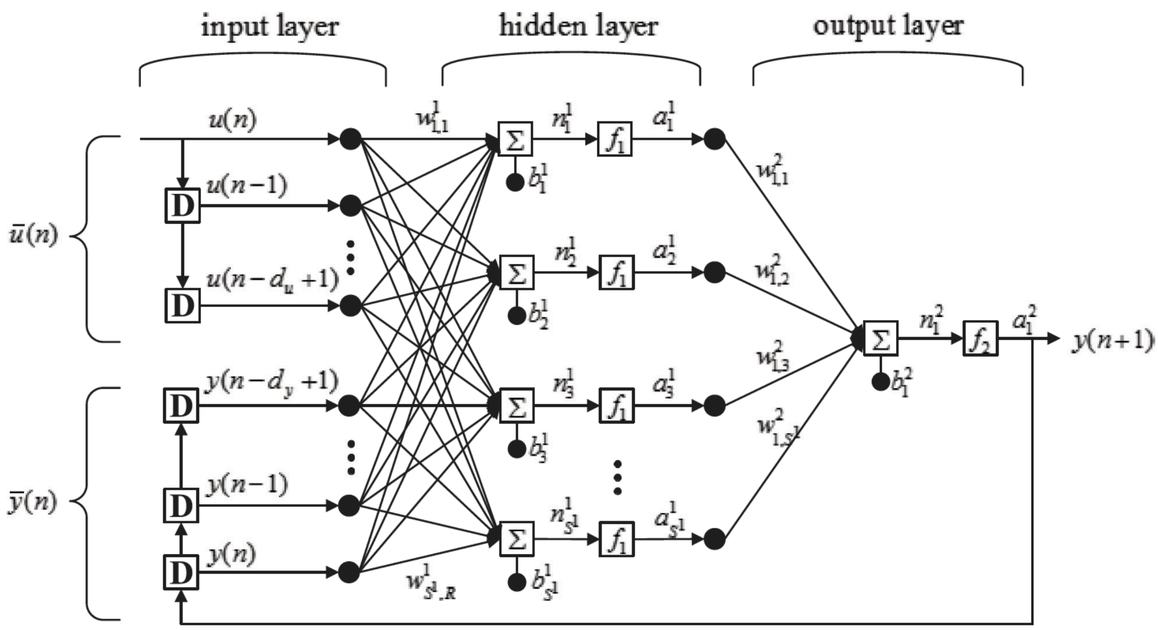

Fig. 3. illustrates the configuration of a NARX [54]

The meanings of the symbols used in Fig. 3 can be found in Table 1.

Table 1: Symbols [53]

Symbol	Quantity
$w_{i,j}^{1}$	Connection weight between the ith neuron in input layer and the jth Neuron j in hidden layer
$w_{1,i}^{2}$	Connection weight between the ith neuron in hidden layer and the output neuron
b_i^{1}	Bias weight of the ith neuron in the hidden layer
b_1^{2}	Bias weight of the output neuron
n_i^{1}	Input value for the ith neuron in the hidden layer
n_1^{2}	Input value for the output layer
$f_1(.)$	Activation function of hidden layer
$f_2(.)$	Activation function of output layer
a_i^{1}	Output value of the ith neuron in the hidden layer
a_1^{2}	Output of network
d_u	The input-memory orders
d_y	The output-memory orders

Fig. 4 displays the two training modes available for a NARX neural network.

1. Parallel (P) mode: In this mode, the estimated outputs are fed back and incorporated into the regressor of the output. The equation for estimating the next output value is represented as [54]

$$\hat{y}(n+1) = \hat{f}[\hat{y}(n), \ldots, \hat{y}(n-dy+1); u(n), u(n-1), \ldots, u(n-du+1)]$$

Here, the hat symbol (ˆ) signifies estimated values or functions.

2. Series-parallel (SP) mode: In this mode, the regressor for the output is constructed solely using the actual values of the system's output. The equation for estimating the next output value is represented as [54]

$$\hat{y}(n+1) = \hat{f}[y(n), \ldots, y(n-dy+1); u(n), u(n-1), \ldots, u(n-du+1)]$$

Here, the hat symbol (ˆ) denotes estimated values or functions.

Both structures can be utilized for network training, depending on the availability of data. The appropriate structure should be selected based on the data characteristics. For example, if the actual system output is obtainable for training, the series-parallel architecture is preferred. This architecture incorporates the real output data instead of the estimated output from the NARX [55]. Utilizing actual data enhances the accuracy of input data during training, leading to improved network performance [55].

Following the identification and training of the suitable neural network for the Digital Twin (DT) model, the subsequent task involves exploring and determining the appropriate maintenance strategy for efficient condition monitoring. This crucial step aims to select the optimal approach that allows the DT model to effectively monitor the system's condition. By choosing the right maintenance strategy, the DT model can proactively detect and address potential issues, leading to enhanced operational efficiency and minimized downtime.

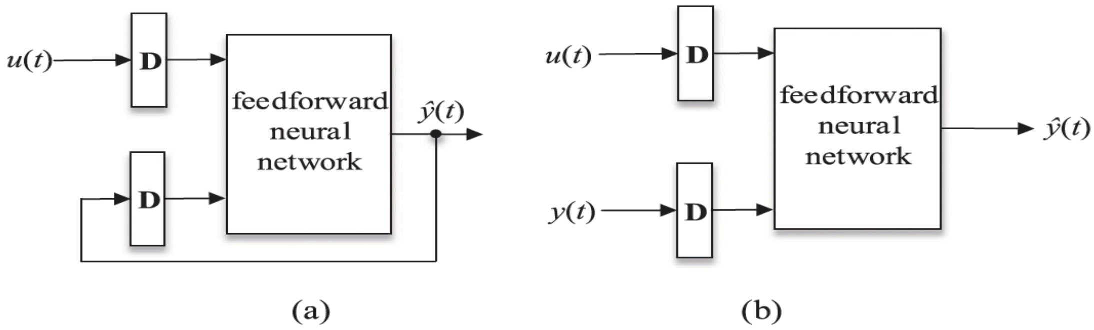

Fig. 4. NARX architectures [54]

2.3 Maintenance Evolution

There are multiple maintenance methods available, each with its own trade-off between complexity and costs. Below are the three most important maintenance methods used within the industry, including:

1. Reactive maintenance: This method involves performing maintenance activities only when a component breaks down. It is commonly employed for components with low cost and minimal risk of hazardous situations. Reactive maintenance can lead to unscheduled machine downtime and is considered the most expensive maintenance approach. It also carries a high risk of catastrophic failures affecting the entire machine [56].

2. Preventive maintenance: Preventive maintenance involves conducting maintenance activities at predetermined intervals. In this approach, the expected lifetime of each component is assessed, and maintenance is performed before the component is likely to fail. Preventive maintenance enables businesses to schedule maintenance activities and minimize machine downtime. However, this method can result in the underutilization of components [56], as there is a tendency to over-maintain machines for safety and service maintenance, which can be costly [57].

3. Predictive Maintenance: Predictive maintenance (PM) is a novel approach in the manufacturing industry that focuses on detecting signs of machine degradation before failures happen. It plays a significant role in the vision of Industry 4.0 and smart manufacturing. By utilizing sensor readings, process parameters, and operational characteristics, PM aims to optimize tool lifespan by minimizing unnecessary repairs and decreasing the occurrence of unexpected failures. Detecting machine failures in advance can lead to more efficient maintenance and repairs, resulting in reduced production costs[14]. Predictive maintenance involves detecting early anomalies or deviations in the system's behaviour or performance to prevent asset failure. By monitoring and analysing various data sources such as sensor readings, equipment parameters, and operational patterns, predictive maintenance aims to identify potential issues and take proactive measures before they lead to the system or asset

failure[13]. Identifying abnormal behaviours in data centres is vital for the purposes of predictive maintenance and safeguarding data integrity [58].

2.3.1 Anomaly Detection

The anomaly detection [59] involves identifying patterns in data that deviate from expected or normal behaviour. It is a highly researched field with diverse applications, including the energy [60], manufacturing [61], network sensors [62], health care, and video surveillance [63]. The goal is to detect and flag instances that differ significantly from the norm, allowing for early identification of potential issues or threats.

Anomaly detection techniques that rely on machine learning can be categorized into various approaches. These approaches include:

1. Supervised Approaches: These methods require a sufficiently large set of training samples with labelled data. The training data consists of both normal and anomalous instances, allowing the model to learn the patterns and characteristics of anomalies [64].

2. Unsupervised Approaches: In this type of approach, only unlabelled measurement data is available. The model learns the normal behaviour from the data and then identifies instances that deviate significantly from this learned behaviour as anomalies. Unsupervised approaches do not rely on predefined anomaly labels [64].

3. Weakly Supervised Approaches: This approach utilizes a large amount of unlabelled data along with a very small set of labelled data. The labelled data serves as weak supervision to guide the learning process. The model can leverage the small, labelled dataset to learn the characteristics of anomalies and generalize this knowledge to detect anomalies in the larger unlabelled dataset [64].

Each approach has its own strengths and limitations, and the choice of the most suitable approach depends on the availability of labelled data, the specific requirements of the application, and the desired trade-off between detection accuracy and resource requirements [13].

After an in-depth review of the relevant literature, a set of challenging questions has arisen, posing significant hurdles for the development and implementation of the digital twin model and predictive maintenance in control systems. These questions highlight the complexities and intricacies involved in integrating digital twin technology and predictive maintenance techniques within control systems. By addressing these questions head-on, this research aims to overcome these hurdles, explore effective solutions, and pave the way for the successful deployment of digital twin models and predictive maintenance strategies in control systems. The ultimate goal is to enhance the performance of control systems, enabling them to effectively facilitate advanced manufacturing processes while mitigating the potentially catastrophic and fatal consequences of system failures.

2.4 Research Questions

After an extensive review of the relevant literature, this research will address the following questions:

Research question 1: What approach can be employed to develop a robust Digital Twin for an industrial control black box system?
This question aims to identify and outline a suitable methodology that ensures the creation of a reliable and accurate Digital Twin model for such systems.

Research question 2: What methodology should be adopted to develop a Predictive Maintenance algorithm specifically tailored for control and automation systems?
This question focuses on exploring and defining the appropriate steps and techniques necessary to design an effective Predictive Maintenance algorithm catering to the unique requirements of control and automation systems.

Research question 3: How can the level of anomalies be quantified within the context of control and automation systems?
This question seeks to develop a quantifiable measure or metric that can accurately assess and evaluate the severity or magnitude of anomalies occurring within these systems.

Research question 4: How can the generalization capability of anomaly detection algorithms be enhanced to accurately classify and detect anomalies in unseen data patterns in control and automation systems?
This question aims to explore techniques and approaches that improve the generalization capability of anomaly detection algorithms, enabling them to effectively differentiate between unseen healthy and faulty operations in diverse operating conditions.

Addressing these research questions will contribute to a better understanding of the methodology for developing a robust Digital Twin, the methodologies used in developing Predictive Maintenance algorithms for control and automation systems, and the quantification of anomalies within these systems.

In this chapter, a comprehensive review of the existing literature on digital twin technology for predictive maintenance in control systems has been presented. The review has shed light on the challenges, research gaps, related work, digital twin modelling approaches, pattern recognition techniques, and maintenance strategies employed in the industry. Drawing upon the insights gained from the literature review, the chapter concludes with the presentation of the research questions that will drive the subsequent phase of this study. To address and answer these research questions, the next chapter, titled 'State-of-the-Art Anomaly Detection Approaches,' will explore the latest advancements in anomaly detection techniques. Specifically, state-of-the-art approaches will be applied to real-time sensor data, providing practical insights into their effectiveness and applicability in the context of industrial control systems.

Chapter 3: State-of-the-Art Anomaly Detection Approaches

This chapter focuses on evaluating the performance of state-of-the-art anomaly detection approaches within an industrial control system using real system data recorded during this research. The objective is to assess their effectiveness in detecting anomalies, quantifying their severity, and distinguishing between healthy and faulty operations. The results presented in the tables and analysis are based solely on the data collected and analysed during this research effort, ensuring the relevance and applicability of the findings.

The evaluated state-of-the-art anomaly detection approaches encompass machine learning algorithms such as Local Outlier Factor, One-Class Support Vector Machine, Isolation Forest, and Robust Random Cut Forest. Additionally, a deep learning approach utilizing an Autoencoder and a statistical approach employing the Mahalanobis Distance were also evaluated. The real-time sensor data used in this study were exclusively recorded from the industrial control system during this research. The recorded data were used to train the state-of-the-art models and the effectiveness of the trained models were validated against the dataset encompasses instances representing healthy conditions, minor anomalies, severe anomalies, and system faults.

By conducting the evaluation of the data recorded specifically for this research, any confusion or potential overlap with other datasets or experiments is eliminated, ensuring the integrity and validity of the results obtained.

3.1. Anomaly Detection

To compare the performance of the different approaches, several tables were created. Table 2 presents a ranking of the approaches based on their effectiveness in detecting minor anomalies, severe anomalies, and system faults. These rankings were derived using data patterns identical to those used for training the algorithms.

Table 2. Anomaly Detection

Training Method	**Algorithms**	**Minor (1)**	**Severe (1)**	**Faulty (1)**	**Total (3)**
Machine Learning	*Local Outlier Factor*	✓	✓	✓	**3**
	One Class Support Vector Machine	✓	✓	✓	**3**
	Isolation Forest	✗	✗	✓	**1**
	Robust Random Cut Forest	✗	✗	✗	**-**
Deep Learning	*Autoencoder*	✓	✓	✓	**3**

Statistical Approach	*Mahalanobis Distance*	✓	✓	✓	**3**

3.2. Anomaly Severity Quantification

Table 3 showcases the effectiveness of the approaches in quantifying the severity of anomalies. The severity quantification is crucial in enabling industries to make informed decisions based on the observed anomaly severity. For minor anomalies, all evaluated approaches accurately quantify the severity, indicating the presence of noise or minor deviations from normal operation. However, in cases where the number of observed anomalies is significantly high, the approaches accurately capture the severity, signalling large-scale disruptions or system malfunctions. This feature allows decision-makers to prioritize actions based on the level of risk associated with the observed anomalies.

Table 3. Anomaly Severity Quantification

Training Method	**Algorithms**	**Minor (1)**	**Severe (1)**	**Faulty (1)**	**Total (Out of 3)**
Machine Learning	*Local Outlier Factor*	✓	✓	✓	**3**
	One Class Support Vector Machine	✓	✓	✓	**3**
	Isolation Forest	✗	✗	✓	**1**
	Robust Random Cut Forest	✗	✗	✗	**-**
Deep Learning	*Autoencoder*	✓	✓	✓	**3**
Statistical Approach	*Mahalanobis Distance*	✓	✓	✓	**3**

3.3. Detected Anomaly Location in Data

Table 4 illustrates how effectively the approaches detect anomaly points and their respective locations within the data. This information is valuable as it provides insights into the nature and specific locations of anomalies. For example, if anomalies are observed only during the high-speed operation of a rotating shaft, it may suggest specific issues related to that particular condition.

The total score was calculated by addition of the % of minor, severe and faulty data. For example Local outlier factor detected 90% (0.9) for minor, 76.19% (0.76) for severe and 68.12% (0.68) for faulty which gave it a total score of 2.34 (0.90+0.76+0.68= 2.34).

Table 4. Detected Anomaly Points and Location

Training Method	**Algorithms**	**Minor (11s)**	**Severe (21s)**	**Faulty (66s)**	**Total (Out of3)**
Machine Learning	*Local Outlier Factor*	10s (90%)	16s (76.19%)	45s (68.18%)	**2.34**
	One Class Support Vector Machine	2s (18%)	3s (14.28%)	33s (50%)	**0.82**
	Isolation Forest	-	-	9s (13.63%)	**0.13**
	Robust Random Cut Forest	-	-	-	-
Deep Learning	*Autoencoder*	-	-	-	-
Statistical Approach	*Mahalanobis Distance*	10s (90%)	16s (76.19%)	52s (78.78%)	**2.44**

3.4. Performance Comparison

Table 5 presents the overall scores and rankings given to the approaches, providing a comprehensive assessment of their performance. The scores are based on a combination of detection accuracy, severity quantification, and anomaly point identification.

Table 5. Results

Training Method	**Algorithm**	**Anomaly Detection (3)**	**Quantification (3)**	**Point Identification (3)**	**Total (Out of 9)**
Machine Learning	*Local Outlier Factor*	3	3	2.34	8.34
	One Class Support Vector Machine	3	3	0.82	6.82
	Isolation Forest	1	1	0.13	2.13
	Robust Random Cut Forest	-	-	-	0
Deep Learning	*Autoencoder*	3	3	-	6

Statistical Approach	*Mahalanobis Distance*	3	3	2.44	**8.44**

3.5. Challenges and Limitations with Generalization

False positive mitigation plays a crucial role in anomaly detection as it refers to the ability of an algorithm to reduce false alarms and accurately classify anomalies in unseen data patterns. In other words, a false positive mitigation approach should not only work well on the data it was trained on but also on new, previously unseen data. Achieving strong false positive mitigation is vital for real-world applications where industrial systems encounter different operating conditions and exhibit diverse patterns over time. Anomaly detection algorithms with robust false positive mitigation capabilities can adapt to novel scenarios and minimize the occurrence of false alarms, even when faced with data patterns that differ from the training set.

However, Table 6 reveals a significant limitation of the evaluated approaches. They struggled to differentiate between unseen healthy and faulty operations. Even when provided with unseen healthy input, all evaluated approaches misclassified it as severe anomalies in the system. This indicates that the approaches are limited to working only on seen data, posing a challenge as industrial systems encounter different tasks daily with varying outputs.

Table 6. Unseen Healthy Data Pattern vs Anomaly Classification

Training Method	**Algorithms**	**Healthy**	**Minor**	**Severe**	**Faulty**
Machine Learning	*Local Outlier Factor*				✓
	One Class Support Vector Machine			✓	
	Isolation Forest			✓	
	Robust Random Cut Forest	-	-	-	-
Deep Learning	*Autoencoder*				✓
Statistical Approach	*Mahalanobis Distance*				✓

This chapter concludes that while the evaluated state-of-the-art anomaly detection approaches demonstrated effectiveness in detecting anomalies, quantifying their severity, and identifying anomaly points, they encountered difficulties in distinguishing between unseen healthy and faulty operations. The statistical approach utilizing Mahalanobis Distance exhibited remarkable performance, outclassing other machine learning and deep learning approaches. However, challenges remain in effectively addressing the false positive issue.

Future research and advancements are necessary to develop approaches that can robustly detect and classify anomalies in unseen data patterns, enabling proactive maintenance and improved decision-making in industrial control systems.

Chapter 6 offers a comprehensive explanation of the testing methodology employed, along with a detailed breakdown of the scores provided in tables 2, 3, 4, 5, and 6. That chapter is a valuable resource for readers seeking in-depth information on the evaluation process.

The next Chapter presents a methodology that not only addresses the limitations of black box system digital twin modelling but also introduces an algorithm capable of detecting anomalies, quantifying their levels, and effectively classifying between healthy and anomaly data in industrial control systems. This methodology aims to provide a comprehensive solution by combining insights from data-driven modelling, anomaly detection, severity quantification, and false positive mitigation.

Chapter 4: Methodology

In response to the research questions outlined in Chapter 2, and the limitations identified in Chapter 3, Chapter 4 delves into the development of two innovative algorithms that address the challenges identified in the literature review. The first algorithm leverages the power of artificial neural networks to construct a high-fidelity digital twin model for control systems. By employing advanced modelling techniques based on artificial neural networks, this algorithm aims to accurately capture the complex dynamics and behaviour of control systems. Building upon the outcomes of the first algorithm, the second algorithm presents a comprehensive methodology for predictive maintenance, utilizing the insights derived from the developed digital twin model. These innovative and novel algorithms represent a significant contribution to the field of industrial control and automation by providing practical solutions to the identified challenges.

4.1: Algorithm 1: Digital Twin of ICBBS (Research Question 1)

For a robust and high-fidelity deep learning model of an Industrial Control Black Box System (ICBBS), the five-step framework (Fig. 5) is proposed in this research that includes system identification, data collection, network architecture, ANN training, validation and testing, and digital twin deployment. The utilization of artificial neural networks (ANNs) has been selected as a machine learning approach to effectively acquire patterns and predict the behaviour of industrial control systems operating as black box systems. ANNs are a potent tool for modelling black box systems due to their capability to comprehend complex relationships between input and output variables, capture non-linear associations, and exhibit noise tolerance. Consequently, ANNs have gained widespread acceptance and have been extensively adopted in the industry to address challenges related to pattern recognition. Aligned with this notion, the current study harnesses the power of ANNs to uncover intricate patterns and forecast the complex behaviour of ICBBS.

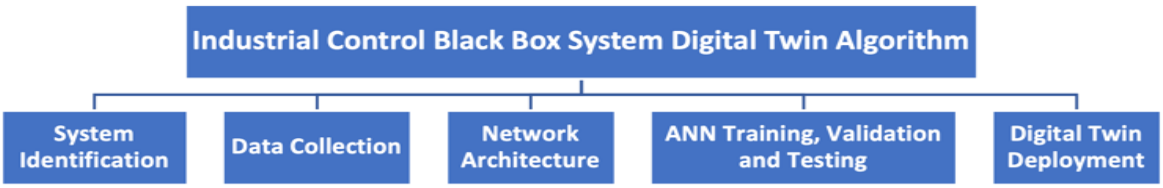

Fig. 5. ICBBS DT Algorithm

4.1.1. System Identification

The accurate selection of a suitable neural network for a system is contingent upon a thorough understanding of the system's inherent characteristics. This understanding involves precisely identifying whether the system exhibits linearity or nonlinearity and whether it possesses static or dynamic properties. Two valuable principles, the Law of Additivity and the Law of Homogeneity, aid in discerning the system's nature [65]. The Law of Additivity states that the system's response to a combination of inputs is equivalent to the sum of its responses to each individual input. Meanwhile, the Law of Homogeneity dictates that scaling the input will result in a proportional scaling of the output response. These principles are applied by utilizing input and output data obtained directly from the system.

To effectively employ these principles, it is essential to have access to an adequate amount of input and output data from the system. The availability of such data sets becomes imperative for facilitating the training, validation, and testing procedures of the neural network. A sufficient volume of training data enables the network to learn and adapt to the system's characteristics, resulting in more accurate predictions and improved performance. Therefore, the precise identification of the system's inherent characteristics, supported by the Law of Additivity and the Law of Homogeneity, along with the availability of ample training data, are crucial factors in the accurate selection and successful training of an appropriate neural network for the system.

The application of the Laws of Homogeneity and Additivity to the recorded data in the experiment is thoroughly explained in Chapter 5, specifically in Section 5.1.1.

4.1.2. Data Collection

Prior to initiating data recording, it is vital to emphasize the significance of ensuring the system's reliability. This precautionary measure is crucial as the utilization of flawed or unreliable data during the training phase can severely impact the accuracy of predictions generated by the network. Consequently, these inaccuracies can render the predictive maintenance algorithm unsuitable for facilitating effective decision-making processes.

To address this concern, it is highly recommended to undertake a comprehensive examination of relevant documents associated with maintenance, troubleshooting, and service records. This examination serves to obtain a holistic understanding of the system's present condition and performance. By meticulously reviewing these documents, valuable insights can be gained regarding the system's historical behaviour, past maintenance practices, identified issues, and overall operational health.

The insights derived from this thorough examination of documents significantly contribute to the overall reliability and accuracy of the predictive maintenance algorithm. This, in turn, enhances its efficacy in providing reliable predictions and facilitating informed decision-making processes. Therefore, the diligent examination of pertinent documents plays a critical role in ensuring the integrity and effectiveness of the predictive maintenance approach.

The specifics of the data collection process, encompassing data sources, sensor utilization, and acquisition procedures, have been extensively detailed in Chapter 5 (Case Study) of the thesis.

4.1.3. Architecture of Artificial Neural Networks

The selection of an appropriate neural network is of utmost importance when it comes to accurately predicting the behaviour of a black box system. It plays a pivotal role in ensuring that the neural network aligns well with the specific characteristics and demands of the system under investigation. This selection process involves careful consideration of various factors and the identification of whether the system is static or dynamic [29].

When dealing with a static system, it is recommended to opt for a static neural network that can effectively capture and model the system's behaviour. On the other hand, for dynamic systems that exhibit time-varying or evolving properties, a dynamic neural network is more suitable. This choice allows for the incorporation of temporal dependencies and enables the network to adapt and respond to changing system dynamics.
In addition to selecting the appropriate neural network type, meticulous attention should be given to the selection of hyperparameters, which significantly influence the network's performance. These hyperparameters encompass various aspects of the network's architecture and configuration. Some key hyperparameters include [44]:

- The total number of layers in the network
- The number of hidden layers
- The number of neurons within each layer
- The number of feedback delays
- The number of input delays

One crucial hyperparameter to consider is the total number of layers in the network. The depth of the network plays a vital role in its capacity to learn complex representations and capture intricate relationships within the data. Another consideration is the number of hidden layers, which determines the level of abstraction and hierarchical processing in the network. The total number of layers in the network encompasses all layers, including input, hidden, and output layers. On the other hand, the number of hidden layers specifically refers to the layers between the input and output layers, where the actual processing and feature extraction occur. Furthermore, the number of neurons within each layer is an essential hyperparameter that affects the network's representational power and capacity to model complex functions. The choice of the number of feedback delays and input delays is also critical, especially when dealing with systems that exhibit memory or temporal dependencies.

Careful selection of these hyperparameters is essential to avoid two common pitfalls: overfitting and underfitting. Overfitting occurs when the network becomes overly complex and starts to memorize the training data instead of learning general patterns. Conversely, underfitting happens when the network is too simple and fails to capture the complexity of the underlying system. To ensure optimal performance and minimize the risks of overfitting or underfitting, it is crucial to tune and select the hyperparameters carefully. This process often involves conducting systematic experiments, exploring different configurations, and leveraging techniques like cross-validation to evaluate the network's performance on unseen data. By choosing the right neural network type, determining the appropriate number of layers, neurons, and delays, and diligently fine-tuning the hyperparameters, the network's accuracy, performance, and generalization capabilities can be enhanced. This comprehensive approach leads to a more reliable and effective predictive maintenance algorithm for control and automation systems, facilitating timely and proactive decision-making.

4.1.4. Training, Validation, and Testing of ANN

In the training phase of neural networks, various training algorithms can be employed to optimize the network's performance. Examples of these algorithms include Levenberg-Marquardt Backpropagation, Scaled Conjugate Gradient, and Bayesian Regularization, among others. Each algorithm has its strengths and limitations, and the choice of algorithm depends on the specific problem and dataset [44].

Once the neural network training is completed, it is crucial to assess its performance using appropriate performance metrics. Mean Square Error (MSE), Sum Square Error (SSE), and Mean Absolute Error (MAE) are commonly used metrics to measure the network's accuracy and deviation from the desired outputs. These metrics provide quantitative measures of the network's performance, allowing for comparisons and analysis [44].

To ensure reliable evaluation, it is important to use separate data for validation and testing. The training data should not be reused for these purposes to avoid bias and overfitting. Instead, new data specifically collected for validation and testing should be utilized. This approach provides a realistic assessment of the network's ability to generalize to unseen data and ensures that the network's performance is not solely optimized for the training dataset [44].

By partitioning the data into distinct groups—training, validation, and testing sets—it becomes possible to assess the network's generalization capability accurately. This data partitioning helps in identifying potential issues such as overfitting, where the network may perform well on the training data but fails to generalize to new data. By evaluating the network's performance on unseen data, it becomes easier to fine-tune the model, adjust hyperparameters, and improve its overall performance and accuracy.

4.1.5. Deployment of Digital Twin

Once the neural network exhibits satisfactory performance across the training, validation, and testing datasets, it signifies a significant milestone in deploying the Digital Twin as a virtual model of the Industrial Control Black Box System (ICBBS). This virtual model accurately mirrors the intricate behaviour and performance of the physical system, providing valuable insights and support for various applications.

However, if the network falls short of meeting the desired performance standards, it is important to take proactive steps to improve its capabilities. This involves an iterative process of refining the network architecture and enriching the training data to enhance its performance and ensure its accuracy in representing the ICBBS.

Refining the network architecture entails carefully adjusting its structure to better capture the complexity of the system. This includes making changes to the number of layers, neurons per layer, and activation functions to optimize the network's ability to learn and understand the underlying patterns and dynamics. These adjustments are like fine-tuning an instrument, ensuring that the network is finely calibrated to accurately replicate the behaviour of the ICBBS.

In addition to architectural adjustments, enriching the training data becomes crucial in further improving the network's performance. By gathering additional data that represents a wide range of operating conditions and scenarios, the network can better understand the nuances of the system and make more accurate predictions.

Through this iterative process of refining the network architecture and gathering more diverse training data, the performance of the neural network can be continuously enhanced. This approach not only addresses initial limitations but also allows the Digital Twin to evolve and adapt alongside the physical system. The resulting Digital Twin becomes a powerful tool for analysing and optimizing the ICBBS, enabling better decision-making, proactive maintenance, and improved efficiency. By continuously fine-tuning the network architecture and expanding the dataset, the Digital Twin becomes a reliable asset for industrial control and automation systems. It helps minimize downtime, maximize system performance, and ensure the smooth operation of the ICBBS.

Once the digital twin reaches a state of readiness for deployment, the subsequent phase involves the development of a robust predictive maintenance algorithm.

4.2: Algorithm 2: Predictive Maintenance Algorithm for Control and Automation Systems (Research question 2)

During the development of Algorithm 1, significant progress has been made with the completion of the initial steps. Now, let's move on to Steps 3, 4, and 5, which are vital in the process as can be seen in Fig. 6. These steps focus on identifying an appropriate condition indicator, detecting anomalies, and raising an alarm for predictive maintenance in the Industrial Automation and Control System.

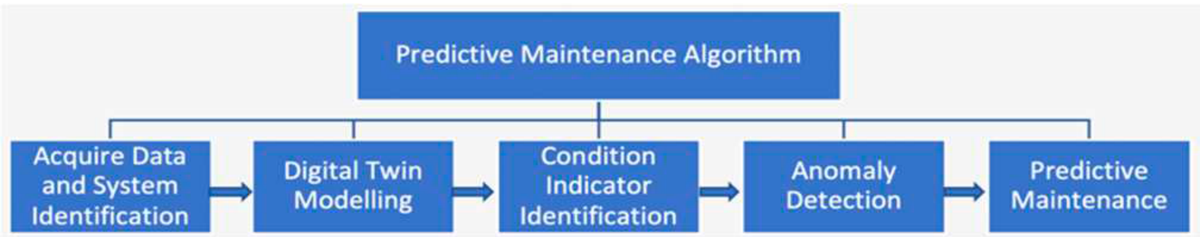

Fig. 6. Predictive Maintenance Algorithm

4.2.1. Identification of Condition Indicators

During the phase of identifying condition indicators, the primary objective was to select suitable metrics that play a crucial role in distinguishing between healthy and faulty data within the Industrial Automation System. The careful selection of condition indicators is essential as they directly impact the accuracy of decision-making processes. Several condition indicators were considered for this purpose:

1. Mean Square Error (MSE)
2. Mean Absolute Error (MAE)
3. Standard Deviation

By utilizing these identified condition indicators, thresholds can be established to effectively detect anomalies within the system. These indicators serve as valuable tools for assessing and monitoring the system's performance and identifying any deviations from expected behaviour. The implementation of appropriate thresholds based on these condition indicators enables timely detection and intervention for abnormal patterns or outliers in the Industrial Automation System. This proactive approach to anomaly detection contributes to the robustness and reliability of the system, allowing for effective decision-making and preventive maintenance to ensure optimal system performance.

4.2.2. Anomaly Detection

To detect anomalies in the physical system, a comparative analysis should be performed between the physical system and the Digital Twin. This involved providing identical inputs to both the physical system and the Digital Twin. The outputs from the physical system should be recorded and compared with the outputs of the Digital Twin, utilizing the previously identified condition indicators from Step 4.2.1, along with their respective thresholds.
By evaluating the performance of the physical system against the threshold determined by the condition indicator, any instances where the performance of the physical system exceeds the threshold are flagged as alerts. These alerts indicate potential anomalies or deviations from the expected behaviour of the system, allowing for timely intervention or further investigation to ensure the system's optimal functioning and reliability.

4.2.3. Predictive Maintenance

Anomalies detected in the system can be attributed to various factors such as environmental changes, temperature fluctuations, equipment aging, or faults. Addressing these anomalies promptly is crucial to prevent equipment failures, as such failures can disrupt advanced manufacturing operations and pose safety risks to workers and operators. To ensure the timely identification and resolution of faults, a fault-finding analysis should be conducted when the performance of the physical system exceeds the safety threshold. This analysis aims to determine the underlying cause of the anomaly and take appropriate measures to rectify the issue. By addressing faults promptly, the risk of equipment failure is mitigated, ensuring the efficiency and safety of the overall industrial processes. Implementing a predictive maintenance approach, supported by anomaly detection, enables proactive maintenance actions to be taken based on the detected anomalies. By identifying and addressing potential issues before they escalate, the system's reliability and uptime are improved, leading to enhanced productivity and cost savings. Additionally, predictive maintenance helps in extending the lifespan of critical equipment and optimizing maintenance schedules, thereby minimizing downtime and maximizing operational efficiency.

In this chapter, two methodologies are presented to address the research objectives outlined in Chapter 2. The first methodology focuses on the development of a high-fidelity digital twin model, aiming to accurately represent the complex dynamics of control systems. The second methodology centres on predictive maintenance techniques, leveraging the insights provided by the digital twin model to enable proactive maintenance strategies. The next chapter will further illustrate the practical application of these methodologies through a comprehensive case study. This case study aims to provide empirical evidence and validate the effectiveness of the proposed methodologies in a real-world setting.

Chapter 5: Case Study for ICBBS Robust Digital Twin Modelling and Predictive Maintenance

In this chapter, a comprehensive case study is presented to demonstrate the practical application and effectiveness of the methodologies introduced in Chapter 4. Building upon the methodologies developed in the previous chapter, this case study serves as a real-world validation of the proposed approaches for high-fidelity digital twin modelling and predictive maintenance in control systems. By applying the methodologies to an actual industrial scenario, this research aims to provide empirical evidence of their performance, reliability, and impact on control systems maintenance.

The proposed frameworks in this chapter were validated using an industrial control system (Fig. 7) comprising specific hardware and software components. The central component of the control system was an Omron programmable logic controller (PLC), which played a crucial role in managing and controlling a 240-volt industrial DC motor. The PLC acted as the brain of the system, executing programmed instructions, and coordinating various tasks to ensure smooth motor operation.

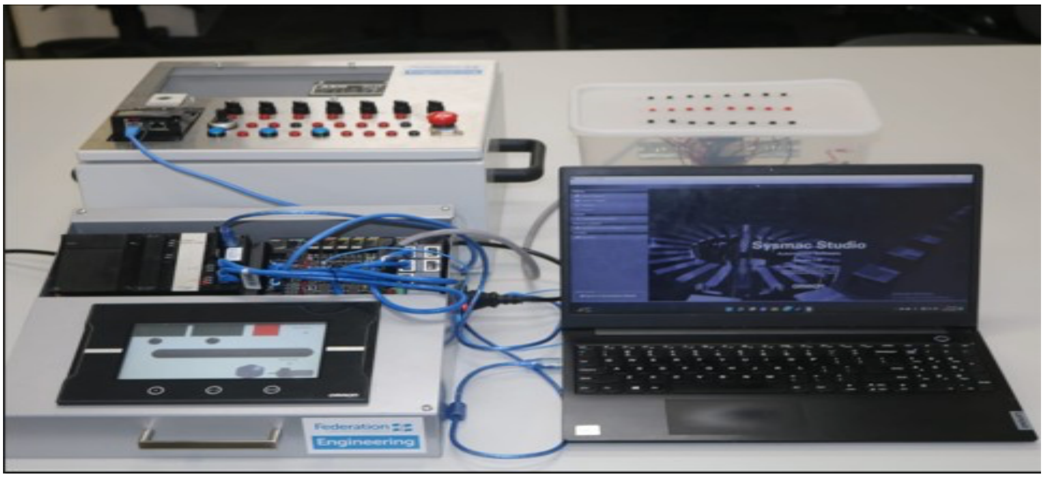

Fig. 7. Industrial Control System

To monitor the real-time performance of the motor and record data, an Omron incremental encoder sensor was employed. This sensor provided precise feedback on the motor's position, speed, and rotational direction, enabling accurate monitoring and analysis of its behaviour during operation. For effective motor control, including synchronization and precise positioning, the control system utilized the Omron MX2 inverter. This inverter served as a power conversion device, allowing efficient control of the motor's speed and torque output. Its integration within the system ensured optimal motor performance for diverse industrial applications.

To facilitate machine automation control, PLC programming, configuration, and simulation, the control system relied on the Omron Sysmac Studio software. This comprehensive software package offered a user-friendly interface and a range of powerful tools for developing and managing automation programs. It allowed engineers to create and optimize control logic, simulate system behaviour, and configure the PLC to suit specific application requirements. The software was executed on an Intel Core i5 Lenovo computer running on the Windows 10 operating system. In addition to the industrial control system, the experiment also involved the utilization of an Apple device with a 7-core CPU equipped with the M1 chip for Digital Twin execution and MATLAB deep learning operations. This Apple device provided the necessary computational power and capabilities to carry out sophisticated simulations, data analysis, and deep learning tasks related to the Digital Twin implementation.

For more comprehensive information about the hardware components used in the experiment, Table 7 can be referred to, which outlines the specific details of each component. Similarly, Table 8 provides detailed information about the software employed, allowing for a comprehensive understanding of the system's technological infrastructure.

Table 7. System hardware

Hardware	**Description**
Omron programmable logic controller	NJ 101-1000: complete integration of logic sequence and motion
Omron inverter	3G3AX-MX2-ECT
Omron incremental encoder	E6C3-C
Omron industrial slim relay	G2RV-SL700
Industrial motor	DC 240 volts, 50 Hz
Intel	Corei5, Windows 10
Apple	7 core CPU with M1 chip

Table 8. Software used for predictive maintenance algorithm

Software's	**Description**
SYSMAC STUDIO	PLC programming, motor control and to read encoder feedback signal
MATLAB	Digital Twin training and execution

5.1: Algorithm 1: DT model of ICBBS

The 5-step algorithm includes system identification, data collection, artificial neural network architecture, DT training, validation and testing and DT deployment, which is based on the methodology presented in Chapter 4.

5.1.1. System Identification

In the context of system identification, two fundamental principles, the Law of Additivity and the Law of Homogeneity, were applied to assess the system's linearity and behaviour. Additivity (Superposition) is a property where the output should be the sum of the responses generated by each input signal individually. In other words, if the system exhibited superposition, it indicated linearity. However, during the experimentation, the system's behaviour did not adhere to the principle of superposition, as the output responses were not a simple linear summation of the individual input responses.

Homogeneity (Scaling) involves scaling the input signals by a constant factor (scalar) to observe its effect on the system's output. For a linear system, a proportional change in the input should result in a proportional change in the output. The observed behaviour of the system revealed a lack of homogeneity, as changes in the input signal amplitude did not result in a consistent linear scaling of the output.

Based on these assessments, it was determined that the system did not follow the principles of superposition and homogeneity. As a result, the system was classified as a non-linear system, reflecting its complex behaviour in response to input changes.

5.1.2. Data Collection

In this phase, OMRON Sensors played a pivotal role in acquiring essential data. The recorded data primarily consisted of Pulse Width Modulation (PWM) frequency signals, providing precise insights into the system's behaviour. The collected data sets exhibited a wide-ranging diversity, encompassing various scenarios, including healthy data sets, data featuring minor anomalies, instances with severe anomalies, and data reflecting faulty conditions. This comprehensive array of data was instrumental in several aspects, serving as valuable input for the training of artificial neural networks and facilitating rigorous validation procedures for the proposed algorithms. The details of the number of data sets have been highlighted in Table 8A.

Table 8A. Data set details

ICS condition	Number of data sets
Healthy operation	3
Minor anomalies	1
Severe anomalies	1
Faulty operation	1

5.1.3. Artificial Neural Network Architecture

Recurrent Neural Network (NARX) was employed in this research to effectively capture the intricate behaviour of the ICBBS. To mitigate the risk of overfitting, the network architecture was intentionally kept simple, taking into consideration the limited variability observed in the data recorded during step A. The inclusion of a complex structure with small variables could have resulted in overfitting, negatively impacting the network's performance. Several combinations of hyperparameters were systematically tested and validated against the recorded data. The selected hyperparameters, as presented in Table 9, consistently yielded the most optimal results in terms of model performance and generalization.

Table 9. Hyperparameters for neural network

Hyperparameter type	**Numbers**
Number of layers	3
Number of hidden layers	1
Neurons in each layer	10
Number of input delay	1:2
Number of feedback delay	1:2

It is important to note that in scenarios where the recorded data exhibits greater complexity or a higher degree of variability, the addition of extra layers and neurons to the network may be necessary. This flexibility allows for adjusting the network's capacity to effectively handle more intricate patterns and capture the full range of system behaviours.

5.1.4. ANN Training, Validation, and Testing

In this research, the network was trained using an open-loop architecture, since real system data was available for training. To facilitate the training, validation, and testing processes, the available data was divided into three subsets, as detailed in Table 10. The training of the model was conducted using the Levenberg-Marquart Backpropagation (LMB) training algorithm. This algorithm incorporates Levenberg-Marquart optimization techniques to update the weight and bias values of the network. Specifically, the algorithm utilizes the Jacobian for calculations, considering the performance metric, which is typically represented as a sum or mean of squared error.

Table 10. Data division for network development

Phase	**Data %**
Training data set	70%
Validation data set	15%
Test data set	15%

In this research, the Mean Square Error (MSE) was chosen as the performance metric for the LMB algorithm, following the default implementation provided by MATLAB. It is important to highlight that separate datasets were used for validation and testing, ensuring independent evaluations of the trained network's performance. At the 18th epoch, the network demonstrated satisfactory performance with an MSE of 2.1. This value indicates the average squared difference between the predicted output and the actual output of the network. The low MSE suggests that the network was able to accurately approximate the behaviour of the system based on the available training data.

Furthermore, it is worth noting that for multi-step ahead prediction, a parallel configuration is highly recommended. This recommendation arises from the series-parallel architecture's tendency to generate errors primarily in one-step prediction scenarios [44]. By adopting a parallel configuration, the network can better handle multi-step predictions and minimize the accumulation of errors over time. Overall, the training process utilized the LMB algorithm with MSE as the performance metric, resulting in satisfactory network performance. The adoption of an open-loop architecture and the appropriate configuration for multi-step ahead prediction contributed to the accurate approximation of the system's behaviour.

5.1.5. Digital Twin Deployment

The performance of the developed Digital Twin was assessed by comparing its output with the output of the ICBBS. The obtained results demonstrate that the developed Digital Twin exhibited effective tracking of the ICBBS's response, particularly during dynamic states. With its demonstrated performance closely mirroring that of its physical counterpart, the Digital Twin was ready to be deployed, offering a robust solution for optimizing operations and ensuring efficient system performance.

5.2: Algorithm 2 for Predictive Maintenance

Once the suitable condition indicator has been identified, the developed Digital Twin from the previous step can be effectively utilized to detect anomalies.

5.2.1. Condition Indicator

In this study, the Levenberg-Marquart backpropagation (LMB) algorithm was employed to train the neural network, and the mean squared error (MSE) was selected as the condition indicator. After the network was trained, its performance was evaluated using unseen data during the validation phase. The validation error, measured as MSE, was found to be 2.1. This validated MSE value of 2.1 was established as the threshold alert for detecting anomalies in subsequent operations. If the performance of the system surpasses this threshold, it serves as an indication of potential anomalies or deviations from the expected behaviour. This threshold can be used to trigger appropriate actions for further analysis or intervention, ensuring proactive maintenance and optimization of the industrial processes.

5.2.2. Anomaly Detection

To evaluate the effectiveness of the condition indicator in detecting anomalies within the automation system, additional experiments were conducted. These experiments involved collecting new data sets from the automation system under both healthy and faulty conditions, utilizing an encoder to record the input and corresponding output in the form of PWM frequency. The Digital Twin, developed using algorithm 1 and operating in a closed-loop configuration using a parallel architecture was used to simulate the automation system's behaviour. The response of the Digital Twin was analysed under different conditions, specifically in a healthy state and in a faulty state. It was found that the developed Digital

Twin model was very effectively able to detect anomalies and distinguish between healthy and abnormal operations.

5.2.3. Predictive Maintenance

The successful detection of anomalies as discussed in the previous section using the proposed algorithm underscores its robust applicability for predictive maintenance in industrial control systems. By effectively identifying deviations from expected behaviour, the algorithm empowers maintenance personnel with timely and actionable insights to address potential issues proactively, minimizing downtime, optimizing system performance, and ultimately enhancing the overall reliability and efficiency of industrial control systems.

This chapter presented a case study where the two algorithms proposed in Chapter 4 underwent rigorous validation using real-time sensor data. In the following chapter, the discussion will centre on the results obtained during the training of the Digital Twin model, the proposed algorithm's capacity to detect anomalies, quantify anomaly severity and address the challenge of false positives. Additionally, the chapter will provide an overarching analysis of the entire research, including the ranking of state-of-the-art approaches.

Chapter 6: Results and Discussion

In the following chapter, a comprehensive analysis and discussion of the obtained results from the case study conducted in Chapter 5 will be presented. The case study serves as a critical evaluation of the methodologies proposed in Chapter 4, which aimed to leverage digital twin technology for predictive maintenance in control systems. This analysis will provide insights into the effectiveness and practical implications of the proposed methodologies. To provide a contextual framework, this chapter will also provide a comparative analysis of the state-of-the-art approaches discussed in Chapter 3. This analysis will highlight the advantages and limitations of these existing approaches, laying the foundation for understanding the innovation and contribution of the proposed methodologies.

Evaluating the performance of a trained neural network is a crucial step in the analysis. The training record of the network, depicted in Fig. 8, illustrates the relationship between errors and epochs. Notably, at 18 epochs, the network demonstrated strong performance, achieving the lowest validation error of 2.15. This indicates that the network successfully learned and generalized the data. It is common for the error to decrease further with additional training epochs. However, caution must be exercised as an overfitted network may exhibit an increase in validation error.

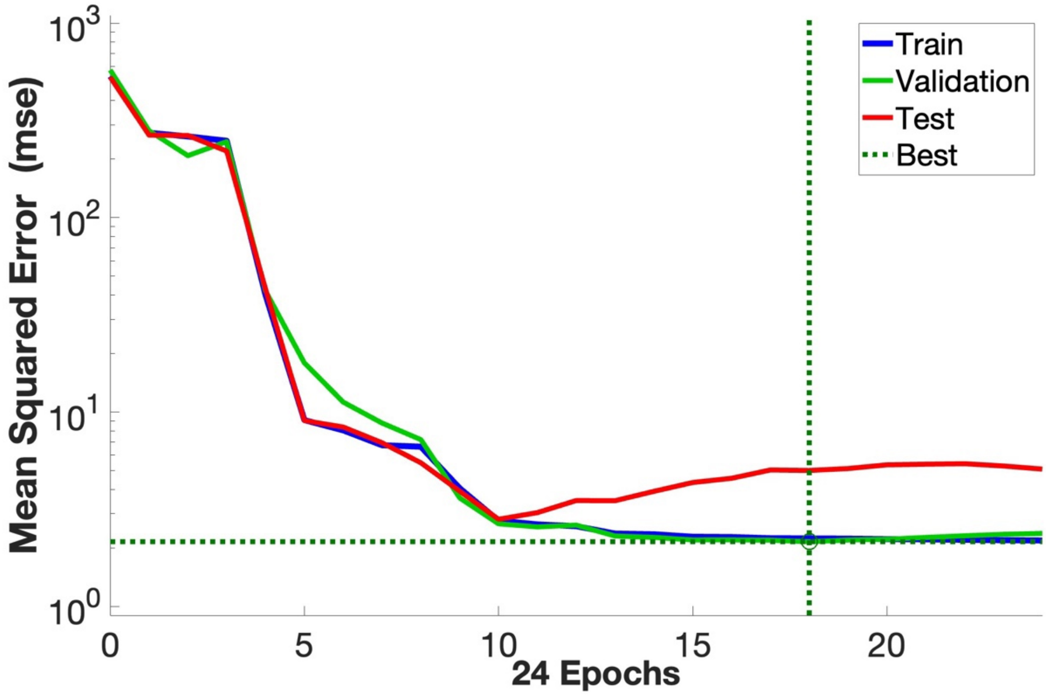

Fig. 8. ANN Performance Matrix

To further assess the performance of the trained network, it is advisable to generate and examine a regression plot. Fig. 9 presents the regression plot, which depicts the correlation between the network output and targets. The plot consists of four distinct sections representing this relationship during training, validation, testing, and the combined data from all three sets. Analysing the regression plot can provide insights into the accuracy and consistency of the network's predictions across different datasets. In each of the plots, the targets are represented by a dashed line, while the solid line represents the best-fit linear regression line that describes the relationship between the network output and the targets. The inclusion of R-values in the plots provides an indication of the strength of this relationship. An R-value of 1 suggests a perfect linear relationship, while an R-value of 0 indicates no linear relationship. In Fig. 9, the R-values for all plots are nearly equal to 1, indicating a highly accurate fit between the network output and the target values. This suggests that the network has effectively captured the underlying patterns and trends in the data.

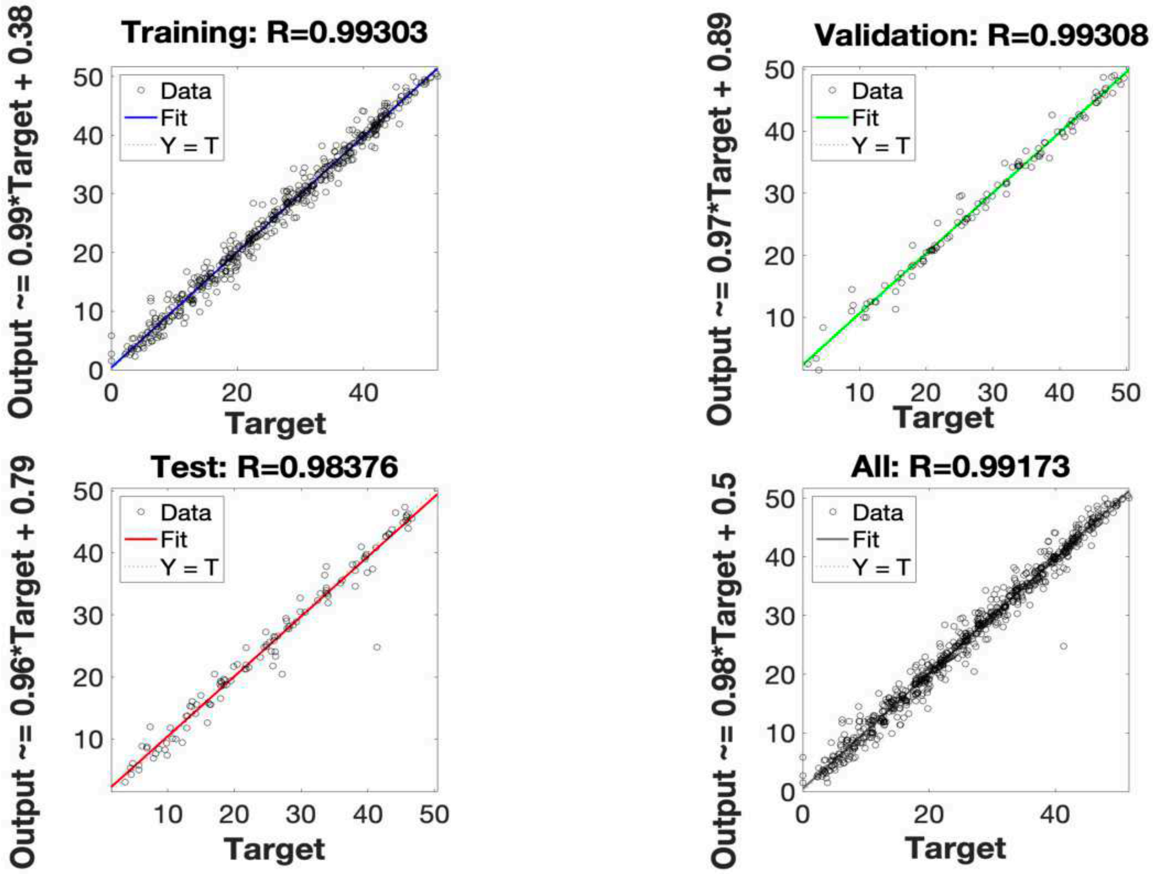

Fig. 9. Regression Plot

Fig. 10 provides a time series response that highlights the selected time points for training, validation, and testing. It also presents the error plotted against time, offering insights into the performance of the network over the duration of the experiment.

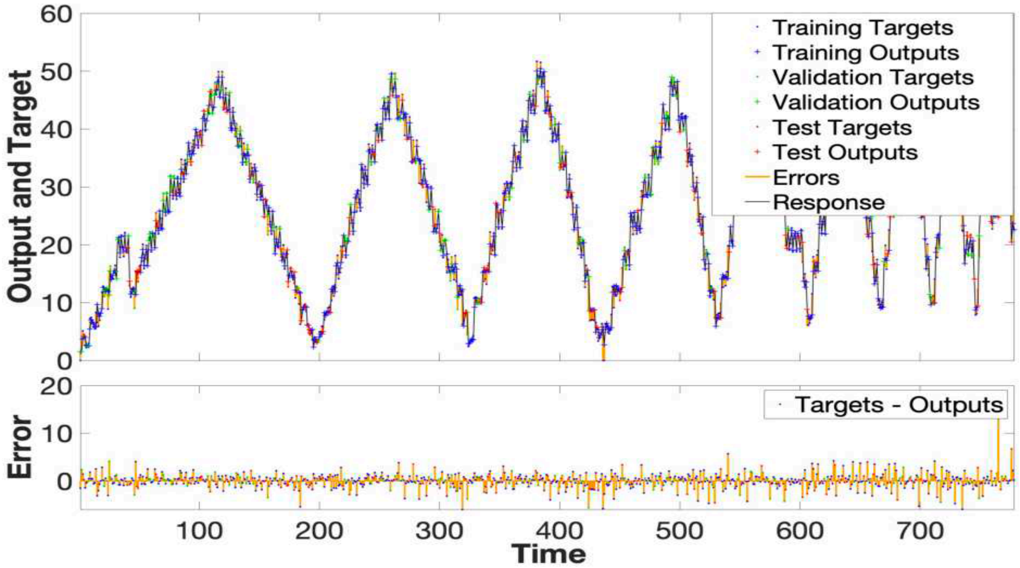

Fig. 10. Time Series Plot

Additionally, Fig. 11 displays a histogram of the error values, with 20 bins, allowing for a visual representation of the distribution of errors in the network's predictions.

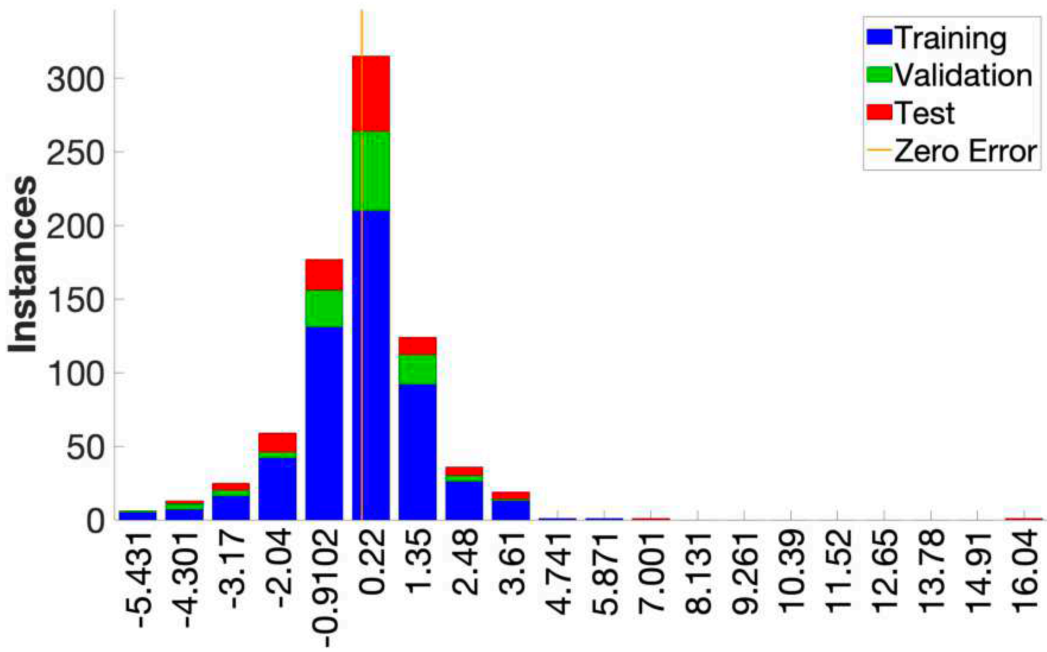

Fig. 11. Error Histogram

the input error correlation, illustrating the relationship between errors and the input sequence can be seen in Fig. 12. The plot provides valuable insights into the performance of the trained network. It is evident from the graph that the network was effectively trained, as

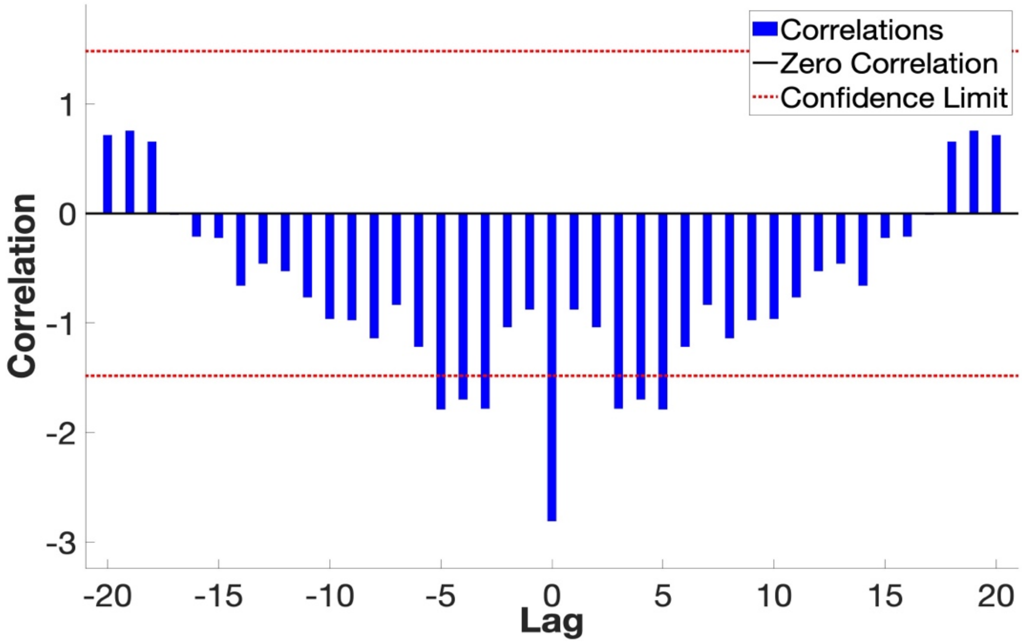

Fig. 12. Input Error Correlation

most of the correlations between errors and the input sequence lie within the confidence limit. This indicates that the network has successfully captured and learned the patterns and dependencies present in the input data. Fig. 13 provides a visual representation of the training states of the network. This plot showcases the progression and evolution of the network's performance throughout the training process. By observing the plot, one can gain insights into how the network's accuracy and error rates change over time, allowing for an assessment of the network's learning dynamics and convergence.

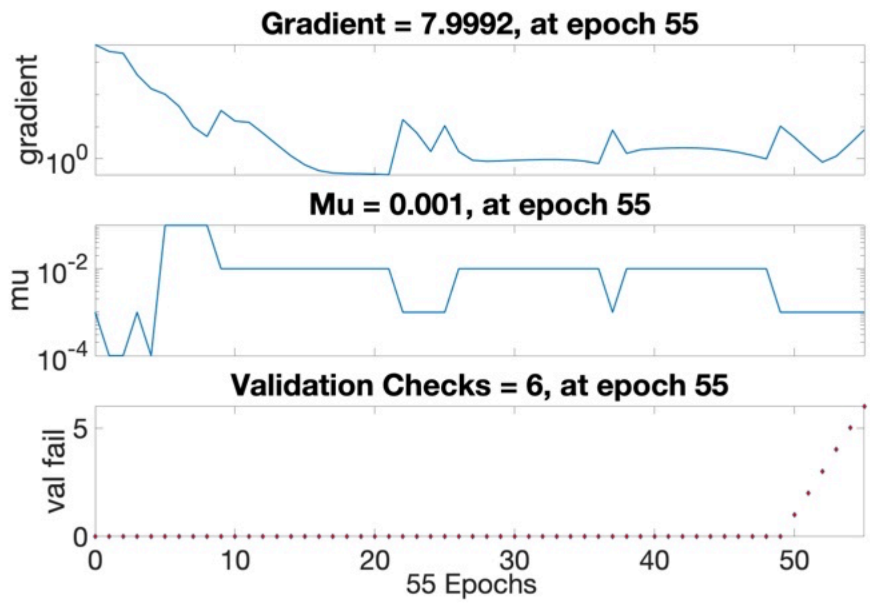

Fig. 13. Training states

The autocorrelation plot in Fig. 14 demonstrates the time-related prediction error. The trained model exhibited excellent performance, as most of the error correlations are within the confidence limit and exhibit independence from each other. The deployment of the Digital Twin (DT) network against the physical system is depicted in Fig. 15. This figure showcases the ability of the network to accurately track the performance of the physical system, particularly in dynamic states.

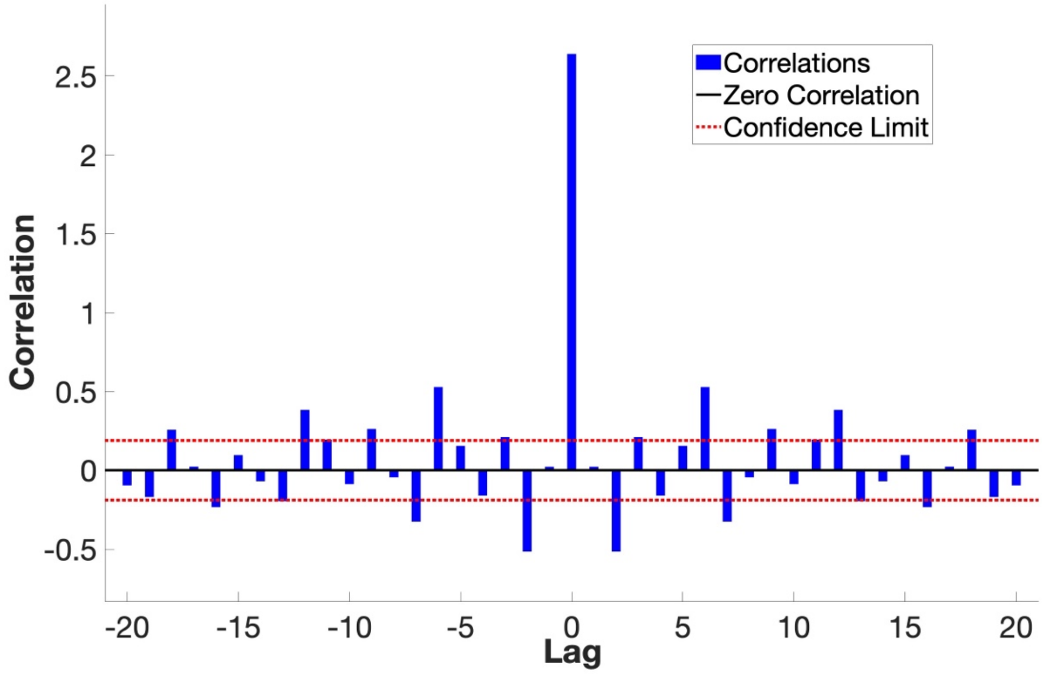

Fig. 14. Autocorrelation of Error

In the assessment of state-of-the-art anomaly detection methods for real-world scenarios, various machine learning, deep learning and statistical approaches were evaluated. These methodologies underwent training using a specific data pattern, as illustrated in Fig. 15. To assess the effectiveness, diverse datasets were employed, including one with minor anomalies (Fig. 16), another with severe anomalies (Fig. 17), and one with instances of faulty operation (Fig. 18). Importantly, all four data sets shared a common input pattern, enabling assessment of their performance on data with similar characteristics.

All these approaches were implemented using MATLAB's built-in models, with a link to the deployment provided in the appendix. Among these methods, the Mahalanobis Distance method demonstrated exceptional performance, achieving the highest score of 8.44 out of 9. It not only adeptly detected anomalies but also quantified their severity and precisely identified their locations in the data. This makes it an excellent choice for detecting anomalies resembling those in the training data. Following closely, the Local Outlier Factor approach achieved a score of 8.34. It effectively detected and quantified anomalies, showing accuracy in identifying anomaly points for both minor and severe cases. However, it had limitations in detecting a few anomaly points within faulty data, placing it in the second position.

The One-Class Support Vector Machine approach earned a score of 6.82 and secured the third rank. While it successfully detected and quantified anomalies, it struggled to identify specific anomaly points within the data. Consequently, its suitability may be restricted in scenarios where precise anomaly point identification is crucial for root cause analysis. The Autoencoder, a deep learning approach, received a score of 4. While it proficiently detected and quantified anomalies, its limitation in pinpointing individual anomaly points significantly limits its applicability. This drawback underscores that the Autoencoder is best suited for scenarios requiring anomaly detection and quantification but falls short in identifying specific anomaly locations.

The Isolation Forest algorithm, ranking fifth with a score of 2.13, demonstrated limited effectiveness in detecting minor and severe anomalies. It also lacked the capability to quantify anomaly severity in these scenarios. Nevertheless, the algorithm exhibited some proficiency in identifying anomalies within faulty data, making it more suitable for reactive maintenance rather than predictive maintenance scenarios. Robust Random Cut Forest received a score of 0 due to its inability to detect any anomaly points within the research dataset, despite using advanced models in MATLAB. These rankings provide a clear comparison of the most effective methodologies, aiding manufacturing industries in informed decision-making regarding the adoption of suitable anomaly detection approaches tailored to specific industrial needs.

However, a significant challenge arose when applying these approaches to unseen healthy data patterns (Fig. 19). Notably, a high Mean Squared Error (MSE) was observed, signifying the misclassification of new, unseen healthy data as anomalies and faulty instances. This indicates that these evaluated approaches struggled to distinguish between normal and faulty operations, resulting in a substantial number of false positives. Consequently, these limitations render them unsuitable for operations involving systems and devices operating on diverse patterns, especially in advanced manufacturing environments.

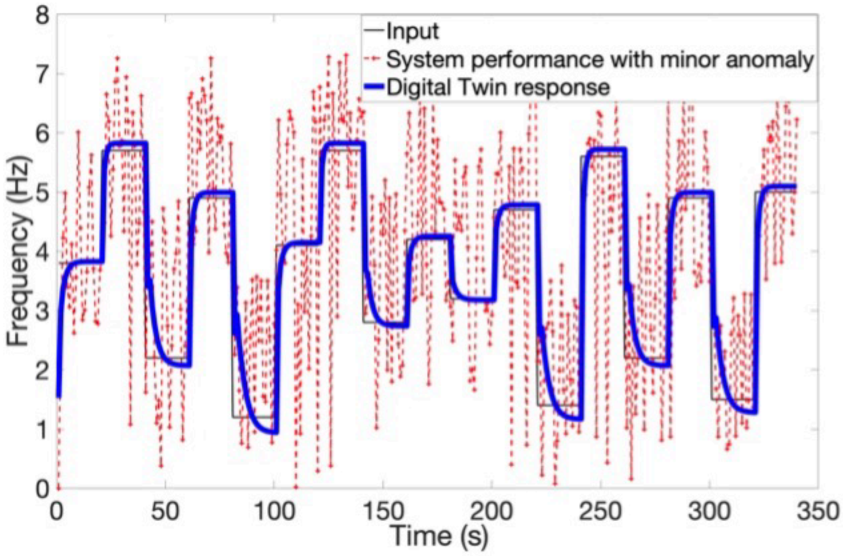

Fig. 15. ICS healthy operation data

Furthermore, the first Digital Twin model deployment was made against the healthy output of the ICS as can be seen in Fig. 19. The recorded MSE was 2.0 which was taken as a condition indicator to locate anomalies in new unseen data. It's crucial to note that the training data used for the DT was entirely distinct from the data encompassing healthy instances, minor anomalies, severe anomalies, and faulty operations. With 780 instances, the training data exhibited unique patterns compared to those shown in other figures. When the system experienced a minor anomaly, as depicted in Fig. 16, the detected error was 2.4 (0.3 above the threshold). This demonstrates the effectiveness of the proposed algorithm in detecting anomalies in distinct patterns.

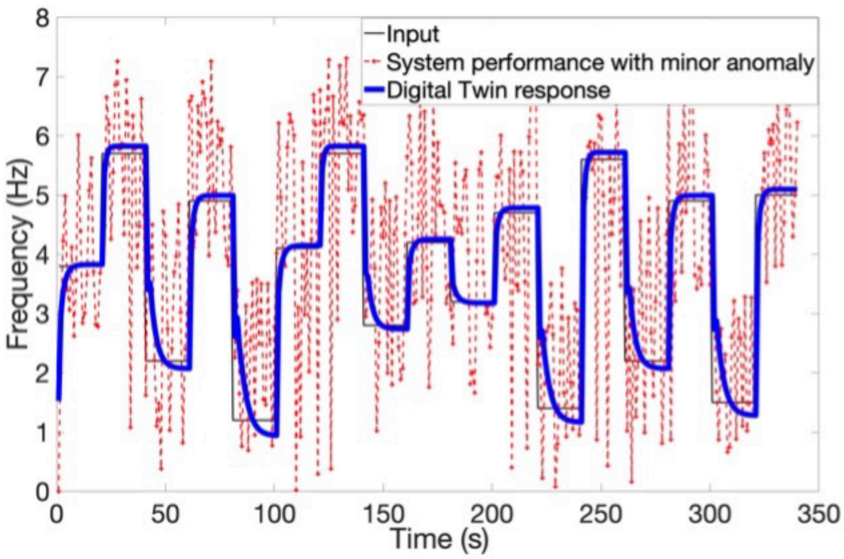

Fig. 16. ICS operation with minor anomaly instances

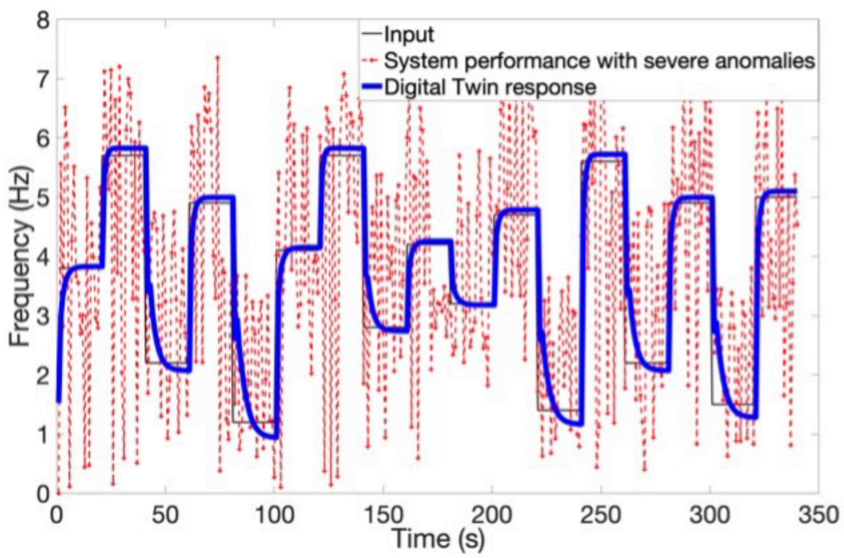

Fig. 17. ICS operation with the severe anomaly instances

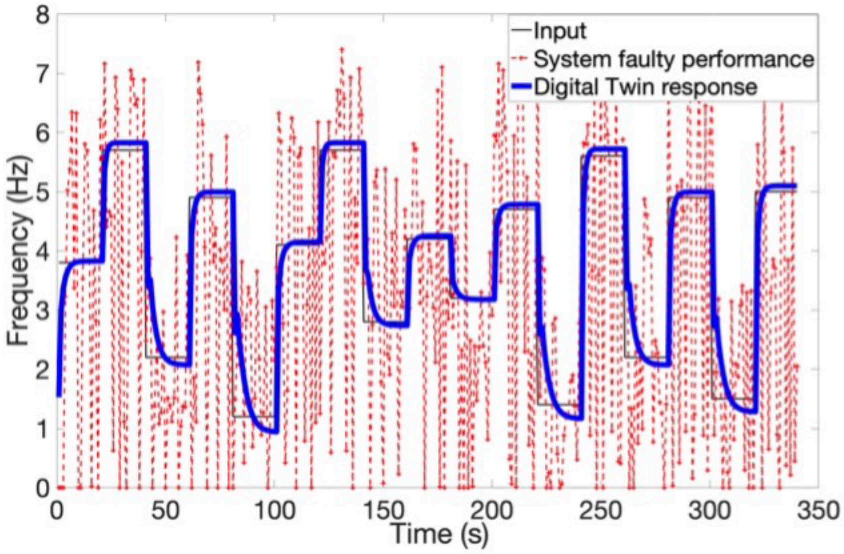

Fig. 18. ICS under fault

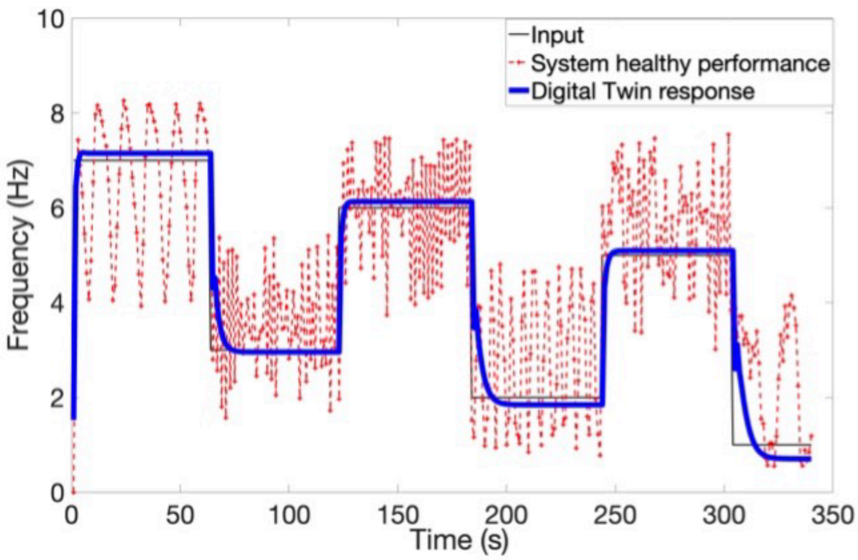

Fig. 19. ICS additional healthy data

To further evaluate the DT's ability to quantify the level of anomaly, its performance was compared when the system encountered severe anomalies as can be seen in Fig. 17 and faulty conditions in Fig. 18. The MSE observed for severe anomalies was 3.4 (1.3 above the threshold), while for faulty conditions, it was 5.4 (3.3 above the threshold). These results clearly indicate that the proposed algorithm not only detected anomalies but also accurately quantified their severity. To further assess the DT's capability in mitigating false positives, additional healthy data were used (Fig. 15). The observed MSE was 2.1 which clearly did not cross the identified alert threshold as well.

Fig. 20. DT Anomaly Detection, Quantification, and False Positive Mitigation

Notably, despite the significant differences in training patterns and instances, the proposed algorithm outperformed state-of-the-art approaches with 100 % accuracy in anomaly detection, quantification, and mitigation of false positives on the recorded data as can be seen in Fig. 20. The trained digital twin exhibits a high level of accuracy, closely resembling the performance of its physical counterpart.

It is also important to acknowledge that a slight deviation in performance can be observed due to the presence of noise in the raw data recorded from the physical system. This noise makes it challenging to use the trained DT model to detect the location of the anomaly points in the data. To further enhance the accuracy of the DT, incorporating noise filtering techniques in real-world applications within industries can be beneficial. By implementing such techniques, the impact of noise on the performance of the DT can be mitigated, enabling more precise identification of anomaly points in the data. Signal filtering techniques, such as low pass and high pass filters commonly used in signal processing, offer significant benefits. Low-pass filters are effective in attenuating high-frequency noise, enabling the extraction of important low-frequency signals that reflect the system's behaviour. Conversely, high-pass filters eliminate low-frequency noise, enabling the identification of rapid changes and transient phenomena. By carefully selecting and configuring these filters, the impact of noise on the digital twin's training data can be minimized. Another valuable tool for data refinement is the MATLAB smoothing toolbox, which provides various smoothing algorithms. For example, the moving average filtering computes the average of neighbouring data points, reducing high-frequency noise while preserving underlying trends. On the other hand, Savitzky-Golay filtering utilizes polynomial regression to estimate smooth curves from noisy data, effectively suppressing noise while retaining significant signal features. The performance of the trained DT model on filtered data can be seen in Fig. 18. The orange line represents the output from the DT while the blue line represents the filtered output of the industrial control system using a low pass filter. It can be clearly seen that the performance accuracy of the trained DT has highly increased when compared with filtered data.

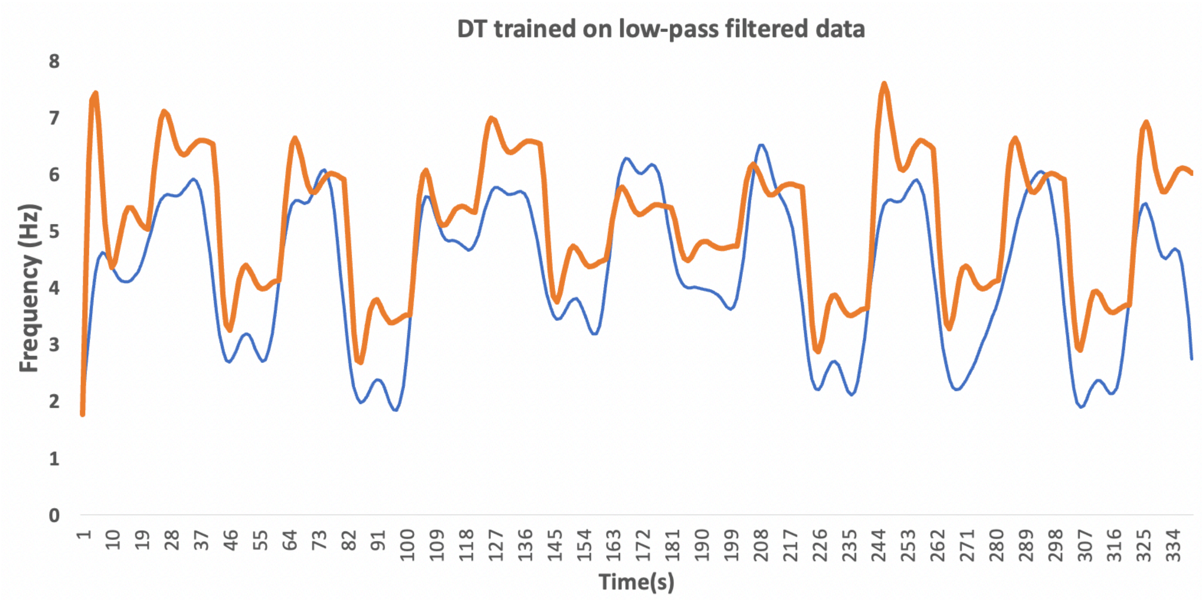

Fig. 18. Digital Twin trained on filtered data.

Nevertheless, it is crucial to emphasize that the primary aim of this research was to develop and train the model on raw data, considering its prevalence and significance in industrial settings. Raw data serves as a valuable source of information in various industries, providing insights into the behaviour and performance of physical systems. By focusing on raw data, this research aligns with real-world practices and facilitates the direct applicability of the trained DT model within industry environments.

Chapter 7: Conclusion

In conclusion, this research has highlighted the immense potential of industrial control systems (ICS) in the context of Industry 4.0 and advanced manufacturing. ICS play a pivotal role as key enablers, offering essential capabilities such as data collection, automation, and analysis, which are crucial for improving product quality and optimizing manufacturing processes. However, the challenge of control system failures poses significant risks, including potential catastrophic effects. The failure of a control system not only disrupts and slows down the advanced manufacturing process but can also result in a substantial loss in overall production and pose serious risks to the safety of the operators operating the plant. The consequences of control system failures can range from financial setbacks due to downtime and production losses to severe injuries or fatalities for the operators. To address this challenge, the utilization of digital twin technology for predictive maintenance algorithms in ICS emerges as a promising approach. By leveraging the power of digital twins, virtual replicas of physical systems, organizations can proactively identify and prevent anomalies, ensuring the smooth operation of control systems and minimizing the risks associated with failures.

This research significantly contributes to the field by presenting innovative solutions and methodologies, which not only fill existing research gaps but also pave the way for more comprehensive studies in the future. A notable contribution of this research is the development of a novel Digital Twin (DT) algorithm tailored explicitly for Industrial Control Black Box Systems (ICBBS). This pioneering approach fills a critical void in the literature and lays a robust foundation for future research endeavours in this specialized domain. In terms of algorithm novelty, this research introduces the use of the NARX model. Unlike previous studies that primarily relied on simulation data for NARX with limited practical applicability, this research meticulously adjusted hyperparameters and employed optimization algorithms.

Another distinct aspect of this research is its novel approach to data utilization. Rather than relying on online data or data generated through simulations, this research utilized six distinct real-world datasets. These datasets provide a comprehensive understanding of system behaviour over an entire year, encompassing various seasons and scenarios. This data diversity is exceptionally rare in the existing literature. Importantly, all experiments were conducted exclusively on raw data, emphasizing real-world applicability and data integrity.

This research further extends its impact by addressing the scarcity of studies focused on quantifying anomaly severity and effective false-positive mitigation within ICS. Notably, a key novelty of this study is the utilization of a novel case study for anomaly detection, quantification, and false-positive mitigation. The case study serves as a crucial component in evaluating the developed algorithms. It provides a real-world context and datasets that are often lacking in existing research. This novel case study encompasses a wide range of real data sets, including healthy system states, minor anomalies, severe anomalies, and faulty data patterns, making it an asset in enhancing the reliability of anomaly detection within the ICS domain.

Another significant and pioneering contribution of this research is the comprehensive comparison of state-of-the-art algorithms. These approaches underwent rigorous assessment and validation against six real-world datasets, covering anomaly detection, quantification, and real positive mitigation within ICS. Furthermore, this research introduced a novel ranking system to evaluate the performance of these approaches based on their application to real-world datasets. It's important to note that this research is ground-breaking in its scope and impact. No prior study has ventured into such a diverse range, utilizing as many real-world datasets for performance assessment. This ground-breaking research significantly advances the state of the field.

The proposed algorithm's performance was highly significant, achieving unparalleled accuracy and efficiency. With the data set recorded from the industrial control system, the algorithms achieved 100% accuracy, not only detecting anomalies and quantifying their severity but also demonstrating robust generalization capabilities by accurately classifying the system's condition as healthy or faulty, even on unseen data patterns. This validation process involved comprehensive datasets recorded during different operational scenarios, including periods when the system was in both healthy and faulty conditions.

The importance of condition monitoring in the industry cannot be overstated. Poor monitoring practices have been shown to contribute to dire consequences, with research indicating that approximately 30% of reported fatalities in the manufacturing environment are directly related to inadequate condition monitoring. Moreover, equipment failures alone can account for up to 60% of total manufacturing costs for companies, highlighting the significant financial burden resulting from insufficient monitoring and maintenance practices. While digital twin technology holds immense potential for improving condition monitoring, the challenge lies in the availability of comprehensive and high-quality data, which limits organizations from fully capitalizing on its benefits.

However, the algorithms proposed in this research address these challenges head-on. They not only tackle the data availability issue but also pave the way for organizations to leverage the full potential of digital twin technology in condition monitoring. By implementing these algorithms, organizations will gain extraordinary advantages, including cost savings, enhanced worker safety, and the achievement of smooth advanced manufacturing processes. These algorithms provide a comprehensive and reliable solution, empowering organizations to proactively monitor the health of their industrial control systems. They can be used to optimize maintenance strategies, enable real-time anomaly detection, prevent equipment failures, and safeguard the well-being of the workforce. This research demonstrates a noteworthy progression in condition monitoring, enabling organizations to unlock substantial operational efficiencies and achieve superior performance in the realm of advanced manufacturing.

Chapter 8: Future Direction

Prescriptive maintenance represents a crucial advancement in maintenance strategies that build upon the foundation of predictive maintenance. While both predictive and prescriptive maintenance play essential roles in optimizing asset performance, they differ in their scope and approach. Predictive maintenance focuses on utilizing historical data, advanced analytics, and machine learning algorithms to predict when equipment failures are likely to occur. By analysing patterns and trends in data, predictive maintenance algorithms can identify potential anomalies or deviations from normal behaviour, providing valuable insights into the health of assets. This enables organizations to schedule maintenance activities proactively, minimizing unexpected breakdowns and optimizing maintenance resources.

Prescriptive maintenance takes it a step further by providing specific recommendations on how to prevent or address the predicted failures. It leverages real-time data and advanced analytics techniques to continuously monitor asset performance and identify potential issues. Based on this information, prescriptive maintenance algorithms generate actionable recommendations for maintenance activities, guiding organizations on the most effective actions to take. Despite the advancements in predictive maintenance, the exploration of prescriptive maintenance has been relatively limited. Given the vast potential and critical significance of prescriptive maintenance, it is evident that further research in this area is imperative.

Publications

1st Conference Paper

1st conference paper has been published in IEEE. The title of the paper is "Artificial Intelligence Enabled Digital Twin for Predictive Maintenance in Industrial Automation System: A Novel Framework and Case Study". Below are the details of the paper and the link.

Sponsored: IEEE Industrial Electronic Society
Host: Loughborough University
Location: United Kingdom
Date: 15th March – 17th March
Link: https://ieeexplore.ieee.org/document/10101971

2nd Conference Paper

The second conference has been accepted for publication. The title of the paper is "Machine Learning Enabled Digital Twin for Industrial Control Black Box System: A Novel Framework and Case Study".

Sponsored: IEEE Robotics and Automation Society
Host: Aston University
Location: United Kingdom
Date: 30th August- 1st September

Journal

The journal paper has been submitted to IEEE Transactions on Industrial Informatics. The title of the journal is "Real-World Anomaly Detection in Control Systems Using Artificial Intelligence Driven Digital Twin: A Novel Framework and Case Study"

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Appendices

Appendix A: Implementation Details

In this appendix, we provide additional information on the implementation of the NARX model and the comparison of state-of-the-art approaches using MATLAB. The NARX model execution was carried out using MATLAB's Deep Learning Toolbox. Also, another way to implement NARX is by using MATLAB APP " nnstart". Below is the link for the app.

(https://au.mathworks.com/help/deeplearning/ref/nnstart.html)

Additionally, MATLAB models were employed to compare state-of-the-art approaches. The models were used using the following links.

(https://au.mathworks.com/help/stats/anomaly-detection.html)

Appendix B: PLC Programming and Data Recording

In this appendix, we provide additional information on the programming of the Programmable Logic Controller (PLC) and the data recording process using SYSMAC Studio

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The PLC programming involved the utilization of Function Block, ST Logic (Structured Text), and Ladder Logic. Each programming language served specific purposes in controlling the PLC's behaviour and executing various tasks within the system. The data were recorded using SYSMAC Studio of Omron.

Appendix C: Digital Twin Training

In order to train the digital twin model, a dataset comprising 780 seconds of healthy data was utilized. This dataset was carefully selected to represent a variety of normal operating conditions and captured various parameters relevant to the system under consideration. The inclusion of such diverse and representative data is crucial for developing an accurate and robust digital twin model.

Appendix D: Algorithm Validation Data

The data used for algorithm validation was collected from an industrial control system located at the Federation University Churchill campus. The industrial control system served as the testbed for evaluating the algorithm's effectiveness in detecting anomalies.