Trustworthy Soft Sensing in Water Supply Systems using Deep Learning

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Thesis submitted to the Faculty of the

Virginia Polytechnic Institute and State University

in partial fulfillment of the requirements for the degree of

Master of Science

in

Computer Engineering

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May 2, 2024

Blacksburg, Virginia

Keywords: Soft Sensor, Water Supply System, Data-Driven, Testbed, Trustworthy AI, Nitrate, Context

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(ABSTRACT)

In many industrial and scientific applications, accurate sensor measurements are crucial. Instruments such as nitrate sensors are vulnerable to environmental conditions, calibration drift, high maintenance costs, and degrading. Researchers have turned to advanced computational methods, including mathematical modeling, statistical analysis, and machine learning, to overcome these limitations. Deep learning techniques have shown promise in outperforming traditional methods in many applications by achieving higher accuracy, but they are often criticized as 'black-box' models due to their lack of transparency. This thesis presents a framework for deep learning-based soft sensors that can quantify the robustness of soft sensors by estimating predictive uncertainty and evaluating performance across various scenarios. The framework facilitates comparisons between hard and soft sensors. To validate the framework, I conduct experiments using data generated by AI & Cyber for Water & Ag (ACWA), a cyber-physical system water-controlled environment testbed. Afterwards, the framework is tested on real-world environment data from Alexandria Renew Enterprise (AlexRenew), establishing its applicability and effectiveness in practical settings.

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(GENERAL AUDIENCE ABSTRACT)

Sensors are essential in various industrial systems and offer numerous advantages. Essential to measurement science and technology, it allows reliable high-resolution low-cost measurement and impacts areas such as environmental monitoring, medical applications and security. The importance of sensors extends to Internet of Things (IoT) and large-scale data analytics fields. In these areas, sensors are vital to the generation of data that is used in industries such as health care, transportation and surveillance. Big Data analytics processes this data for a variety of purposes, including health management and disease prediction, demonstrating the growing importance of sensors in data-driven decision making.

In many industrial and scientific applications, precision and trustworthiness in measurements are crucial for informed decision-making and maintaining high-quality processes. Instruments such as nitrate sensors are particularly susceptible to environmental conditions, calibration drift, high maintenance costs, and a tendency to become less reliable over time due to aging. The lifespan of these instruments can be as short as two weeks, posing significant challenges. To overcome these limitations, researchers have turned to advanced computational methods, including mathematical modeling, statistical analysis, and machine learning. Traditional methods have had some success, but they often struggle to fully capture the complex dynamics of natural environments. This has led to increased interest in more sophisticated approaches, such as deep learning techniques. Deep learning-based soft

sensors have shown promise in outperforming traditional methods in many applications by achieving higher accuracy. However, they are often criticized as “black-box” models due to their lack of transparency. This raises questions about their reliability and trustworthiness, making it critical to assess these aspects.

This thesis presents a comprehensive framework for deep learning-based soft sensors. The framework will quantify the robustness of soft sensors by estimating predictive uncertainty and evaluating performance across a range of contextual scenarios, such as weather conditions, flood events, and water parameters. These evaluations will help define the trustworthiness of the soft sensor and facilitate comparisons between hard and soft sensors. To validate the framework, we will conduct experiments using data generated by ACWA, a cyber-physical system water-controlled environment testbed we developed. This will provide a controlled environment to test and refine our framework. Subsequently, we will test the framework on real-world environment data from AlexRenew. This will further establish its applicability and effectiveness in practical settings, providing a robust and reliable tool for sensor data analysis and prediction. Ultimately, this work aims to contribute to the broader field of sensor technology, enhancing our ability to make informed decisions based on reliable and accurate sensor data.

Dedication

To my parents and my beloved sisters, thank you for always having my back.

Acknowledgments

First and foremost, I would like to express my deep gratitude to Dr. Feras Batarseh for his mentorship and for welcoming me into the A3 Lab family. As I navigated the ups and downs of my M.S., Dr. Batarseh supported me with his advice and challenged me not only to be a better researcher but also to step out of my comfort zone.

I would like to express my appreciation to the members of my committee, Dr. Dong S. Ha and Dr. Sook Ha, for their insightful feedback and dedication to my work. Their support and challenging questions have helped me improve my work and sharpen my skills as a researcher.

I would like to extend my sincere gratitude to AlexRenew for their invaluable contribution to my thesis* study by providing datasets. I appreciate their generosity and the opportunity to utilize such resources in my research.

To my A3 labmates, you have been the best comrades one could ask for during my M.S. program. A special note of thanks to Justice, Ajay, and Nazmul for their extra efforts in ensuring I had all the support and advice I needed.

Finally, I want to express my sincere gratitude to my parents, Leangheng and Kosalmony, for showering me with love and support and for being my role models. They taught me to be resilient, optimistic, kind, and empathetic. I also want to thank my big sister, Leakhena, for her care, and my sister Nalin, for being the wise one who always has my back.

*I acknowledge the use of ChatGPT-4 and Grammarly, solely in Chapters 1 and 2 for grammar checks, rephrasing and editing purposes.

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List of Abbreviations

$^\circ c$ Celcius

mg/L Milligram per liter

ACWA AI & Cyber for Water & Ag

AI Artificial Intelligence

AlexRenew Alexandria Renew Enterprise

ANN Artificial Neural Network

BPNN Back Propagation Neural Network

CPT Centrate Pretreatment Process

DBN Deep Belief Network

DBN-EL DBN with Event-Triggered Learning

DO Dissolved Oxygen

EC Electrical Conductivity

F Fahrenheit

FNN Feedforward Neural Network

GDBN Growing Deep Belief Network

LoRa Long Range

MAE Mean Absolute Error

MAPE Mean Absolute Percentage Error

MGD Million Gallons per Day

NH3 Ammonia

NO3 Nitrate

NSE Nash-Sutcliffe Efficiency

PBIAS Percent Bias

PLC Programmable Logic Controller

RBFNN Radial Basis Function Neural Network

RSR Root Mean Square Error- Observation Standard Deviation Ratio

SWaT Secure Water Treatment

TDS Total Dissolved Solid

WAS Waste Activated Sludge

WSS Water Supply System

WWTP Wastewater Treatment Plant

Chapter 1

Introduction

Sensors are pivotal in various Cyber-Physical systems, offering myriad benefits. Essential in measurement science and technology, they enable reliable high-resolution measurements at low cost, affecting areas such as environmental monitoring, medical applications, and security [15]. In food and water safety, advances in sensors involving engineered nanomaterials address challenges such as detection limits and complex environmental interactions [21]. In general, the continuous development of sensor technology holds promise for further breakthroughs and social benefits, underscoring its indispensableness in modern science and technology.

The significance of sensors extends to the fields of Internet of Things (IoT) and Big Data Analytics. In these areas, sensors are crucial for generating data used in industries such as healthcare, transportation, and surveillance. Big data analytics processes this data for various purposes, including healthcare management and pandemic prediction, illustrating the growing importance of sensors in data-driven decision-making [4].

In the context of biological wastewater treatment, hardware sensors encounter several challenges, highlighting the need for advanced solutions and continuous innovation. One major challenge is the variability in influent quality, particularly in managing sequencing batch reactors (SBRs), a type of activated sludge process for wastewater treatment, for the biological treatment of urban and industrial wastewater [9]. This variability makes online instrumentation crucial for characterizing influent and assessing process efficiency. Techniques such as set-point titration and UV spectrophotometry have been effectively used to monitor and control SBRs despite these challenges, demonstrating the adaptability of current methods in the face of influent variability. However, these traditional monitoring methods are limited in providing reliable, online, real-time monitoring due to the need for sample preparation and expensive equipment [34].

In environments such as wastewater treatment plants (WWTPs), sensors are prone to malfunction due to harsh conditions. Yoo et al. [81] implemented monitoring methods that can reconstruct sensor data in the presence of redundancy between sensors that can improve monitoring efficiency, demonstrating the need for robust and resilient sensor technologies in these environments. For instance, toxicity measurement in biological WWTPs is particularly daunting. These systems are vulnerable to toxicants in their influent and most toxicity measurement methods are performed offline, limiting their adaptability to online monitoring for early warning. Although the development of biosensors for toxicity assessment in aquatic environments and biological WWTPs is expanding, there is still a need to improve sensitivity and develop a matrix of biosensors to address these challenges [79] adequately.

In real-time or online monitoring, especially biosensors, the accuracy of existing hardware sensors is often insufficient, and maintenance problems such as electrode fouling are common. To overcome these limitations, software sensor techniques have been developed, utilizing correlations between different parameters to estimate water quality, offering a workaround for the limitations of hardware sensors [11]. In addition, researchers have also turned to advanced computational methods. Techniques such as mathematical models, statistics, and machine learning have been used to predict parameters such as pH, biochemical oxygen demand (BOD), and nitrate levels. These efforts aim to supplement or replace physical sensors that are susceptible to disturbances. Despite some successes, traditional methods often fail to capture the complex dynamics of natural environments, leading to a growing interest in more sophisticated models. For example, Ooi et al. [56] demonstrated the use of machine learning techniques, such as Random Forest and Support Vector Regression, to predict BOD5, a sample of BOD during 5 days period, in water samples, highlighting the shift towards advanced computational methods for environmental monitoring.

1.1 Background

Nitrate pollution in aquatic ecosystems has emerged as a significant environmental concern, impacting both aquatic life and human health. The prevalence of nitrates, which come from natural and anthropogenic sources, has led to an increase in the eutrophication of water bodies [10]. Addressing this issue is imperative, yet high costs and operational complexities often hinder current methods for nitrate removal [36, 40, 60, 61, 69].

Wastewater treatment plays a critical role in mitigating nitrogen compound pollution. Biological wastewater treatment processes, especially Biological Nitrogen Removal (BNR) systems, have been widely adopted due to their effectiveness in removing nitrogen from wastewater. However, these systems face challenges related to high energy consumption and complexities of control[31, 35, 52, 76]. Traditional monitoring methods, such as titration and spectral analysis, are limited in providing real-time, online, and durable monitoring due to the need for sample preparation and expensive equipment [34].

Various challenges are encountered in biological wastewater treatment, mainly due to stricter environmental regulations and technological advancements. These challenges include the need for updated treatment processes in WWTPs for improved effluent quality, which increases operational and management costs [32]. Additionally, reliable field measurements are difficult to obtain due to issues such as solids deposition and instrument fouling, making real-time analysis challenging [32]. To address these problems, WWTPs have turned to soft-sensors, which are computer programs that model process data, categorized into phenomenological, data-driven, and hybrid models [32]. Although data-driven modeling offers promising solutions for process monitoring and fault detection, its adoption is not as widespread as in other sectors [32]. Furthermore, the process data in WWTPs are subject to various disturbances, such as seasonal trends and variations in industrial processes, which require robust backup systems and real-time process monitoring to ensure efficient operation [32].

1.2 Motivation

Physical sensors are subject to environmental conditions, calibration drift uncertainties, are expensive, difficult to set up, and are unreliable [25, 67]. Over time, these regular sensors can get less accurate due to aging, while in contrast, data-driven models such as soft sensors get better over time due to accumulating data, consequently leading to better accuracy [77], as shown in Figure 1.1.

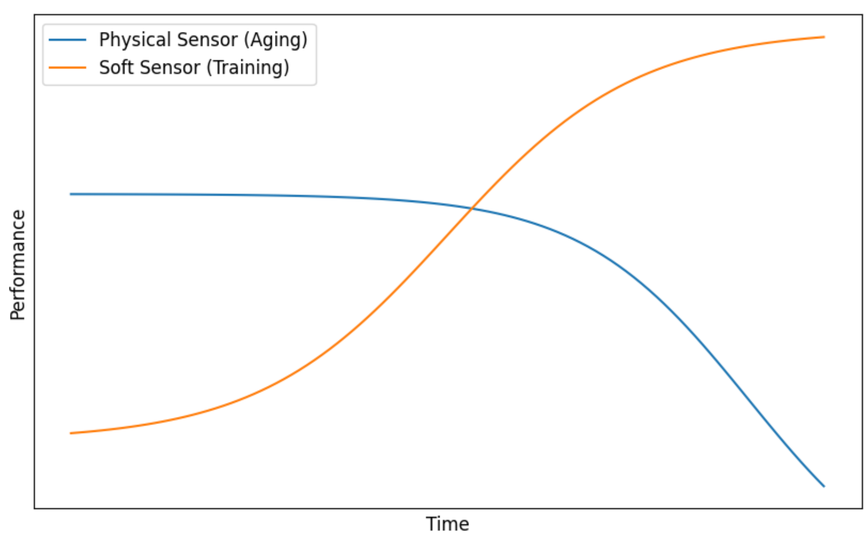


Figure 1.1: Representation of comparing the performance between a physical sensor and a soft sensor (over time).

Considering these aspects, this work focuses on investigating and developing a framework for creating trustworthiness in utilizing soft sensors.

Implementing data-driven soft sensors in biological WWTPs is a complex task, with several key challenges impacting their effectiveness and reliability. Sensor reliability in the hostile environments of WWTPs also presents a significant challenge. The quality of the collected data is often compromised due to harsh conditions, which adversely affects the effectiveness of soft sensors that estimate critical process variables, such as nitrate level [12]. The quality of the data and the selection of input variables are crucial to developing effective soft sensors. Poor data quality and the challenges of selecting the right variables can significantly affect the accuracy of soft sensors in estimating water quality variables, underscoring the need for careful data management and analysis [43]. The design of effective soft sensors requires a careful selection of variables suitable for calibration. This process can be challenging due to the variability and complexity of the data typically available from WWTPs [51].

1.3 Contributions

This thesis work consists of two main contributions:

1. AI and Cyber for Water and Agriculture testbed (ACWA), a water Cyber-Physical Testbed, aimed at advancing water resources' management using AI and cybersecurity experimentation. This testbed can address data availability and data quality issues.

2. Trustworthy Soft Sensing: developing a soft sensing framework, using deep learning that can empower non-AI experts. It is achieved by estimating predictive uncertainty and conducting context-based evaluations for nitrate, taking into account various factors such as water conditions, weather factors, and anomaly events.

Chapter 2

Literature Review

This chapter reviews the evolution of soft sensors, including a model-driven and data-driven approach, focusing on applications in biological wastewater treatment and their challenges. The transition from traditional model-driven approaches to AI-enhanced data-driven models in soft sensors highlights their crucial role in handling complex dynamic data in various industries. The review also addresses the challenges faced in biological wastewater treatment, emphasizing the need for advanced monitoring and control methods. Furthermore, it explores the significance of data availability in Artificial Intelligence (AI) applications, particularly in sectors such as agriculture and water management, and discusses the development of testbeds to tackle data-related challenges. This comprehensive review aims to provide insight into soft sensors and AI's current state and future prospects in addressing critical environmental and technological issues.

2.1 Soft Sensors

A soft sensor, also known as a virtual sensor, is a software-driven process that uses mathematical models to simulate the behavior of an actual, physical sensor [46]. Soft sensors are used to estimate real-time process conditions or product properties that are difficult, expensive, or currently impossible to measure directly with hardware sensors and also often refer as "hard-to-measure" variables. They often utilize input data from various sources, including readily available measurements from other physical sensors, process conditions, and historical data, often referred to as ”easy-to-measure” variables, to predict the variables of interest, as shown in Figure 2.1. Soft sensors can be categorized into two main types: model-driven and data-driven soft sensors [38].

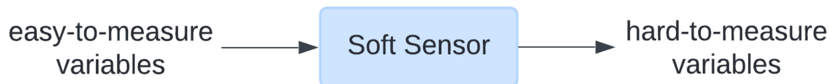


Figure 2.1: General representation of a soft sensor

Model-driven models, also known as first principle models, are typically based on the fundamental principles of the process, such as physical laws, chemical reactions, and thermodynamics. These models use equations to describe the behavior of a system, taking into account parameters such as mass and energy balances, reaction kinetics, and transport phenomena [38]. For example, a mathematical model for water distribution systems was developed to predict the steady-state flow pattern in a system consisting of conduits, pumps, pressure-reducing valves, and reservoirs, solving a system of nonlinear equations through the Newton iteration method [83]. Teppola et al. [72] developed a Kalman filter to address process drifting issues in activated sludge wastewater treatment plants, demonstrating the ability to recursively estimate model coefficients for improved prediction accuracy. This method depends on how much is known about the system. When the internal mechanisms are known, it is common to model them using known relationships from physics, chemistry, biology, among others. However, in many cases, some elements of the model are unknown and have to be determined using parameter estimation. In addition, ensuring the models remain effective under varying conditions, such as changing weather patterns or water usage behaviors, poses a significant challenge [26].

Data-driven soft sensors are models that use statistical or machine learning methods to infer the values of difficult-to-measure process variables from more easily measured variables.

Unlike model-driven soft sensors, which rely on physical and chemical laws to describe a process, data-driven soft sensors rely on historical data to learn the relationships between input and output variables. Kadlec and Gabrys [37] discusses the evolution and importance of AI in developing soft sensors. Soft sensors have transitioned from model-driven approaches, based on physical and chemical principles, to data-driven models, which rely on process data and are often referred to as black-box models. This shift towards data-driven models has been driven by the increased complexity and instrumentation in processing plants. AI plays a critical role in these data-driven soft sensors, enabling them to handle complex data and adapt to changing process conditions. The future of soft sensors lies in the development of robust, adaptive AI models that can handle the dynamic nature of industrial data, with AI being central to achieving this goal. Kadlec and Gabrys [37] proposed a framework for soft sensor development, emphasizing automated data processing, model validation, and adaptation, to address the current challenges in soft sensor application.

2.1.1 Soft Sensing using Deep Learning

The advancement of soft sensors in wastewater management is a rapidly evolving field, marked by significant research efforts aimed at improving their performance, accuracy, and reliability. Researchers are employing techniques such as iterative regression methods to better predict water flow rates, addressing challenges such as missing data and variable selection [84]. Deep learning approaches are also being explored to improve the estimation of pollutants in industrial settings, addressing data scarcity issues [30]. Graziani and Xibilia [30] implemented neural network-based soft sensors for pollutant estimation in a water stripping plant, adopting a deep learning approach to address data scarcity issues. Their approach significantly improved the performance of neural network-based soft sensors, highlighting the potential of AI in augmenting soft sensor trustworthiness in complex industrial settings. Yan et al. [80] introduced a novel soft sensor modeling method utilizing deep learning. Their approach, which integrated denoising autoencoders with a neural network, was adept at capturing essential input data information, thereby enhancing the performance and generalization of data-driven soft sensors to estimate the amount of oxygen in flue gasses.

2.1.2 Predictive Uncertainty Estimation

Although Deep Learning methods have proved to work on complex problems, they cannot achieve true confidence in prediction [53]. Quantifying uncertainty in Deep Learning not only provides the interpretability of Deep Learning models, but also guides decision-making processes in critical areas such as healthcare, autonomous driving, and process monitoring [41]. Furthermore, the failure to identify overconfident predictions may lead to undesirable consequences. Integrating uncertainty quantification can improve model generalization by effectively managing overconfident predictions on unseen data, leading to advancements in model trustworthiness and safety in AI deployments.

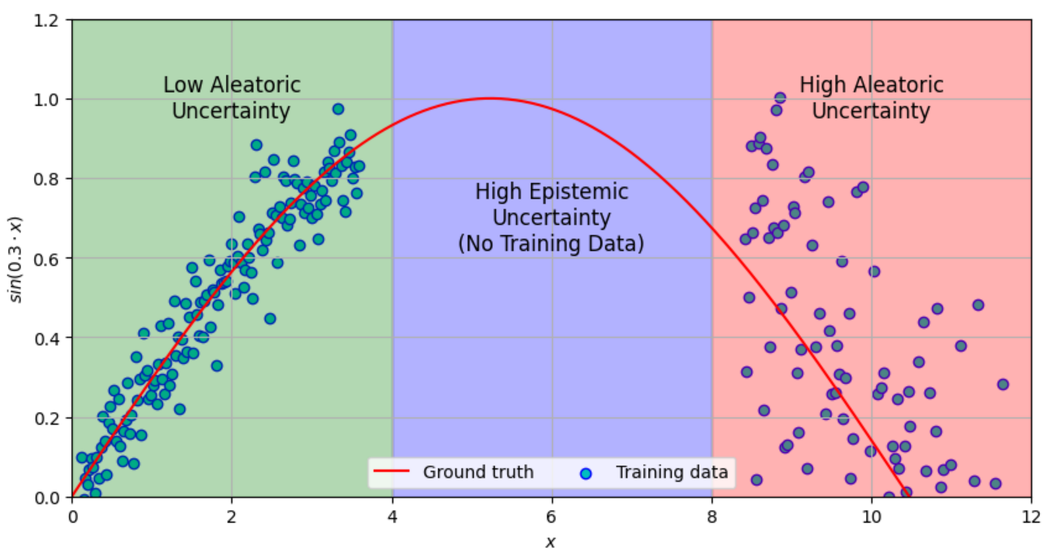


Figure 2.2: Illustration of the Epistemic and Aleatoric uncertainty. (This figure is adapted from Tuna et al. [74])

Uncertainties can be aleatoric or epistemic [75]. Aleatoric uncertainty refers to the random and unpredictable nature of the physical system inherent in physical phenomena and cannot be reduced. In soft sensors, this uncertainty results from measurement noise, namely the intrinsic variability found in sensor readings. This uncertainty is difficult to reduce even when more data are collected. However, the epistemic uncertainty is due to the model's lack of knowledge. It can be reduced with more data. Epistemic uncertainty is often captured using ensemble methods, where variation in predictions across different models indicates uncertainty. For example, if training data are insufficient, the uncertainty would be introduced in the parameters/weights of high-capacity empirical models such as deep neural networks. However, these uncertainties are usually combined and predicted as a single value, called predictive uncertainty [23]. Figure. 2.2 show the illustration of the epistemic and aleatoric uncertainty.

2.2 AI Assurance

AI models are typically evaluated on the basis of their ability to make accurate predictions during development. However, the ability and performance of these models may be influenced by context or domain-specific may evolve over time [22]. Batarseh et al. [7] define AI Assurance as a comprehensive process applied in all AI systems. This process aims to ensure that AI systems can produce outcomes that are not only accurate, but also valid, verified, data-driven, trustworthy, and explainable to non-experts. Furthermore, it stresses the importance of AI systems being ethical, unbiased, and fair in their deployment context. AI systems are often built upon specific domain and subareas; therefore, Sikder et al. [66] introduced two model-agnostic AI Assurance (AIA) pipelines, meaning they can be applied regardless of the specific AI algorithm used. These pipelines, based on game theory and Bayesian approaches, offer a way to assess AI systems across six goals: Explainable AI (XAI), Trustworthy AI (TAI), Fair AI (FAI), Ethical AI (EAI), Secure AI (CAI), and Safe AI (SAI) (see Table 2.1). This approach effectively bridges the gap between the theoretical underpinnings of AI assurance and its practical application, enabling stakeholders to gauge the trustworthiness and efficacy of AI systems in a dynamic and evolving technological landscape.

Table 2.1: AIA Goals definitions [68]

Term	**Definition**
Explainable AI	the AI algorithms can be explained or interpreted on how it came to a decision.
Trustworthy AI	Users are confident that the AI system works properly.
Fair AI	The AI system makes decisions without taking into account demographic, reverse reasoning, affiliation, or individual preferences.
Ethical AI	The AI system can make 'correct' decisions that benefit both affected and affected people, not only people who have technology power.
Secure AI	AI systems can prevent attacks or other threats that can undermine the system's proper functioning.
Safe AI	AI systems ensure the lives and well-being of people who use it and are affected by it.

2.3 Data Availability in Water Supply System

Deep learning models, such as Artificial Neural Networks (ANNs), are indeed known for requiring large amounts of data to train effectively [59]. This data-hungry nature can pose challenges, particularly in domains where collecting data is difficult or expensive, or when dealing with rare events. Several research papers and works address issues related to data availability, offering insight, methodologies, and innovations to mitigate these challenges. Elbasi et al. [19] discuss the application of AI in agriculture, which directly impacts water management. They highlight the use of sensors and soil sampling for data collection, which is crucial for managing water resources in agriculture. The paper emphasizes the role of AI in improving farmers' profitability and the overall economy, which is closely tied to efficient water use [19]. Mueller et al. [50] identify significant gaps in datasets for water assessment, particularly in the measurement and reporting of geographic water shortfalls. They underscore the need for comprehensive datasets to enable effective water management decisions in businesses [50]. Aani et al. [1] review the application of AI in water treatment and desalination. They point out challenges related to data structuring and the potential of AI to optimize operational conditions once these issues are addressed [1]. Suchetana et al. [70] introduce AI techniques on water data to promote sustainable usage. They discuss AI's insights for both short-term and long-term water policy decisions, highlighting the potential and challenges of using AI in water management [70]. Li et al. [44] detail AI's role in optimizing drinking water treatment processes. They discuss AI's potential in water quality diagnosis, decision-making, and operation process optimization, although they also note challenges in data availability and quality [44].

2.3.1 Water Cyber-Physical System Testbeds

Researchers are actively engaged in developing testbeds to address the critical issue of data availability in data-driven applications. These testbeds are designed to simulate real-world scenarios and generate comprehensive datasets that can be used to train, test, and validate various data-driven models and algorithms.

WaterBox

Kartakis et al. [39] presented WaterBox; a small-scale testbed that allows the simulation of monitoring and control processes of smart water systems. The WaterBox is a closed-loop structure consisting of three individual layers, as shown in Figure 2.3. The upper layer is the Supply, which simulates the reservoir and a pumping station. The WaterBox also has pressure sensors and controllable values to monitor the water transfer to the middle layer. The middle layer indicates three District Metered Areas (DMAs) represented by tanks of different sizes that provide water to the lower layer. The lower layer represents Demand, which mimics the water demand variation in time using valves. Each output from the DMA in the lower layer has a flow sensor and valve installed. In the end, the water from the lower layer is collected in a large tank and recycled to the reservoir using an underwater pump. The details on information on preliminary experiments using WaterBox are provided by Kartakis et al. [39].

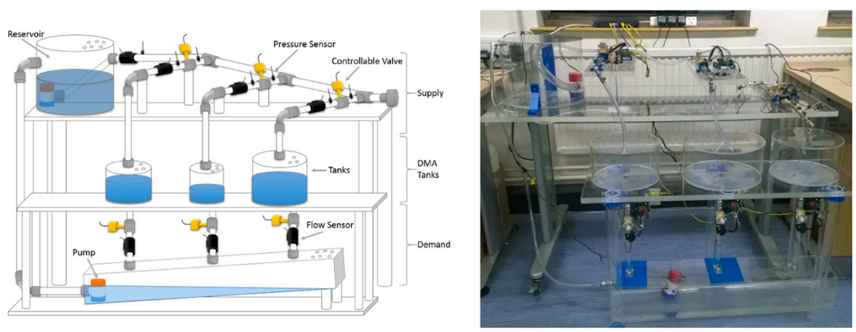


Figure 2.3: WaterBox testbed is a closed-loop structure with three individual layers [39]

Secure Water Treatment (SWaT)

Goh et al. [28] presented a six-stage Secure Water Treatment (SWaT) testbed, a scaled-down version of real-world water treatment plant. SWaT utilises membrane-based ultrafiltration and reverse osmosis units to produce 5 gallons per minute of filtered water. The overall process layout and the architecture of SWaT are presented in Figure 2.4. SWaT has six main processes: taking raw water (P1), pre-treatment (P2), filtration via membranes (P3), dichlorination (P4), reverse osmosis (P5), and distribution (P6). The authors collect data from these processes. Network traffic data are also collected from commercial equipment via Check Point Software Technologies Ltd. The additional details of data generation and attacks simulation using the SWaT testbed are discussed in Goh et al. [28].

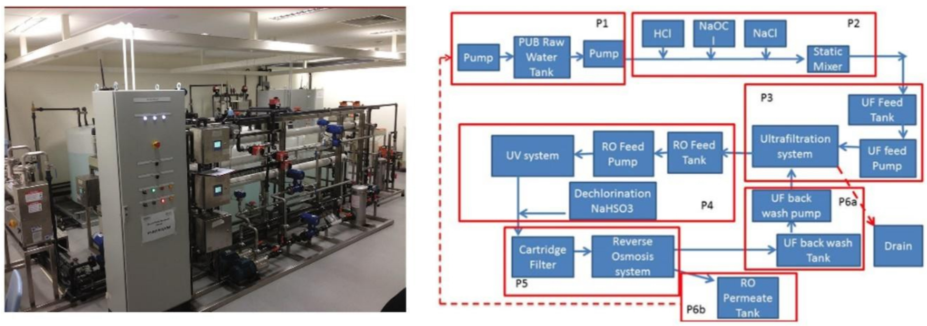


Figure 2.4: Overall process layout and architecture of SWaT testbed [28]

PLC-based water system

Laso et al. [42] presented a dataset generated from the physical water testbed to enable the detection of anomalies and malicious acts in cyber-physical systems. This testbed utilises two tanks (one with a 7-Litre capacity and the other with a 9-Litre) for storing water or fuel, one ultrasound depth sensor, four discrete sensors, and two pumps. As shown in Figure 2.5, the physical components are controlled and monitored using a computer connected to a Programmable Logic Controller (PLC). This water testbed simulates 15 unique situations affecting ultrasound sensors, discrete sensors, the underlying network, or the whole subsystem.

Smart Water Campus

Oberascher et al. [55] described the Smart water campus testbed for monitoring water networks that can be useful for fault detection in real-time along with involving cross-system improvements like rainwater harvesting. The authors noted that the Smart water campus is

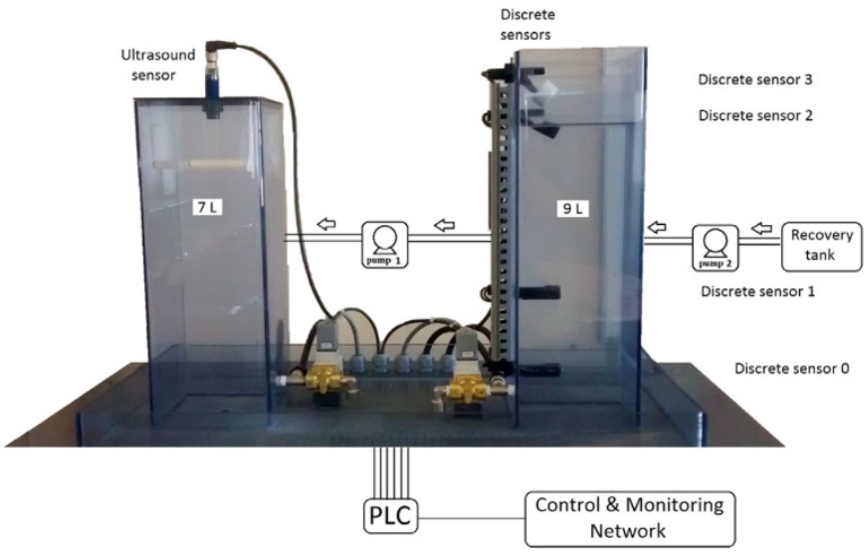


Figure 2.5: A physical water testbed used by Laso et al. [42]

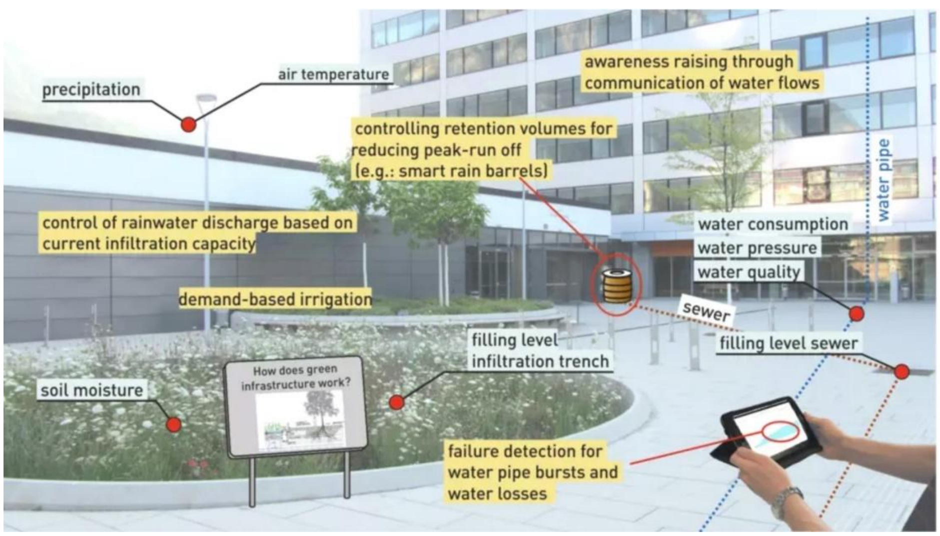


Figure 2.6: Illustration of features of the Smart water campus [55]

a network-based urban water infrastructure that integrates a water distribution network, an urban drainage network, and nature-based solutions. The testbed leverages perception, communication, middleware, and processing layers. An illustration of the Smart water campus testbed is provided in Figure 2.6.

Chapter 3

Problem Statement

In various industrial and scientific applications, accurate and reliable sensor measurements are crucial to making informed decisions and maintaining high-quality processes [58]. However, hardware sensors are subject to environmental conditions, calibration drift uncertainties, are expensive, difficult to set up, and are unreliable [25, 67]. Over time, these regular sensors can get less accurate due to mechanical degradation, while in contrast, data-driven models such as soft sensors get better over time due to accumulating data, consequently leading to better accuracy [77]. Considering these aspects, this work focuses on investigating and developing a framework for creating trustworthiness in utilizing soft sensors in the water sector.

3.1 Research Questions and Hypothesis

- RQ#1: Are soft sensors (nitrate) effective in sensing the nitrate level in water systems compared to the physical sensors?
- RQ#2: Can water testbed (ACWA) be used for developing a baseline nitrate soft sensor for a real-world water utility?
- RQ#3: How can the soft sensor be assessed for trustworthiness and uncertainty?

Chapter 4

Experimental Setup

This chapter presents the AI & Cyber for Water & Ag (ACWA) lab's experimental setup, a cyber-physical system that combines computational resources with a physical infrastructure of sensors and water management equipment. It details the creation of specific network topologies—Line, Star, and Bus—using water tanks and pipes to mimic water supply systems. The lab integrates a variety of sensors to monitor water parameters, which are essential for the development of deep learning models driven by data.

4.1 ACWA lab

ACWA lab is a cyber-physical testbed that comprises a cluster of computational resources, CPUs, GPUs, sensors, water tanks, pumps, valves, pipes, and soil beds. The lab's primary goal is to address pressing challenges in the water and agricultural domains by utilizing cutting-edge AI and cyber technologies. Some of these challenges include cyber security, resource management, sustainability, and decision making [6]. In addition, the AI assurance [5] aspect of AI, which is generally overlooked in biological domains, are also at the core while developing and promoting AI-driven solutions for these systems. Considering ongoing innovations and collaborations, the ACWA lab is developed to bridge the gap between research and practical applications to empower industries and communities while accelerating positive change in the global water and agricultural landscapes.

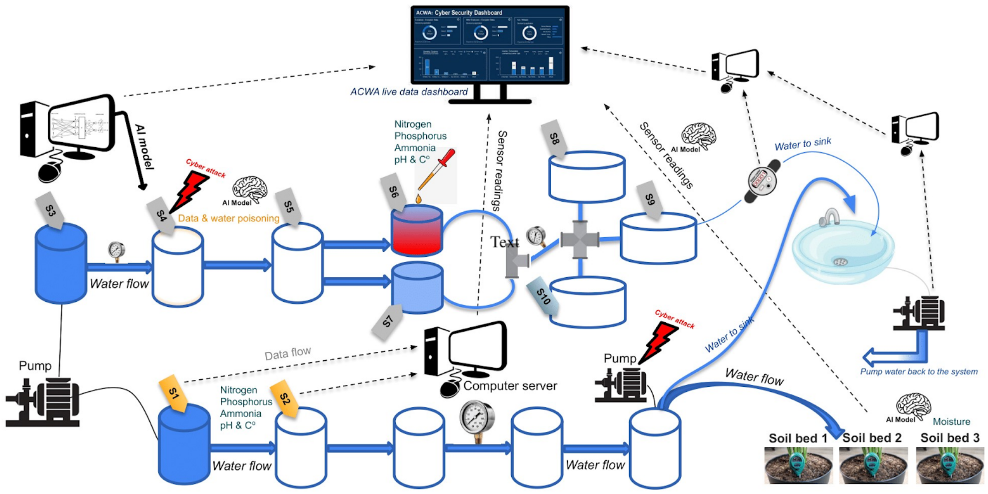
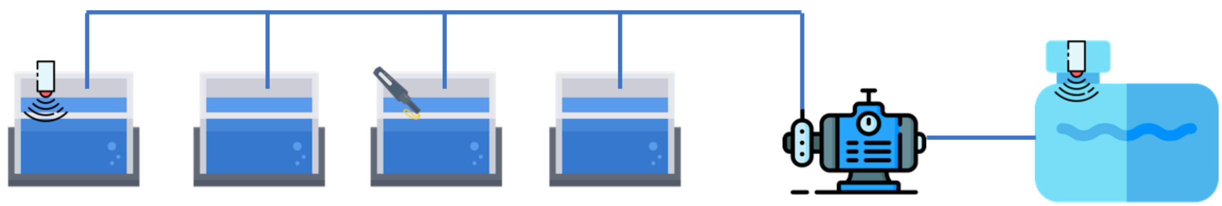


Figure 4.1: High-level design of the ACWA Lab, featuring water tanks, soil beds, pumps and sensors S1 through S17. These sensors are configured to measure water quality parameters, including water level, pH, electrical conductivity (EC), dissolved oxygen (DO), temperature, moisture, and other relevant variables.

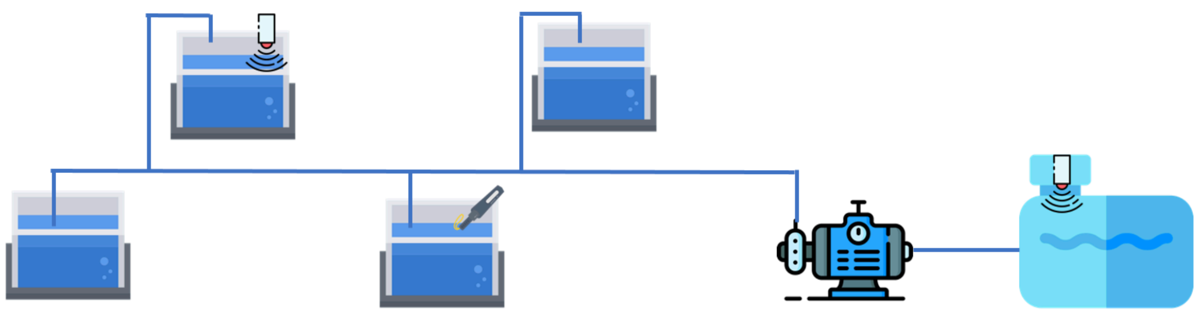
4.1.1 Water Testbed

In water system network design, a topology refers to the arrangement of nodes and their interconnections. Common network topologies, as highlighted in the literature [48, 57], include Line, Bus, Star, Ring, Mesh, Tree, and Hybrid, which form the basis of computer networks. Similarly, Water Supply Systems (WSS) adopt distinct structures like Grid-Iron, Ring, Radial, and Dead-End [3], which can be modeled using these fundamental computer network topologies. For example, the dead end WSS [13] resembles the bus topology, featuring a central line with branching sub-mains. The Ring WSS, a circular system [13], can be emulated by connecting the endpoints of a Line topology. The Radial WSS, with a central reservoir distributing water [13], aligns with the Star topology.

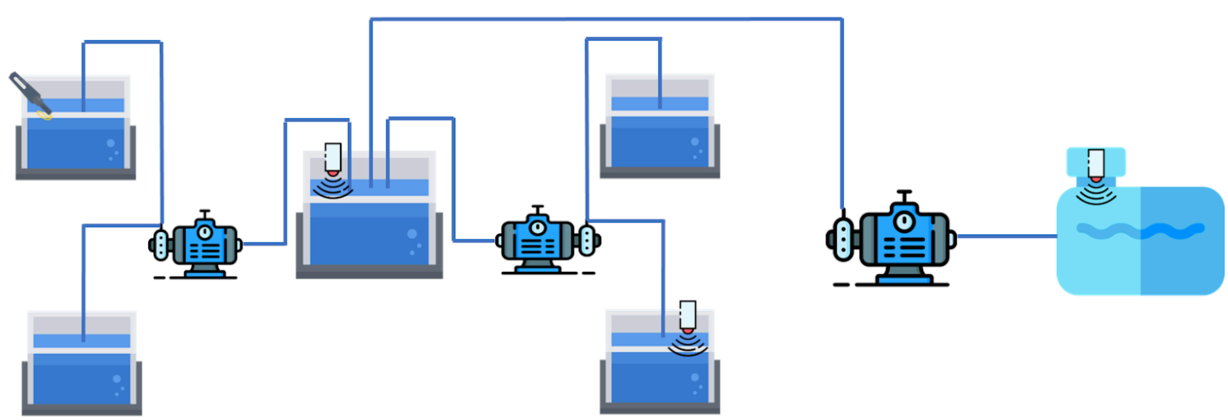
In this setup, the line, star, and bus topologies have been constructed to reflect these principles, as shown in Figure 4.2b. The water tanks, which represent the nodes, are connected



(a) Line topology



(b) Bus topology

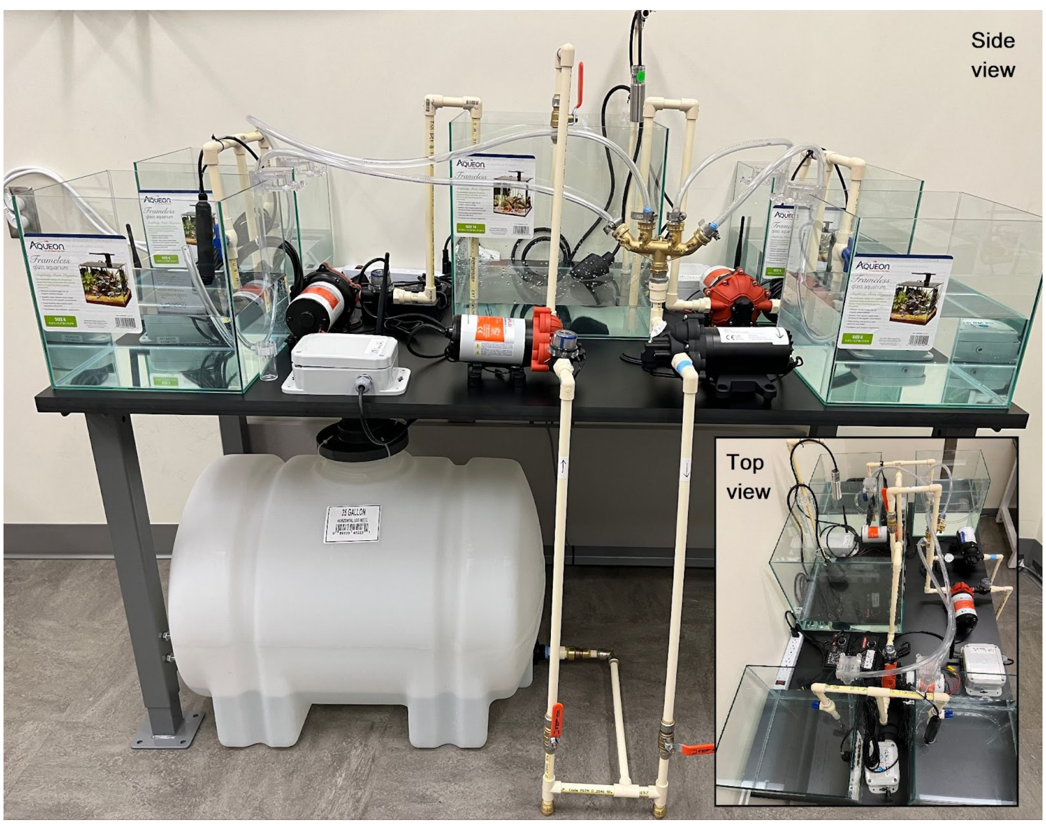


(c) Star topology

Figure 4.2: Representation of water testbed topologies [8]

(a) Line topology

(b) Bus topology



(c) Star topology

Figure 4.3: Water testbed topologies [8]

through pipes and tubes to pumps and reservoirs. These topologies, each on tables measuring 5 x 2.6 x 2.5 inches (length x width x height), can be combined into a hybrid topology using PVC or CPVC pipes. Two large 35 gallon tanks, measuring 29 x 20 x 23 inches (length x width x height), serve as water reservoirs for the testbed.

Specifically, the Line topology (Figure 4.3a) includes three 20.25 x 12.625 x 10.5 inch tanks (10-gallon capacity) connected via ½ inch PVC pipes, with two diaphragm water pumps and manual valves for control. This setup, equipped with water level, nitrate, pH, and temperature sensors, enables real-time data collection. The Bus topology (Figure 4.3b) utilizes two pumps and connects four smaller 16.25 x 8.375 x 10.5 inch tanks (5.5-gallon capacity) using ¾ inch C-PVC pipes, incorporating water level, EC, and pressure sensors. Lastly, the star topology (Figure 4.3c) features a medium-sized 15.25 x 15.25 x 15.25 inch tank and four 9.25 x 9.25 x 9.25 inch tanks, connected by 1 2 inch C-PVC pipes, four diaphragm water pumps, and a water splitter. This setup, equipped with water level, pH, temperature, and EC sensors, is designed for diverse data collection.

4.1.2 Sensors and System Architecture

The setup has computational resources, hardware, and software to conduct water and soil experiments that simulate different real-world scenarios of WSS and applications of precision and smart farming. This is possible due to the modularity and flexibility of components in ACWA such as pumps, valves, pipes, tanks, sensors, and soil beds. To simulate and collect real-time data on different scenarios of WSS, the lab sensors capture water parameters such as pH, temperature, dissolve oxygen (DO), nitrate, and Electrical Conductivity (EC), see Table 4.1. In addition, essential water-related variables such as water level, pressure, and flow rate are captured. These data are stored in the MongoDB database for analysis, and

Table 4.1: Technical details for sensors

Label	Name	Communication Protocol	Type	Topology
S01	S01_NCD_EcTempDo	Zigbee	EC/Temp/DO Sensor	Bus
S02	S02_NCD_EcTempDo	Zigbee	EC/Temp/DO Sensor	Star
S03	S03_NCD_PhTemp	Zigbee	pH/Temp Sensor	Line
S04	S04_NCD_PhTemp	Zigbee	pH/Temp Sensor	Star
S06	S06_Senix_WL	LoRa	Tough Sonic 50 Level Sensor	Line/Bus (Reservoir)
S07	S07_Senix_WL	LoRa	Tough Sonic 50 Level Sensor	Star (Reservoir)
S09	S09_Senix_WL	LoRa	Tough Sonic 14 Level Sensor	Line
S10	S10_Senix_WL	LoRa	Tough Sonic 14 Level Sensor	Bus
S11	S11_Senix_WL	LoRa	Tough Sonic 14 Level Sensor	Star
S12	S12_Keyence_Pressure	Modbus	Pressure sensor (GP-MT)	Bus
S13	S13_Keyence_Flow	Modbus	Flow rate sensor (FD-H)	Line
S15	S15_ECD_Nitrate	Modbus	S80 Nitrate Ion Sensor	Line

model development, which can assist in tackling challenges in the water and agricultural domains as found in recent literature [6, 16, 62].

4.1.3 Data Collection Process

Before initiating the data collection process, proper calibration of the sensors is essential. This step ensures the accuracy and reliability of the data obtained. Calibration is crucial for reducing potential measurement errors and biases. A list of standard calibration solutions is shown in Table 4.2 to facilitate this. These solutions are used to correct sensor readings to improve accuracy.

The data collection process varies depending on the network configuration, such as line, bus, or star topologies. The duration of this process ranges from 20 minutes to 60 minutes for each experiment, depending primarily on the sensor's response time to environmental changes.

The objective is to gather a comprehensive set of data points that covers a wide range of numerical values. For this purpose, a series of experiments have been designed, as outlined in Table 4.3. These experiments involve the adjustment of key environmental parameters, such

Table 4.2: Chemical Solutions at ACWA

Type	Concentration(s)	Usage
pH	4.01, 7, 10.01	Calibration of pH sensor for three-point calibration
EC	12.88, 64 (mS/cm)	Calibration of EC sensor for two-point calibration
Nitrate	10, 100 (ppm)	Calibration of nitrate sensor for two-point calibration
DO	Zero Oxygen	Calibration of DO sensor
Distilled Water		To remove mineral buildup from sensors

Table 4.3: Experiment for populating the dataset

No.	Experiment description
1	Utilize tap water to circulate through all topologies. Monitor and collect data during the water pumping process. The dynamics of water flow can influence various water quality parameters such as pH, DO, nitrate, and water temperature [18, 63].
2	In this experiment, the water source is replaced with water collected from the Duck-pond, a pond located on the Virginia Tech campus in Blacksburg, Virginia. This substitution introduces natural variability into the water.
3	This experiment introduces a range of water quality conditions by adjusting parameters using chemical solutions listed in Table 4.2. The aim is to diversify the dataset.

as pH, EC, dissolved oxygen (DO), and nitrate levels. This is achieved by adding specific solutions to the system, thus altering the environmental conditions.

Communication Protocols

The ACWA testbed's data acquisition system is designed to handle a complex array of sensor information, crucial for analyzing and optimizing water and agricultural resources. At the core of this system lies a sophisticated data storage mechanism that ensures the integrity and accessibility of the data collected from the multiple of sensors deployed throughout the lab. Sensors within the lab communicate through different protocols such as Modbus, LoRa, and Zigbee, each with a unique way of transmitting data. These diverse data streams are then converted into TCP/IP protocols facilitated by dedicated gateways. This conversion is critical to maintaining a consistency of network protocol to the centralized data server, as shown in Figure 4.4.

Within this setup, the three communication protocols play an important role. Modbus is a widely used communication protocol in industrial automation and control systems. It allows different electronic devices, such as sensors, actuators, and PLCs, to exchange data and control commands over a network [73]. LoRa, or Long Range, is a wireless communication technology for long-distance data transmission with low power consumption [14]. It enables devices to communicate wirelessly over extended ranges. Zigbee is a wireless communication protocol [20] developed to create short-range low-power networks between various devices. It is designed for home automation and industrial control. The Zigbee protocol enables efficient and reliable data exchange [20].

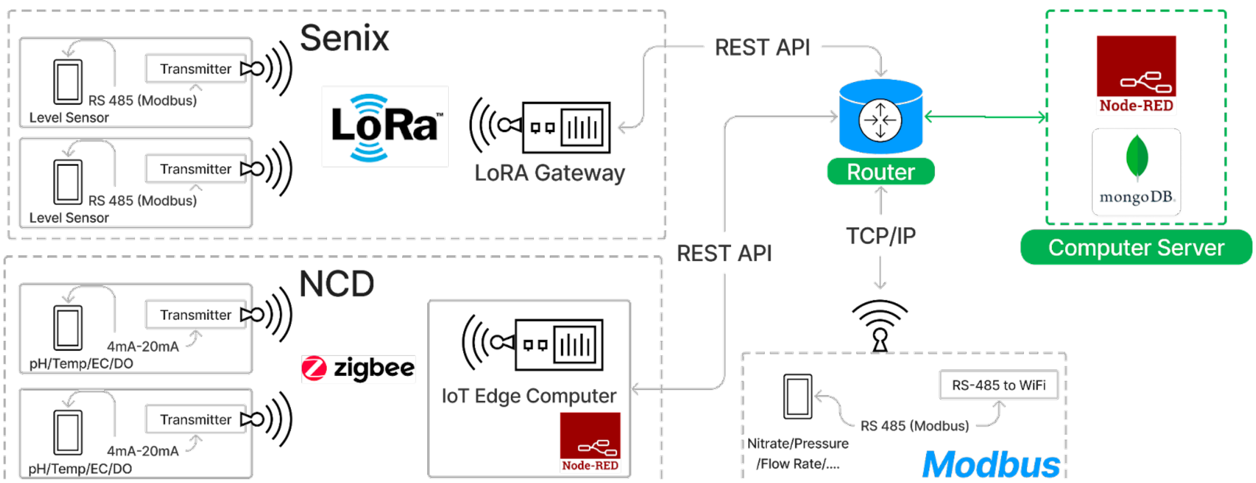


Figure 4.4: Overall sensors connectivity diagram

Data Storage

Node-RED is deployed as the backend server within this setup. It is a versatile tool that simplifies the data management process. Its primary function within the ACWA lab is to manage the flow of data from the sensors, ensuring that readings are collected efficiently and sent to the database without loss or corruption.

MongoDB, a NoSQL database, is chosen for storing data because of its flexibility to manage diverse data structures from different sensors. This database accommodates various data formats, eliminating the need for uniform data structures, a limitation often found in traditional databases. This adaptability is particularly advantageous in research environments where data types and requirements can rapidly evolve.

Chapter 5

Datasets

This chapter presents the datasets used in this study. The ACWA lab dataset, a water testbed with computational resources, sensors, and water systems, simulates real-world conditions to address data quality and availability issues in AI water system research. I also present the AlexRenew dataset (from a real-world wastewater treatment plant), reflecting external factors like weather changes and events. Both datasets are used in the experiments.

5.1 ACWA lab dataset

The ACWA lab [8], presented in Chapter 4, integrates advanced computational resources, sensors, and water management systems to address challenges in water and agricultural sectors using AI and cyber technologies. It focuses on cyber security, resource management, sustainability, and decision making. The versatility of the lab, with its array of sensors and equipment, allows for comprehensive simulations and data collection in water supply systems. Data from these simulations are stored in a MongoDB database, supporting AI model development and assurance. The testbed's data acquisition system utilizes various communication protocols, such as Modbus, LoRa, and Zigbee, ensuring effective data transmission and integrity to optimize water and agricultural resources. The data created and used to develop the soft sensor for this study are presented in Table 5.1.

Table 5.1: Data description for ACWA lab sensor variables [8]

No.	Parameter	Description (unit)
1	EC_s01	Electrical conductivity ($\mu S/cm$)
2	TDS_s01	Total Dissolved Solid (mg/L)
3	salinity_s01	Salinity level (mg/L)
4	temperature_water_s01	Water temperature ($°c$)
5	DO_s01	Dissolved oxygen level (mg/L)
6	DO_saturation_s01	Dissolved oxygen saturation (mg/L)
7	temperature_s01	Air temperature ($°c$)
9	pH	pH level
10	water_level_06	Water level of reservoir in line/bus topology (inches)
11	water_level_09	Water level in line topology (inches)
12	water_level_10	Water level in bus topology (inches)
13	water_level_11	Water level in star topology (inches)
15	flow_gpm	Flow rate in line topology (gpm)
16	flow_acc_g	Cumulative Flow (gallon)
17	nitrate	Nitrate level (mg/L)

5.2 AlexRenew dataset

AlexRenew is the wastewater treatment facility focused on transforming water pollution into clean water for Alexandria and parts of Fairfax County [33]. The AlexRenew provides real-world dataset and appears to cover a comprehensive range of parameters for wastewater treatment processes. The dataset , see Table 5.2, includes measurements of flow rates, such as total effluent flow, which indicates the volume of wastewater treated. Crucial water quality indicators, such as DO, ammonia (NH3), nitrate (NO3), pH levels, and temperatures for multiple reactors, are collected. In addition to water quality attributes, water systems such as AlexRenew are influenced by various factors beyond the treatment process. These include weather conditions (such as rain, snow and flooding) and anomalous events.

In addition to the primary dataset for AlexRenew, I have incorporated a comprehensive dataset of weather parameters, including precipitation and atmospheric temperature, sourced from the National Oceanic and Atmospheric Administration's (NOAA) National Weather

Table 5.2: Data description of AlexRenew

No.	Parameter	Description
1	Effluent Q	Final effluent flow (MGD)
2	Flow MGD Eff	Total Effluent Flow (MGD)
3	Flow MGD	Total Inffluent Flow (MGD)
4	Solid TSS	Average Dewatering Centrate TSS (mg/L)
5	Avg DO	Average DO (mg/L)
6	Min DO	Minimum DO (mg/L)
7	Max DO	Maximum DO (mg/L)
8	Avg NH3	Average NH3 (mg/L)
9	Min NH3	Minimum NH3 (mg/L)
10	Max NH3	Maximum NH3 (mg/L)
11	Avg NO3	Average NO3 (mg/L)
12	Min NO3	Minimum NO3 (mg/L)
13	Max NO3	Maximum NO3 (mg/L)
14	Min pH	Minimum pH
15	Max pH	Maximum pH
16	Avg Temp	Average Temp (F)
17	Min Temp	Minimum Temp (F)
18	Max Temp	Maximum Temp (F)
19	Flow MGD Eff	Reactor Decant Flow (GPD)
20	WAS Flow	Waste Activated Sludge (GPD)
21	Process Air	Process Air to CPT ($scfm$)
22	Carbon	Carbon transfered to CPT (gal)
23	Temp F	Average Centrate Temperature (F)
24	precipitation[1]	Precipitation ($inch$)
25	avg_t[1]	Air Temperature (F)

[1]NOAA

Service (NWS). This additional data has been seamlessly merged with the AlexRenew dataset. By doing so, I aim to provide a more holistic view of the impact these external conditions have on the study's result.

Chapter 6

Methodology

This chapter delves into the framework of trustworthy soft sensing. Afterwards, it presents how context-based evaluation works and how S2 score is formulated to provide comprehensive insight of how well the soft sensor performs in water systems.

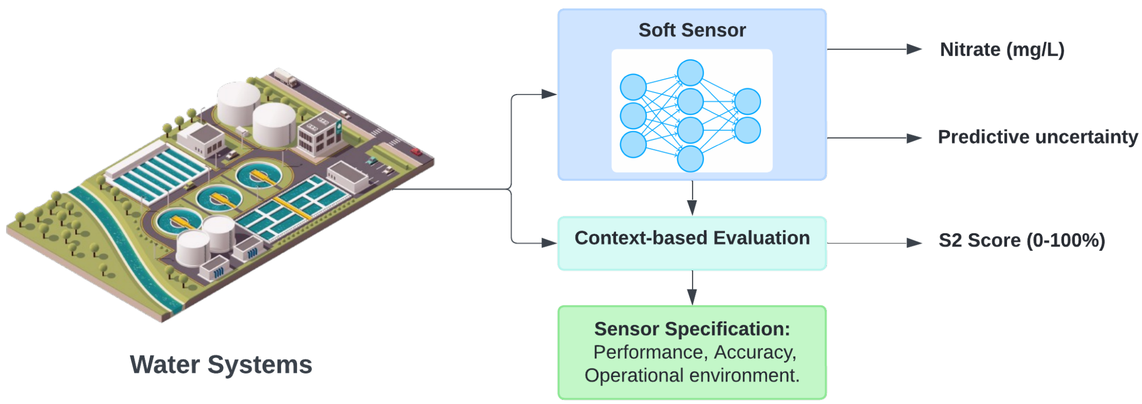


Figure 6.1: Trustworthy Soft Sensing Framework

6.1 Trustworthy (Nitrate) Soft Sensing

6.1.1 Data preprocessing

In the data preprocessing phase of the study, it begins by dividing the dataset into three subsets for different phases of model development: 50% is allocated for training, 50% for testing. Although this allocation seems unusual compare to previous studies, we want to

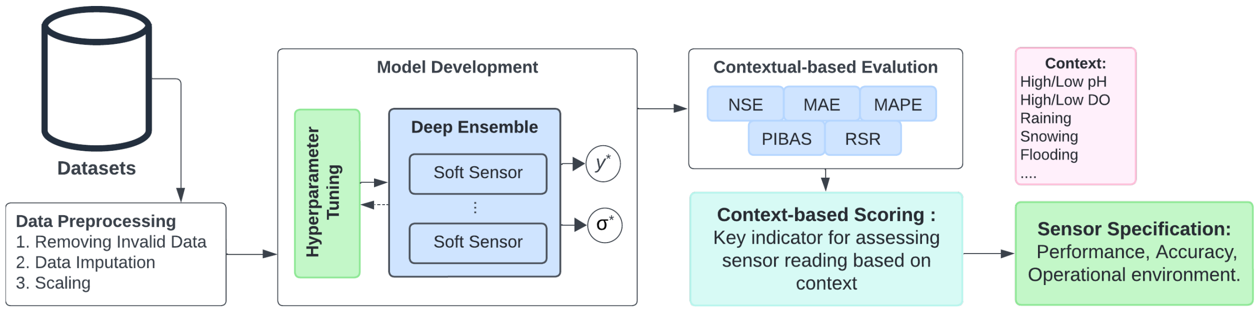


Figure 6.2: Overview of Trustworthy Soft Sensing Development

maximize the amount of data in testing set so that I can increase sample size in each class of context-based evaluation, potentially to increase improve confidence on the peformance result.

The preprocessing stage includes two primary techniques: data imputation and normalization. Data imputation, specifically through linear interpolation, addresses gaps in the dataset, a common issue in time-series data in water systems [27]. Despite its simplicity, linear interpolation is favored for its effectiveness in bridging these gaps, thereby maintaining the continuity and integrity of the dataset. To ensure uniformity in the data range and distribution, standardization scaling technique is applied to datasets.

6.1.2 Model Development

ANN is a computational model inspired by the networks of biological neurons found in brains. It is a key component of AI and machine learning, designed to simulate the way human brains analyze and process information. It is made up of nodes, or artificial neurons, that are connected by edges that represent the synapses of a biological brain [2].

Among the existing soft-sensing models of WWTP, ANN is the most popular data-driven method to predict water quality parameters [77]. In particular, they played an important role in the simulation of industrial WWTPs and provided the feasibility for other practical applications [29]. There are many types of ANN, e.g., Back Propagation Neural Network (BPNN), Radial Basis Function Neural Network (RBFNN), Feedforward Neural Network (FNN), Deep Belief Network (DBN), Growing DBN (GDBN) and DBN with Event-Triggered Learning (DBN-EL).

The performance of an ANN model is highly dependent on the selection of its hyperparameters [82]. Optimal models are selected through a process known as hyperparameter tuning. As noted by Yu and Zhu [82], random search is highly effective in most cases comparing the other algorithms such as grid search. This technique involves defining a hyperparameter space, randomly sampling from it, training and evaluating models with different hyperparameter combinations, and selecting the best-performing model. The advantage of random search is that it can efficiently explore the hyperparameter space and often yields good results with less computational cost compared to exhaustive search methods such as grid search.

6.1.3 Predictive Uncertainty Estimation using Deep Ensemble

Predictive uncertainty in deep learning is crucial for assessing the reliability of model predictions [24]. Deep ensemble models, which consist of multiple model instances, allow one to capture prediction variability and uncertainty, as shown in Figure 6.3.

Our study uses ensemble methods to capture the diverse predictive behaviors of individual neural networks. I improve model prediction variation by initializing each network with random weights, leading to different learning outcomes. Additionally, we use data augmentation techniques on the input data for each model, promoting further variance in predictions. The diversity in model training, along with our uncertainty calculation techniques, provides a robust framework for assessing predictive confidence. In this study, we use the number of models in the ensemble, M = 10 in the experiment using ACWA dataset and M = 11 in the

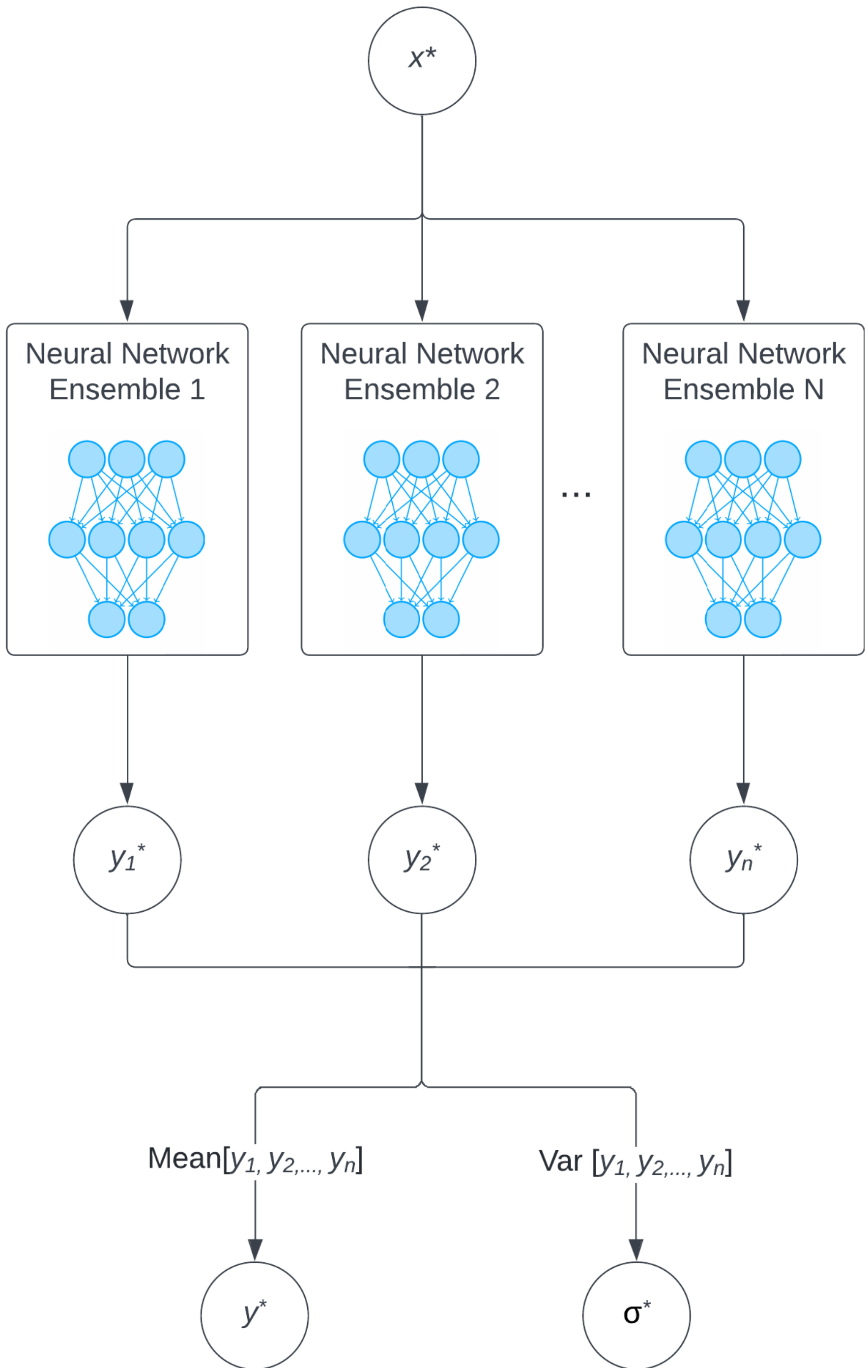


Figure 6.3: An illustration showcasing the core principles of uncertainty modeling in deep ensembles for neural networks. Each method provides a prediction y^* and a measure of model uncertainty σ^* for a specific input sample x^*. (This figure is adapted from Gawlikowski et al. [24])

experiment using AlexRenew dataset based on the performance metrics (RMSE, NSE, and RSR) and computation aspects, as shown in Figure 7.1.

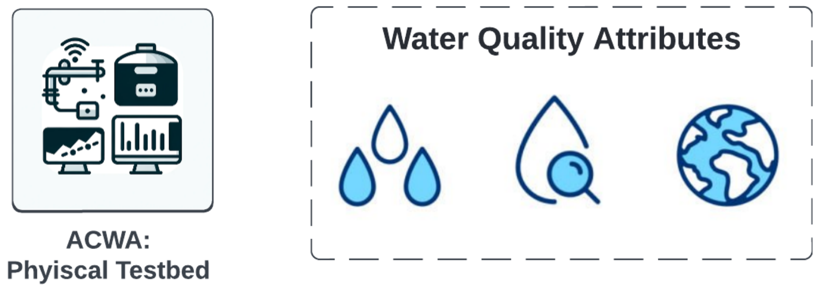


Figure 6.4: Water physical testbed characteristic

Figure 6.5: Real-world water systems characteristic

6.1.4 Context-Based Scoring Methodology

Researchers typically comprehensively assess model performance in a holistic manner. Some explore evaluating their models across various timelines or categories, yet it remains a challenge due to models' context-specific performance. Understanding this enables us to leverage models more effectively by concentrating on their strengths in specific context.

In the biological processes of the treatment plants, nitrate levels are largely influenced by water quality attributes such as pH, DO, NH3, and temperature [54, 78]. In addition, due to physical limitations in collecting nitrate levels, they can be influenced by external factors such as weather and extreme events, including overflow, flooding, rain, and snow, making accurate prediction and monitoring challenging.

In this study, I develop a scoring system that incorporates historical data to assess the likelihood that the soft sensor performs well in sensor readings based on context. By evaluating the soft sensor separately in the context of water quality attributes, weather factors, and extreme events, it provides more confidence the soft sensor reading's outcomes.

The experiment is divided into two parts: initially, it focuses on a controlled environment dataset, influenced solely by water quality parameters and flow dynamics. This allows for a thorough evaluation of the soft sensor within a controlled water quality context. Subsequently, the experiment extends to real-world water system datasets, incorporating additional factors such as weather changes and extreme events such as rain, snow and flooding, allowing a thorough evaluation of the soft sensor under varied conditions, as in Figure 6.5.

Evaluation metrics

The evaluation metrics selected below for assessing the performance of the nitrate soft sensor are widely recognized within the hydrological system and have been previously utilized in numerous studies [17, 64, 65]. The soft sensor are evaluated based on five metric: Nash-Sutcliffe Efficiency (NSE); Mean Absolute Error (MAE); Mean Absolute Percentage Error(MAPE); Percent Bias (PBIAS); and root mean square error-observation standard deviation ratio (RSR). The formulas for these metric are provided as follows:

$$NSE = 1 - \frac{\sum_{i=1}^{n}(y_i - p_i)^2}{\sum_{i=1}^{n}(y_i - \overline{y})^2} \tag{6.1}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - p_i| \tag{6.2}$$

$$MAPE = \frac{100\%}{n}\sum_{i=1}^{n}\left|\frac{y_i - p_i}{y_i}\right| \tag{6.3}$$

$$PBIAS = \frac{\sum_{i=1}^{n}(y_i - p_i)}{\sum_{i=1}^{n} y_i} \times 100\% \tag{6.4}$$

$$RSR = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - p_i)^2}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \overline{p}^2}} \tag{6.5}$$

In Equations. 6.1, 6.2, 6.3, 6.4, and 6.5, y_i is the observed data, p_i is the prediction of the model, and $\overline{y}$ is the mean of the observed data.

Context clustering using K-means Clustering

This section describes the approach used to create context classes based on each of water quality parameters such as pH, DO, Water Temperature, Air Temperature, and NH3 and so on, by using K-means clustering [45]. The objective is to segment water quality data into distinct groups that reflect similar water quality characteristics. This segmentation help to identify patterns or anomalies within the data, enabling context-specific evaluation. Before performing clustering of K-means on water quality attributes (such as pH, DO, temperature, NH_3, etc.), I used the silhouette score to determine the optimal number of clusters for each attribute. The silhouette score is often utilized in determining the suitable number of clusters in K-means clustering because of its effectiveness in quantifying how similar an object is to its own cluster compared to other clusters [71].

Table 6.1: Guidelines for evaluating the performance of hydrological modelling

Satisfactory Rating	References
NSE >0.5	Duda et al. [17], Moriasi et al. [49]
MAE <20	Shyu et al. [65]
MAPE <25%	Shyu et al. [65]
PBIAS <25%	Duda et al. [17], Moriasi et al. [49]
RSR <0.6	Duda et al. [17], Moriasi et al. [49]

$$J = \sum_{i=1}^{m} \sum_{k=1}^{K} \|x^i - \mu_k\|^2 \tag{6.6}$$

In Equation. 6.6, μ_k is the centroid of the cluster. The technique involves minimizing J with respect to the other variables, assigning the data point x^i to the closest cluster based on its sum of squared distance from the cluster's centroid.

S2 Score Methodology

The evaluation of nitrate soft sensing is conducted using a composite score derived from multiple metrics. According to the suggested guidelines in Table 6.1 for evaluating the performance of hydrological modeling, each metric is assigned a point. Each method is then scored as meeting criteria (1) or not (0).

Let's denote the S2 score as S2, and let $x_1, x_2, x_3, ..., x_n$ represent the different parameters, which could include pH, DO, Temperature, NH3, precipitation, events whether it is operating under flooding, overflowing, raining, or snowing. The normalized score S that ranges from 0 to 100% (or equivalently, 0 to 1 for a proportion) can be calculated using the following formula:

$$S2 = \frac{\sum_{i=1}^{n} w_i \cdot f_i(x_i)}{\sum_{i=1}^{n} w_i M_i} \tag{6.7}$$

Where:

- w_i are the weights assigned to each parameter x_i, indicating its importance in the overall score. These weights allow for the flexibility to prioritize certain environmental factors over others based on the context or objectives of the evaluation. For simplicity, we will assume that all $w_i = 1$ which means all context are equally important.
- $f_i(x_i)$, is the number of criteria met by x_i in a particular context class, contributing into a score to the overall score. For each parameter x_i, the function f_i evaluates the following conditions in Table 6.1 and sums the number of true statements.
- M_i is the maximum possible score or value that $f_i(x_i)$ can yield.

Scoring is based on a testing set from historical records under diverse contextual scenarios. This approach provides a holistic view for water utility operators and AI practitioners. For instance, Lin et al. [47] developed four unique flood indices by incorporating data of geographies, demographics and historical flooding records, with the intent of providing comprehensive insights for decision support at the federal level.

Chapter 7

Results

This chapter presents both overall and context-based performance result of nitrate soft sensor. The result of evaluating soft sensor in various of context are evaluated and providing estimated score by testing against the state of the art recommended performance for hydrological systems. The S2 score are used to evaluate the trustworthiness and robustness of the sensor outputs.

The results of hyperparameter tuning using the random search algorithm, as shown in Table 7.1. The differences in the best configurations of the ACWA and AlexRenew datasets are due to the varying network capacities and complexity requirements of the models. Both models are trained for approximately 200 to 300 epochs, with batch sizes of 64 and 128, respectively, to optimize performance based on the mean square error (MSE) criterion.

Table 7.1: Hyperparameters tuning result for soft sensors

Hyperparameters	**ACWA**	**AlexRenew**
No. of hidden layers	14	18
Learning rate	0.001	0.001
Layer 1 to 5	66, 672, 800, 32, 672 (ReLU)	770, 672, 672, 928, 608 (ReLU)
Layer 6 to 10	224, 160, 160, 32, 320 (ReLU)	704, 416, 160, 224, 672 (ReLU)
Layer 11 to 14	512, 576, 928, 512 (ReLU)	192, 992, 32, 32 (ReLU)
Layer 15 to 18	-	32, 32, 32, 32 (ReLU)

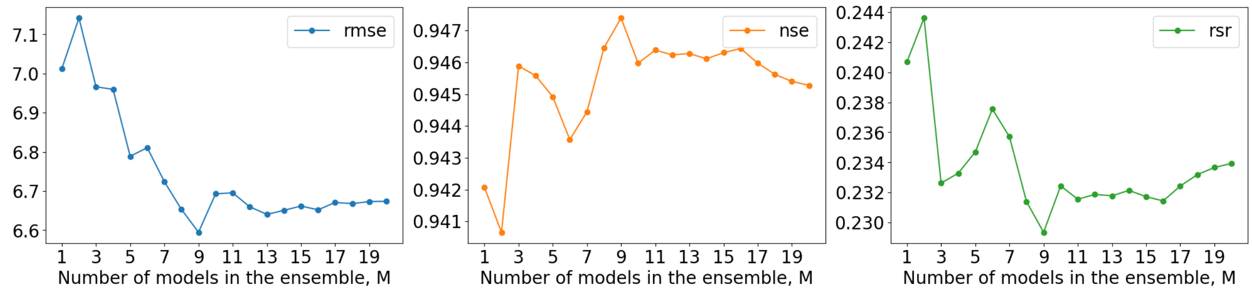
Table 7.2: Overall performance of soft sensor

Dataset	NSE	MAE	MAPE	RSR	PBIAS
ACWA	0.948	3.183	450.323	0.22	-0.911
AlexRenew	0.719	17.686	0.537	0.529	-1.938

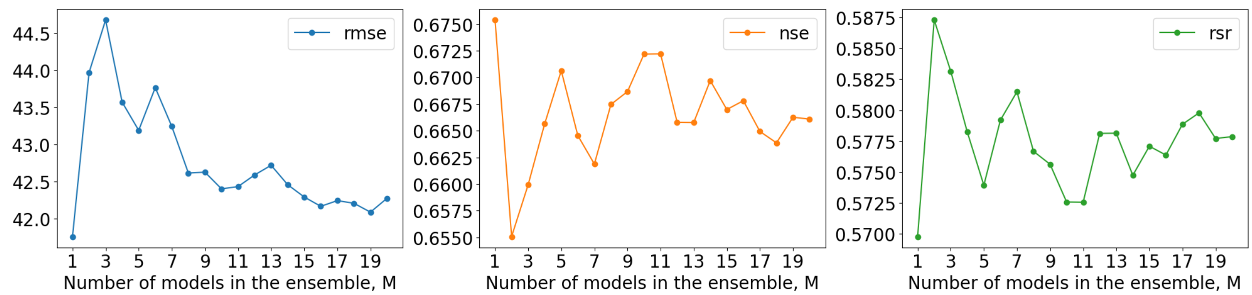
7.1 Overall evaluation

In this section, Table 7.2 present the results of the Soft Sensor in estimating nitrate level in water systems. We have selected five key performance metrics to evaluate the sensor based on NSE, MAE, MAPE, RSR and PBIAS that are commonly used to assess performance in hydrological systems [17, 49, 65].

According to the result, the soft sensor performs very well on the ACWA dataset, with high accuracy reflected by NSE of 0.948 and a low MAE of 3.183. The unexpectedly high MAPE of 450.323 with a low MAE, which may suggest the presence of skewed data, particularly if the actual values in the dataset are very small or close to zero. In this case, even minor absolute errors can produce large percentage errors. For the AlexRenew dataset, the sensor shows good but lesser performance with an NSE of 0.719 and a much higher MAE of 17.686. The MAPE is significantly lower than ACWA's at 0.537, indicating more consistent percentage errors. RSR is acceptable for both datasets, with ACWA at 0.22 and AlexRenew at 0.529, implying satisfactory performance. The hyperparameter configurations detailed in Table 7.1 may contribute to the model's tendency to slightly underestimate nitrate levels in both datasets. A more pronounced underestimation is observed in the AlexRenew dataset, as indicated by a PBIAS of -1.938, in contrast to the -0.911 recorded for ACWA. Overall, the soft sensor appears to be more accurate and reliable for the ACWA dataset than for the AlexRenew dataset, although there are concerns such as outlier or skewed data about the high MAPE value for ACWA (also given it a controlled environment) that should be further investigated.



(a) ACWA



(b) AlexRenew

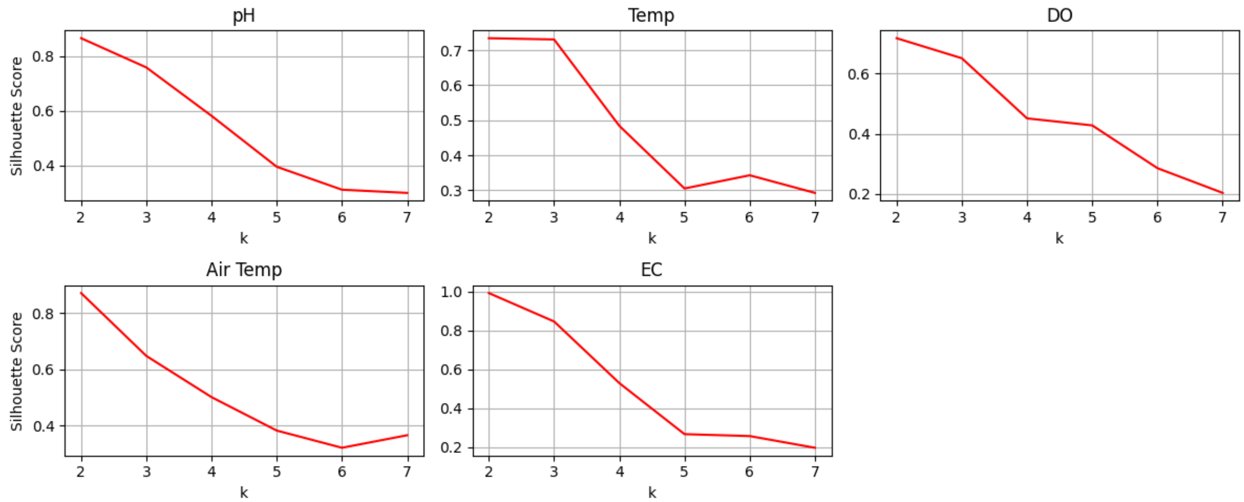
Figure 7.1: Improving Performance through Deep ensemble: A graph showing the relationship between the number of models in an ensemble and overall performance. As the number of models increases, performance initially sees significant gains, reaching an optimal point before plateauing, illustrating the diminishing returns of adding more models.

7.2 Context-based model evaluation

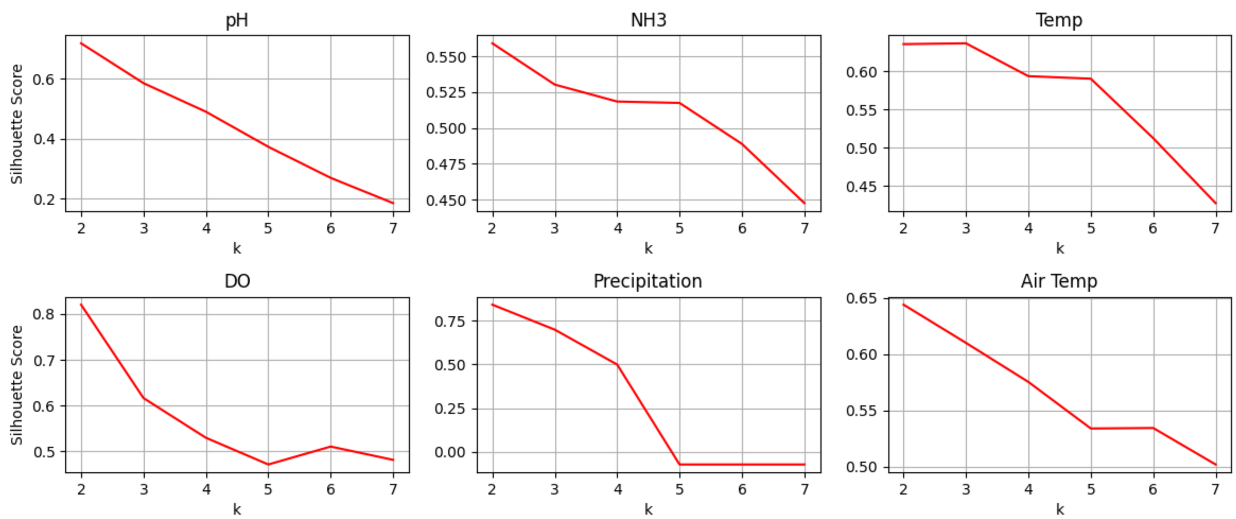
To evaluate the performance of soft sensors based on context, it is important to first define contexts that are going to be assessed. In this study, we employed K-means clustering to establish multiple context-specific groupings, each characterized by differing ranges of values for water quality attributes and other external factors.

Within the ACWA dataset, the silhouette plots illustrated in Figure 7.2a indicate that for all water attributes (pH, Temp, DO, Air Temp and EC), a configuration of groups $k = 2$ is most suitable based on achieving the highest silhouette scores.

In the AlexRenew dataset, as illustrated in Figure 7.2b, the silhouette analyzes suggest that two groups ($k = 2$) are optimal for pH, NH_3, DO, precipitation, and air temperature, in



(a) ACWA



(b) AlexRenew

Figure 7.2: Silhouette Score Diagram for K-Means Clustering

terms of achieving the highest silhouette scores. However, the score suggests that three clusters ($k = 3$) have the temperature score.

The following section presents the evaluation and interpretation of the context-based performance result that was performed on both the physical water testbed of the ACWA data set and the real-world water utility of the AlexRenew dataset. All result will be tested against the guidelines for hydrological modelling in Table 6.1 and produce a score for each context.

7.2.1 ACWA Results Evaluations

The Table 7.3 presents evaluations of different contexts or ranges, with performance metric in the ACWA dataset. For DO, the NSE is satisfied at 0.709 and 0.963 for a range of 10.74 to 338.36 and 5.46 to 10.72, suggesting that the model performs well. The MAE and MAPE indicate that the model's output can be quite off, with the lowest error at a higher DO range.

For EC, the model shows high performance in one context (0.0 to 360.26) with an NSE of 0.878 and low MAE/MAPE, but it's less accurate at higher ranges of conductivity, indicated by a lower NSE of 0.858.

For pH, the model has a high NSE across all pH ranges, indicating accurate predictions, with the highest accuracy in the range of 5.73 to 6.48. The negative NSE in the range of 6.49 to 7.11 suggests the model predictions are worse than an average-based prediction.

For air temperature, the model's performance is poor in the range of 21.28 to 22.43, as indicated by negative NSE values. Conversely, in the range of 22.51 to 23.77, despite the high MAPE, the MAE remains low, and the NSE exceeds the satisfactory benchmark. These results suggest that the model can capture the dynamics of the system; however, the high MAPE with the low MAE is likely due to actual nitrate values being close to zero.

For water temperature, the model performs well in estimating nitrate levels with a good NSE in the lower temperature range. However, at a slightly higher range of 21.97 to 23.39, the NSE drops considerably, indicating reduced model accuracy.

The model tends to overestimate nitrate levels (positive PBIAS) except at the highest EC range. The RSR values are generally low, suggesting that the model errors are modest relative to the variability of the observed data.

For validation, we plot the physical sensor against the soft sensor with predictive uncertainty

Table 7.3: Context-based evaluation of water quality attributes on ACWA dataset

Context		NSE	MAE	MAPE	RSR	PBIAS	count	Score
DO	10.74 to 338.36	0.709	7.943	1.883	0.537	3.589	98.0	3
	5.46 to 10.72	0.963	3.296	0.638	0.189	0.619	590.0	3
EC	0.0 to 360.26	0.878	4.692	0.167	0.342	1.055	293.0	4
	900.64 to 1092.82	0.858	3.413	1.296	0.375	2.112	395.0	3
pH	5.73 to 6.48	0.894	3.307	1.168	0.324	2.12	463.0	3
	6.49 to 7.11	-0.774	5.297	0.09	1.302	0.777	225.0	2
Air temp	21.28 to 22.43	-0.607	5.209	0.088	1.239	0.942	239.0	2
	22.51 to 23.77	0.882	3.291	1.203	0.343	2.009	449.0	3
Temp	21.55 to 21.76	0.861	3.228	1.279	0.371	2.037	419.0	3
	21.97 to 23.39	0.411	5.094	0.093	0.75	1.083	269.0	2

using our model and showing the S2 score, as shown in Figure 7.3. It seems that the soft sensor line closely follows the physical sensor line, providing a good estimate of the nitrate levels. The deviation between these lines indicates the error in the soft sensor's estimates. In general, the soft sensor seems to follow the trends of the physical sensor quite closely, suggesting that it is a good estimator for the physical readings. The confidence interval ($\pm 2\sigma$) shown in purple around the soft sensor readings is crucial to understanding the uncertainty in the soft sensor estimates. The width of the confidence interval indicates the level of confidence we can have in the soft sensor's predictions. A narrow confidence interval suggests that the soft sensor predictions are relatively precise. This occurs at several points along the time index where the purple band is small, indicating less uncertainty in the sensor's readings. A wider confidence interval indicates greater uncertainty in the estimates. This is noticeable during periods where the nitrate readings show high variability or spikes; the interval widens significantly, reflecting less certainty in the soft sensor's ability to predict accurately during these periods. The notable spikes in nitrate levels, where both sensors show a significant increase, could be due to external events or anomalies due to sensor readings. For instance, tampering with physical or water flow dynamics can influence the sensor measurements. If these spikes are accurate reflections of the nitrate levels, both sensors capture them, but

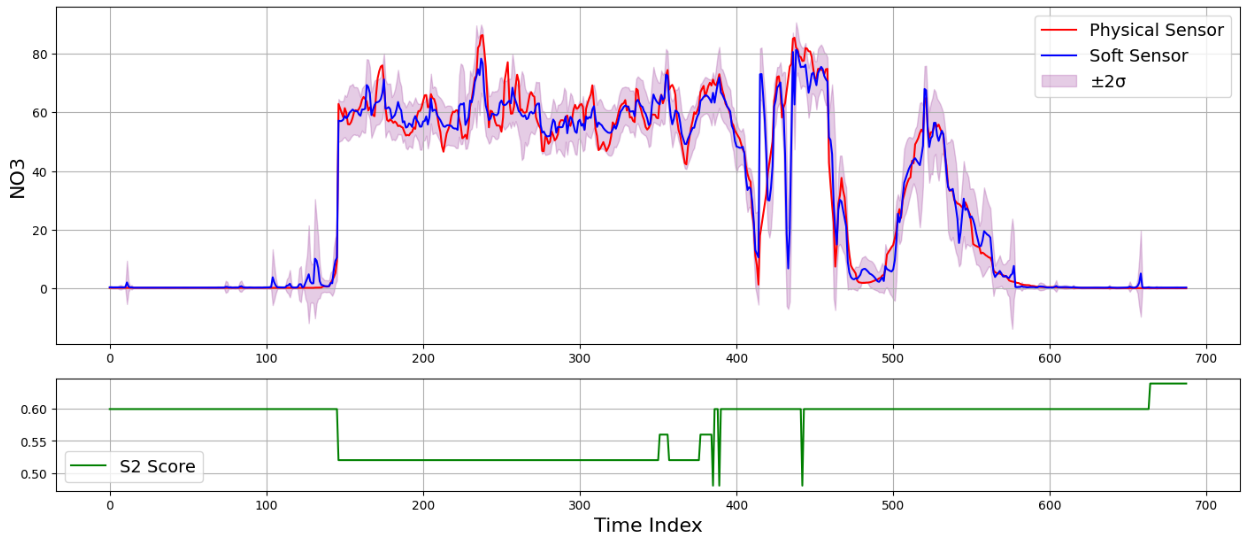


Figure 7.3: ACWA plot of physical sensor vs soft sensor (NO3)

during these periods, the uncertainty of the soft sensor increases, as shown by the widening of the confidence interval. There are times when the soft sensor readings fall within the confidence interval of the physical sensor. This overlap is a positive indication that within the uncertainty bounds the soft sensor is performing well.

7.2.2 AlexRenew Result Evaluations

Tables 7.4 and 7.5 presents evaluations of different ranges, with performance metric in the AlexRenew dataset.

For DO, the soft sensor's accuracy is moderate to low in predicting nitrate levels based on DO. It has an acceptable NSE of 0.771 for the lowest range but drops significantly for the mid-range (1.65 to 5.01), and slightly improves for higher DO levels.

For NH3, the NSE indicates that the sensor performs poorly for lower and higher ranges, with the best performance at a mid-range (134.07 to 384.32) with an NSE of 0.815.

Table 7.4: Context-based evaluation of water quality attributes on AlexRenew dataset

Context		NSE	MAE	MAPE	RSR	PBIAS	Count	Score
DO	0.0 to 1.65	0.771	18.689	0.183	0.478	-0.282	670.0	4
	1.65 to 5.01	0.08	35.914	0.971	0.951	29.049	111	0
NH3	0.03 to 133.1	0.117	22.34	0.43	0.935	8.077	383	0
	134.07 to 384.32	0.815	19.98	0.166	0.427	-1.15	398	4
Temp	60.85 to 79.2	-0.102	41.032	1.064	1.04	27.272	112	0
	79.7 to 90.06	0.796	17.271	0.195	0.45	-1.071	308	4
	90.13 to 100.34	0.768	18.263	0.142	0.48	-0.145	361	5
pH	3.71 to 7.17	0.762	19.705	0.22	0.486	0.737	587	4
	7.18 to 10.0	-0.215	25.469	0.522	1.093	10.953	194	0

Table 7.5: Context-Based Evaluation of weather factors on AlexRenew dataset

Context		NSE	MAE	MAPE	RSR	PBIAS	Count	Score
Air Temp	17.0 to 60.5	0.413	23.879	0.387	0.763	5.066	364	0
	61.0 to 91.0	0.782	18.744	0.215	0.466	-0.164	417	5
Precipitation	0.0 to 0.27	0.603	21.631	0.291	0.629	2.614	673.0	1
	0.27 to 3.44	0.793	17.816	0.318	0.452	0.381	113	3

For temperature, The model performs poorly at predicting nitrate levels for the lower temperature range (60.85 to 79.2), as suggested by the negative NSE. The performance improves significantly in higher temperature ranges, indicated by NSE values of 0.796 and 0.768 for mid and higher temperature ranges, respectively.

For pH, the sensor shows good accuracy in a lower pH range (3.71 to 7.17) with an NSE of 0.762, but a negative NSE (-0.215) for the higher pH range (7.18 to 10.0), indicating poor model predictions in more alkaline conditions.

For air temperature, the sensor's accuracy improves with higher temperatures, with moderate performance at lower temperatures (NSE of 0.413) and better performance at higher temperatures (NSE of 0.782). Prediction error, as indicated by MAE and MAPE, decreases in the higher temperature range, and PBIAS indicates a trend from overestimation to slight underestimation as temperature increases.

For precipitation, the model performs moderately well at lower precipitation levels (NSE of 0.603) and even better as precipitation increases (NSE of 0.793). Prediction accuracy increases and errors decrease in the higher precipitation range, with a PBIAS closer to zero indicating less bias.

The PBIAS indicates a general trend towards model overestimation in higher ranges of DO and pH, and underestimation in lower ranges of NH3 and temperatures, except for the lowest temperature range which shows overestimation. The MAE and MAPE values, which indicate average absolute and percentage errors, are relatively high across all contexts, particularly in DO and pH, suggesting that the model predictions can be considerably off from the actual measurements.

The RSR values are moderate, indicating that the model errors are reasonable compared to the observed data variation, except for the lower temperature range where the RSR is high, suggesting less reliable model performance.

Based on these scores, the model performs best at higher air temperatures and higher precipitation levels. The RSR values, which offer a standardized assessment of model error, are better (lower) in the higher ranges for both air temperature and precipitation, aligning with the other indicators of improved model performance.

Table 7.6: Context-based evaluation of anomaly events on AlexRenew dataset

Context	NSE	MAE	MAPE	RSR	PBIAS	Count	Score
Normal	0.66	21.3	0.23	0.58	0.87	500	3
Overflowing	0.902	14.17	0.188	0.308	-8.42	17	4
Raining	0.483	20.793	0.435	0.718	6.115	257	0
Snowing	0.673	22.105	0.172	0.554	0.3	23	3

Table 7.6 assesses the performance of a soft sensor in estimating nitrate levels during different weather or anomaly events. In normal conditions, the sensor has an NSE of 0.66, indicating a moderate fit to the observed data. The MAE and MAPE are relatively low, suggesting

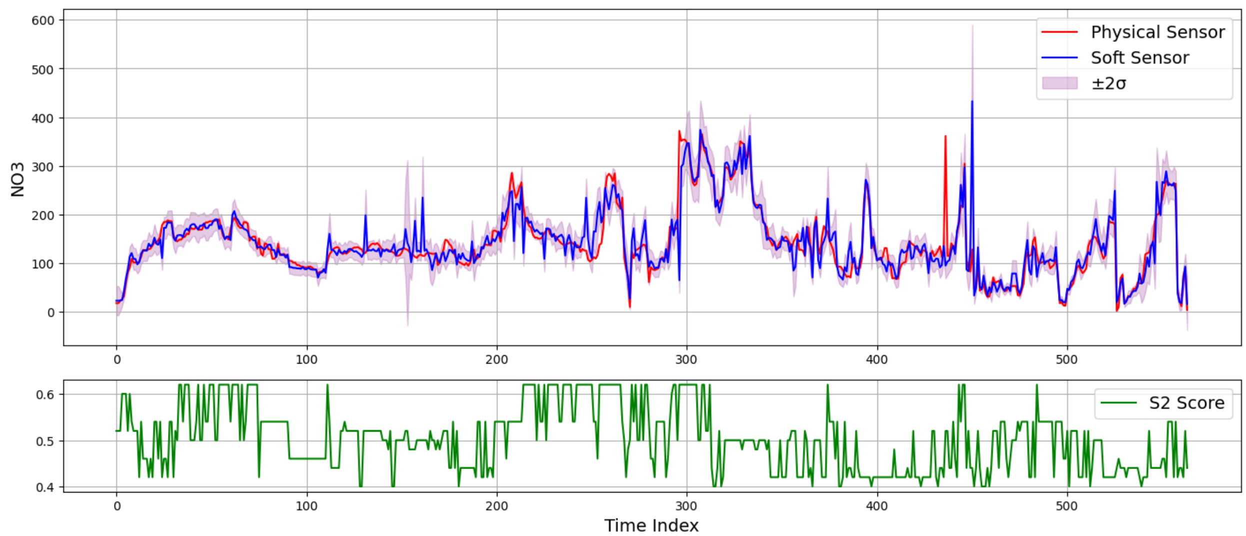


Figure 7.4: AlexRenew plot of physical sensor vs soft sensor (NO3)

decent accuracy in normal weather. PBIAS is slightly negative, showing a minor tendency for underestimation.

The soft sensor performs best under overflowing conditions with an NSE of 0.902, which denotes a high level of accuracy. The MAE is the lowest among all events, and the MAPE is also quite low, which suggests accurate estimation during overflowing. However, the PBIAS is highly negative (-8.42), indicating significant underestimation of nitrate levels during overflowing.

During rainfall, the model's performance drops (NSE of 0.483), with higher MAE and MAPE values compared to normal and flooding conditions. The PBIAS is very positive, indicating a substantial overestimation of nitrate levels.

For snowy conditions, the model has a relatively high NSE of 0.673, similar to normal conditions. MAE and MAPE are modest, comparing to among all events and in the guidelines Table 6.1, and the PBIAS is close to zero, indicating minimal bias.

We plot the physical sensor against the soft sensor with predictive uncertainty using our model and showing the S2 score, as shown in Figure 7.4. Both sensors' readings show nitrate levels fluctuating over time with some periods of increased variability and spikes. These could represent natural variations in nitrate concentration or response to specific environmental events. There are points, especially noticeable in the later part of the time index, where the soft sensor shows significant divergence from the physical sensor readings. This could be due to the soft sensor's model not fully capturing the dynamics of the system or due to anomalies in either the physical or soft sensor's data.

The scoring might correlate with the readings from the sensors in the upper graph. For instance, where there's a significant divergence between the soft and physical sensor readings, the S2 score may drop, suggesting that the soft sensor's performance is less reliable during these periods. The S2 score provides additional insight into the reliability and accuracy of the soft sensor's estimations.

Chapter 8

Discussions

The experiment of developing trustworthy nitrate soft sensors using deep learning in water systems provides substantial evidence towards addressing the research questions posed in this study. Through overall and context-based evaluations, the performance of soft sensors has been scrutinized across controlled environments (ACWA dataset) and real-world conditions (AlexRenew dataset), using metrics such as NSE, MAE, MAPE, RSR, and PBIAS, alongside a novel context-based scoring methodology.

The soft sensors demonstrate high effectiveness in the ACWA dataset, achieving a notable NSE value, indicative of their robust predictive capabilities in a controlled setup. However, the high MAPE suggests certain limitations, possibly due to anomalies caused by human interference and water flow dynamics during the data collection process. The performance in the AlexRenew dataset, although slightly reduced, still showcases the soft sensor's competency in real-world applications. The differences in performance underscores the soft sensor's potential and areas for improvement when transitioning from controlled environments to complex, real-world scenarios.

The study has shown that the ACWA water testbed serves as a valuable platform for developing and refining soft sensor methodologies. The controlled environment allows for detailed analysis and adjustment of models, which can then be adapted and potentially mimic against the complexities of real-world systems such as AlexRenew. The context-based evaluation, in particular, highlights how different environmental conditions and operational factors influence sensor performance, providing insights how well soft sensor performance in context-specific.

The context-based evaluation methodology and scoring developed in this study offer a novel framework to assessing soft sensor trustworthiness. By segmenting the dataset into different contexts—ranging from water quality parameters to weather conditions and anomaly events—the study quantifies the sensor's performance in each scenario, providing a different results based on context. The S2 score , crafted from the context-based evaluation, plays an important role in translating complex performance metrics into understandable and actionable insights. By assigning scores to different contexts, the study illustrate the sensor's strengths and areas for improvement. This S2 scoring system, rooted in the assessment against established hydrological modeling guidelines, as shown in Table 6.1, offers a clear and concise method for evaluating soft sensor performance across a spectrum of real-world conditions.

8.1 Conclusions and Future Work

In this study, we present ACWA, a Cyber-Physical testbed for water management, designed to leverage AI and cybersecurity experimentation to address challenges in data availability and quality. We have developed a Trustworthy Soft Sensing framework using deep learning, which is designed to be accessible to non-AI experts. This framework enables users to evaluate and quantify the robustness and trustworthiness of AI systems by estimating predictive uncertainty and conducting context-based evaluations. These evaluations consider various factors, including water conditions, weather factors, and anomaly events.

Our investigation highlights the significant potential of soft sensors in water quality monitoring and identifies specific areas for future improvement. The research findings affirm the effectiveness of soft sensors, the benefits of controlled environments for framework development, and the critical role of context-based evaluation in assessing sensors trustworthiness. This study lays a foundation for advancing soft sensor technologies, steering towards more accurate, reliable, and context-based monitoring solutions that promise to support sustainable water management practices.

Future research includes addressing sample size limitations in context-based evaluations, refining the scoring methodology, expanding the scope of sensor applications, and exploring other machine learning algorithms. Implementing soft sensors in real-world scenarios and integrating mechanisms for continuous adaptation will further enhance their reliability and utility in water resource management.

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