Forecasting Ammonia Concentrations and Color Levels using Machine Learning for Reclaimed Water Treatment Operation and Management

by

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Abstract

Water scarcity is a global challenge, and one of the promising ways to mitigate the water resource crisis is via wastewater reclamation. Chlorine is commonly used for reclaimed water disinfection and requires precise dosing to satisfy endorsed quality standards. Ammoniacal nitrogen (NH_3-N) and colour substances exist in the reclaimed water, which consumes chlorine and affects the chlorine dosing. Therefore, the on-line monitoring of NH_3-N and colour are usually practiced in reclaimed water facilities. However, the conventional on-line analyzers are wet-chemistry-based, and the measurement takes time. The limitation creates a potential issue: there may not be sufficient time for the downstream chlorine dosing system to respond to sudden surges in color and ammonia levels. To tackle this challenge, this thesis work developed time-variant models based on machine learning to predict the NH_3-N concentrations and colour levels in the reclaimed water three hours into the future. For the training dataset, the NH_3-N and colour data were collected by an on-line analyzer and a customized auto-sampling spectrophotometer, respectively. Both are installed in a reclaimed water treatment facility in Hong Kong. Baseline models for forecasting ammonia concentrations and colour levels were first developed with five machine learning algorithms. Long Short-Term Memory (LSTM) was found to be the most effective algorithm, with the lowest MSE values of 0.0405 and 0.0148 for ammonia and colour forecasting models, respectively. In the training processes, novel data pre-processing methods and feature engineering techniques were implemented to en-

hance predictive model performance. The data pre-processing methods were proved to enhance the quality of training datasets and improved the performance of ammonia and colour forecasting models by reducing the MSE values by 4.2% and 8.1%. The feature engineering results supported that the daily fluctuations in NH_3-N and colour have correlations with the urban water consumption patterns. This finding further enhanced the NH_3-N and colour forecasting model performance by reducing MSE by 8.9% and 28.6% compared to baseline models. The established models can be used to assist the disinfection control strategies based on the model predictions with the use of traditional process control systems. This research offers novel methods and feature engineering processes for NH_3-N concentrations and colour levels forecasting in reclaimed water for treatment optimization.

CHAPTER 1

INTRODUCTION

1.1 Background

Urban water challenge increases as the cities grow larger. The World Bank estimates that the urban population worldwide will double by 2050—with severe implications of escalating water demands in cities by 50–70 percent (TheWorldBank, 2021). Global climate change has primarily affected the amount, distribution, and quality of the available fresh water in the urban water cycle. The report from (UNICEF, 2021) points out that one in four cities is facing challenges in supplying adequate water to inhabitants, and the situation is even worse in cities in the developing world. The rise of urban water usage will generate more wastewater. Thus, converting municipal/industrial wastewater into reusable water has recently drawn much attention. Reuse water increases availability by substituting freshwater for non-potable (drinkable) uses for agricultural irrigation, industrial and urban water reuse, etc. The alternative reuse water can supply many activities and save drinking water for other purposes elsewhere (Adewumi et al., 2010).

The construction of reclaimed water facilities often requires a huge amount of capital investment. Upgrading available wastewater treatment plants with reuse water treatment facilities is an economical solution accompanied by the potential of realizing resource recovery (e.g., nitrogen and phosphorus recovery) (Maryam and Büyükgüngör, 2019; Kehrein et al., 2020). The primary concern of reusing treated wastewater is the potential risks caused to public health. Under unexpected circumstances, the reclaimed water facilities can produce unqualified reclaimed water, which is harmful to the living beings (i.e., as reused water is ingested directly or through irrigated crops) and irrigated soil (Adewumi et al., 2010). In Hong Kong, reclaimed water quality is regulated with up to 10 or more water quality parameters, and any parameters that fail to meet the standard will lead to disqualification. The common practice for controlling the treated water quality is achieved through water quality control strategies. The market controllers have evolved from a simple on-off logic controller called Programmable Logic Controller (PLC), to a more advanced multi-step response controller called proportional-integral-derivative (PID), and finally to the controller consists of machine learning models.

The uses of machine learning models in the water quality controllers for assisting water quality control strategy are ground-breaking applications. Many research papers have proposed various machine learning models for replacing the PLC and PID controllers and demonstrated the benefits of machine learning models. From the study of (Librantz et al., 2018), PID and machine learning-based controllers were deployed to compare the operational costs of dosing the chlorine to the setpoint concentration in a drinking water treatment plant. The results showed that the Artificial Neural Network-based model has a more satisfactory cost reduction in a chlorination dosing control system than the PID controller. Another research finding suggests using a Support Vector Regression (SVR) model as the controller required less time to reach the setpoint concentration of free chlorine residual compared to the PID controller in both simulation and experimental conditions Wang et al. (2020). Incorporating machine learning models in traditional process control systems has also been practiced by Santín et al. (2015) for avoiding violations of total nitrogen in the effluent using the decisions made by Artificial Neural Networks. Long Short-term Model was also used to predict which process control strategy should be selected for eliminating violations of total nitrogen concentrations in the effluent Pisa et al. (2019). Forecasting water quality or predicting future events using machine learning are proved to be effective measures for controlling effluent water quality in wastewater treatment plants, making these approaches to be promising solutions for the reclaimed water treatment operation and management.

The superior performance of machine learning models comes from training high-quality datasets with a good amount of data that can fairly represent the system's dynamic. Most studies have only focused on evaluating the model performance by comparing the test loss values between models and the improvements over PID controllers without considering the collected dataset's quality. The noises in the data and the number of features (i.e., inputs or variables) are the two critical factors affecting machine learning models' accuracy and robustness. Many data pre-processing techniques are proposed and applied to enhance the dataset's quality. For instance, some papers discussed pre-processing data for removing the noise in raw datasets using data smoothing filters (Cheng et al., 2020), or creating new features in addition to the original ones (Mamandipoor et al., 2020) to achieve data augmentation. Despite the efforts being made, the influences of the proposed data pre-processing techniques on the final model performance have not yet been established.

Machine learning models for water quality control have two main types of algorithms, regression and classification. The former provides forecasting results of specific values, while the latter provides a decision of yes or no (i.e., 1 or 0). The regression model is also called the forecasting model, which plays a vital role in water quality control in drinking water treatment plants (DTPs) and wastewater treatment plants (WWTPs) by forecasting the future water quality. The need to use forecasting models is due to the unpredictable nature of water quality. Yet, the treatment operations are required to produce effluent satisfying the government regulation Chen et al. (2003) regardless of how the influent water quality may vary daily. In the reclaimed water system in Shek Wu Hui Effluent Polish Plant (SWHEPP), forecasting models are recommended for effluent treatment management and operation. However, only limited online sensors are available onsite. Despite the limited data for model training, it is still possible to train forecasting models with one feature, which is known as the univariate forecasting model. In this study, we will attempt to build machine learning models for forecasting water quality parameters in reclaimed water. Meanwhile, data pre-processing methods will be proposed and evaluated to address the research gap of insufficient understanding of data pre-processing in modeling in the wastewater treatment industry.

1.2 Objectives

The specific objectives of this thesis work are:
(1) To build baseline univariate forecasting models using machine learning and deep learning models.
(2) To develop data pre-processing techniques for removing data noise for enhancing model performance.
(3) To extract relevant information from reclaimed water system using domain knowledge for feature engineering.
(4) To create new features for augmenting dataset's quality for further improving forecasting model performance.

1.3 Organization of the thesis

In Chapter 1, "Introduction," the background information, objectives, and organization of the thesis were presented.

Chapter 2, "Literature Review", provides an overview of water quality control strategies in water treatment plants, wastewater treatment plants, and reclaimed water systems.

In Chapter 3, "Materials and Methods," the instruments for data collection of ammonia concentrations and colour levels, computer programming environment, and data preparation techniques were summarized. The processes of formulating extra features for training forecasting models were illustrated.

In Chapter 4, "Results and discussion," the performance of machine learning and deep learning models were compared. Forecasting models trained by different data preprocessing techniques and the influences of feature engineering on model performance were compared with the baseline model performance in test loss.

In Chapter 5, "Conclusions and Recommendations," the findings obtained from this thesis work were summarized, and possible future studies were recommended.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction to water quality control

2.1.1 Automated system for water quality control

A programmable logic controller (PLC) is an industrial computer system designed for any process requiring a series of devices and equipment to operate cohesively to achieve multiple purposes in manufacturing or treatment processes. The main components of PLC include a central process unit (CPU), input modules, and output modules (I/O). CPU is responsible for processing digital signals from input modules and sending commands through output modules based on the control logic programmed on the PLC. For chemical dosing control in water treatment plants (WTPs), the PLC system receives readings from turbidity and pH sensors and uses pumps to dose aluminum solution automatically (Andhare and Palkar, 2014). The PLC system with the capability of producing real-time output commands in response to the input signals also makes it widely used in wastewater treatment plants (WWTPs). For oxygen concentration control in the aeration tank, the PLC system receives signals from dissolved oxygen (DO) detectors and transmits signals to open or close the electric butterfly valves to alter the DO concentration (Zhu and Qiu, 2017). Although PLC systems are the most used systems across industries for their easy programming and reliable control, PLC system is merely a device that can be programmed to control operative devices with on-off logic (i.e., a logic control with two states). The straightforward implementation of the PLC system compromised its ability to perform complex tasks in a more dynamic water treatment environment. In reality, many WTPs or WWTPs require precise control of the treatment processes. Being aware of the limitations of the PLC systems, a more advanced controller called proportional–integral–derivative (PID) controller for receiving analog signals was developed to obtain more sophisticated controls over the operative devices.

To react to rapidly-changing environments in wastewater treatment plants, a PID controller generates an output value based on the continuous calculation of an error value e(t), which is the difference between the desired setpoint (SP) and a measured process variable. Then, the controller applies a correction based on proportional, integral, and derivative terms in the control functions. The use of the "P," "I," and "D" allows the system to quickly reach steady-states with feedback control systems (i.e., the system output is returned to the system input, which is included in the decision-making process of PID controller). Generally speaking, a PID controller is a technology (i.e., a specialist algorithm) for controlling a single device with more complex logic, while a PLC system is a physical system consisting of different modules capable of controlling dozens of devices only with two-state logic. In addition, A PID controller can be designed to operate on a PLC device and provide a more specific control strategy to a designated device. In WWTPs, a single-variable feedback analog control loop in PID can be used to control the temperature in the activated sludge treatment by stabilizing the system temperature in a shorter time (Bados and Morejon, 2020). The feedback control scheme is also applied in DWTPs to adjust the addition of chlorine dosage (i.e., also known as the disinfection process, chlorination, or post-chlorination) to reach the target concentration of free chlorine residual (FRC) (Wang and Xiang, 2019). The disinfection process is carried out in a chlorine contact tank, which provides sufficient time for the chlorine to disinfect pollutants. Since the chlorine added by the dosing device requires time to travel from the entry to the exit, the system output can only reflect the changes in water quality in a delayed time of 30 minutes. In the case of chlorination, the time lag makes feedback control difficult (Kobylinski et al., 2006) as the system is delayed in responding to any sudden surge of the pollutants when it can only receive output at the end of the disinfection process. PID controllers in WWTPs also encounter similar challenges as the increasing complexity of water quality and stricter regulations on the discharged water quality.

Many control strategies are proposed to address the challenges encountered in the process control system. For instance, feed forward-feedback control, linearized and optimal control, model-predictive control, fuzzy control (Demir and Woo, 2014), etc. Among the algorithms used in control strategies, Artificial Intelligence (AI) modeling has gained the most attention in recent years compared to modeling based on mathematical or empirical formulas. In DWTPs or WWTPs, fully understanding the treatment plants' physical, biological, and chemical interactions is very difficult. The unpredictable behaviors during the water treatment can be the significant changes in influent flow rate, water quality fluctuations, the complexity of the biological treatment process, and the large time delay between control variables and the process inputs, etc. Therefore, AI modeling shows great potential in dealing with the highly complex conditions in the treatment process (Li et al., 2021). The next sections will discuss the applications of different AI modeling methods.

2.1.2 Artificial Intelligence

Artificial intelligence (AI) can perform cognitive tasks with the development of computational solutions. The concepts of AI are usually confused, and in fact, AI is a broad term, and any kind of algorithms or models involved in decision-making with computation fall in the domain of AI. For example, AI can be fuzzy logic and optimization algorithms, which are formulated with human design and involved in the computer decision-making processes. Another subset of AI is called machine learning (ML), but generating an ML model is different from generating a fuzzy logic model. ML uses learning algorithms to generate a model via learning from the historical or large amount of data without being explicitly programmed. ML algorithms can be classified into three categories, which are Supervised, Unsupervised, and Reinforcement learning. In the training process of supervised learning, input variables (x) and output variables (Y) will be provided. The model will learn from the provided datasets to map the x to the Y. A supervised model can generate a prediction based on the new input data (i.e., also called the unseen data). Unsupervised learning is when the dataset is not labeled, the model can learn to infer patterns in the dataset without reference to the known outputs. This type of algorithm can find similarities and differences in the data. In reinforcement learning, models are designed to constantly interact with the environment in a try-and-error way and receive rewards and punishments based on the purpose of the tasks. Generating an optimal action to achieve the lowest penalties is the primary function of a reinforcement learning model. Supervised learning is commonly used for machine learning in water quality control strategies. Regression is a supervised machine learning technique used to predict continuous values. A regression model can estimate the relationship between the input variables in the system and the output target from given datasets and then use the nonlinear relationship to map the unseen input data to predicted output data. This type of applications best fits for water quality prediction (Librantz et al., 2018), and sensor fault detection (Cecconi and Rosso, 2021), etc.

2.1.3 Machine learning and deep learning

In machine learning, popular models which researchers frequently use for training predictive models are Supporting Vector Machine (SVM), Random Forest (RF), and Artificial Neural Networks (ANN). RF models are popular due to their superior performance compared to typical machine learning algorithms. Xu et al. (2021) built an RF-based model to predict total nitrogen concentration in water bodies and proved RF models outperformed models such as K nearest neighbor (KNN), Ridge Regression, and Multilayer Perceptron (MLP). The other two widely used models, ANN and SVM, were compared carefully with the reliability and accuracy in predicting 1-day interval T-N concentration in a WWTP (Guo et al., 2015). The results showed that the SVM model has higher accuracy while the ANN model is more reliable for decision-making. Although most of the studies did not focus on the underlying causes of why SVM, RF, and ANN models have more excellent model performance, it would still seem that these models are reliable options for predicting water quality empirically.

As the computing power doubles every 18 months according to Moore's law, implementing Deep Learning (DL)—a subset of machine learning, requires less and less computing time and becomes universal for researchers to solve everyday tasks. One way to explain a DL model is with the definition of having neural networks with more than two hidden layers (i.e., the model complexity increased and required more computing power to calculate). In DL, various architectures are specifically structured based on the problems we attempt to solve. For image processing, Convolutional Neural Network (CNN) is designed to extract essential features from the image vectors. Another famous DL architecture is the Recurrent Neural Network (RNN), which is powerful in solving time series-related applications and Natural Language Processing (NLP) tasks (Li et al., 2018). In particular cases, different DL architectures can be stacked in series to solve specific tasks. A rainfall-runoff prediction model was built using CNN and RNN (Li et al., 2022). The raw data features were extracted by convolution and entered into the RNN models for processing time-series patterns. The results showed a low Kling–Gupta efficiency (KGE) of 0.75 in the high-water period. DL models can be compelling when multiple architectures are stacked into a single model to perform a specific task, which machine learning models cannot realize. That being said, DL models can achieve higher model performance in terms of prediction accuracy compared to ML models.

2.2 Water quality control with machine learning

A drinking water treatment plant (DWTP) produces potable (i.e., drinking water) water for human consumption by removing contaminants from the source water, such as lakes or streams, or from underground aquifers. The raw water enters DWTPs and goes through treatment units of coagulation, flocculation, sedimentation, filtration, and disinfection in sequence as the primary treatment scheme in the conventional DWTPs (Li et al., 2021). During the treatment process, colloids, suspended matter, pathogenic microorganisms, and organic matter are removed to meet the regulated standard. However, raw water quality is not always stable, and corresponding actions must be promptly adopted when events like the surge of pollutants or the large variability of the influent flow. In any event, the treated water from DWTPs should generate drinking water that complies with the World Health Organization's Guidelines (i.e., WHO guideline) for drinking water quality. Otherwise, the treated drinking water would either be discharged, resulting in the short-term outage of water supply to the downstream cities; or the users will receive contaminated drinking water, which can transmit diseases and cause illness.

Turbidity is one of the critical water quality indicators, which can be defined as the "optical quality" of water. The unit describing the turbidity is the Nephelometric Turbidity Unit (NTU). High turbidity levels in raw water can impede the effectiveness of filtration and chlorination processes and potentially cause short-term outages of the water supply. Heavy rainfall and fissures within the aquifer can also lead to turbidity events that are most likely to cause high turbidity (World Health Organization, 2017). The challenge in the event of high turbidity in raw water is that it occurs rapidly, and mitigating activities must be actionable immediately. To address the sudden event of such, Stevenson and Bravo (2019) trained forecasting models based on general linear model (GLM) and RF to predict the time when the turbidity reaches higher than 7 NTU. The results indicate that both models can successfully predict the events (i.e., with accuracy between 0.81 and 0.86), and the RF model is found to have higher precision due to its ability to capture the nonlinear relationship between rainfall (mm) and turbidity (NTU).

To maintain operational costs and water quality in the coagulation process, the amount of coagulant, mainly subject to the turbidity and alkalinity in the raw water, is traditionally determined through manual sampling and analysis. Jar tests are designed to find the optimal chemical dosage for coagulation to remove the turbidity in raw water. The entire process includes on-site sampling and more than 40 minutes of laboratory work (Gani et al., 2017). To replace the laborious jar tests, Wang et al. (2022) proposed using principal component regression (PCR), support vector regression (SVR), and long short-term memory (LSTM) neural network to build predictive models for estimating daily chemical dosage. Compared with the linear PCR model, nonlinear SVR and LSTM models capture more relationships between the chemical dose (e.g., ferric sulfate) and the raw water quality based on a higher R-squared value of 0.70.

Disinfection is the last step of water treatment processes in drinking water treatment plants to generate safe potable water. In this step, chemical disinfectants such as chlorine, chloramine, or chlorine dioxide are added into the water to inactivate any remaining pathogenic microorganisms. However, the chlorination process requires precise dosing of disinfectant—too high will lead to the formation of disinfection byproducts (DBPs), and too low will result in insufficient levels of the residual disinfectant concentration. In both scenarios, the treated drinking water can pose health threats to the end-users. Although the PID controller can achieve automatic dosing of disinfectants according to the change in water quality, Wang et al. (2020) proposed a model predictive control based on machine learning models to improve the dosing process further. The study indicated that the predicted chlorine dosage from a Support Vector Regression (SVR) model could help the free chlorine residual in the water reach the setpoint concentration in a shorter time compared to the PID controller in both simulations and experimental conditions. Machine learning models can not only reduce the time required to reach setpoint concentration but also decrease the chemical usage required in DWTPs. An Artificial Neural Network-based model has proved to optimize the treatment operation by reducing the chemical usage in a chlorination dosing control system compared to using PID controller (Librantz et al., 2018).

The invariability of the raw water quality is always a big issue for disinfection. For instance, chlorine dose can be excessively dosed when the treated water contains fewer pollutants (e.g., non-organic matters and ammonia nitrogen). Exessive chlorine in water results in the waste of chemicals, which is reflected in the increased operational cost and the generations of undesired disinfection by-products (e.g., trihalomethanes (THMs), which are carcinogenic to humans). Xu et al. (2022) trained an ANN model for predicting the occurrence of THMs in tap water using simple and straightforward water quality parameters (e.g., pH, temperature, UVA_{254} and residual chlorine (Cl_2)). Despite the fact that the results showed a good model accuracy in predicting for THMs (i.e., T-THMs, TCM, and BDCM), the applications of the model are largely limited in reality due to the lack of dataset regarding quantity and quality. In fact, the lack of high-quality datasets for training ML models is a common issue, which explains, until recently, mathematical or empirical-based AI models like fuzzy logic (Gamiz et al., 2020; Godo-Pla et al., 2021) is still widely used for process control in WTPs.

2.2.1 Wastewater treatment plants

Human activities produce wastewater and discharge it from homes, businesses, factories, and commercial activities to the sewage systems which connect to wastewater treatment plants (WWTPs). The function of WWTPs is to remove contaminants from sewage and water so that the treated water can be returned to the natural water body without dangering any living beings residing in the ecosystem. Undertreated wastewater can lead to harmful algal blooms or cause oxygen deficit in the water (i.e., low oxygen content can kill the fish). The steps for treating municipal wastewater involve three major categories—primary treatment, secondary treatment, and tertiary treatment. Most of the particular matters will be removed in primary treatment via settling or floating; a secondary treatment is mainly responsible for removing BOD_5 in the biological processes; in the final tertiary treatment, membrane filtration, adsorption by activated carbon, and addition of disinfectant are applied optionally to further eliminate the undesired pollutants in the water.

Wastewater is categorized and defined according to its sources of origin. Domestic wastewater is water discharged from residential sources generated by kitchen wastewater, cleaning, and personal hygiene. Industrial/commercial wastewater is generated and discharged from manufacturing and commercial activities, such as the textile industry and food and beverage processing wastewater. Institutional wastewater is generated by large institutions such as hospitals and educational facilities. Regardless of the source of the wastewater, WWTPs have to achieve at least three sustainability targets: environmental protection (i.e., minimum pollutants discharge), social acceptance (i.e., human sanitary protection), and economic development (i.e., feasible operational and management costs) (Mannina et al., 2019). To effectively achieve these goals, process control is required to reduce energy consumption, improve effluent quality, and save costs in plant operation and management. The focus of this study is on discussing the development of using process control for treatment operation and management.

Under known operational conditions of a WWTP, machine learning models can be trained to assist the plant operators in optimizing treatment processes to improve effluent quality. Wang et al. (2021) proposed a machine learning framework, utilizing a model based on Random Forest to predict the effluent Total Suspended Solid (TSS) and phosphate (PO_4). This study uses data from six on-line sensors (i.e., flow rate, TSS, pH, PO_4, temperature, and total solids (TS) meters) across the treatment line to train the RF model. The results indicated that the influent temperature is the most influential variable for both TSS and PO_4 in the effluent, and PO_4 depends strongly on the TSS in aeration basins, etc. It has been suggested that the combined use of the RF model and analytical tools allows the author to pinpoint the critical factors influencing the effluent quality, which is regarded as an innovative approach. However, several significant drawbacks hinder such model developments using on-line sensors to collect training data. Many of the existing WWTPs and DWTPs are not equipped with on-line sensors, and a lack of automation and instrumentation is universal. The difficulties in installing on-line sensors include the extra costs of purchasing hardware, extra labor works for maintenance, and most importantly, the optimal locations for sensor installation.

In secondary treatment, the relationships between the sludge and wastewater quality are complex due to the complex interactions between the microorganisms and the organic matters in the reactor (Wilén et al., 2018). To fully understand and describe the interactions in such systems requires a substantial amount of data. However, installing on-line sensors everywhere in the system is impossible. Zaghloul et al. (2021) attempted to find out the ideal locations and adequate number for on-line sensor installation. The author used the data collected from the on-line sensors installed in three lab-scaled secondary treatment reactors to train machine learning models to predict effluent quality. In addition, considering the intricacy of operational conditions in the secondary treatment, the author claimed that with the use of feature selection and ensemble model (i.e., average results from multiple model outputs), overfitting could be prevented.

Like the secondary treatment units, an electrocoagulation reactor is also a complex system in which the operation and management are based on pH value, current density, flow rate, and the initial concentration of heavy metal ions, etc. Interestingly, instead of using an ensemble model to prevent the overfitting issue claimed by Zaghloul et al. (2021), Zhu et al. (2021) used a deep learning Long and Short-term model (LSTM) and an error compensate Autoregressive Integrated Moving Average model (ARIMA) to predict the removal rate of heavy metal ion concentration in wastewater. An LSTM-ARIMA model has strengthed the model performance compared to the solely used LSTM or ARIMA model in predicting removal rate shown by the Results. A possible rationalization of using an LSTM model without worrying about model overfitting is that deep learning is sophisticated enough for learning the nonlinear patterns in complex systems, while machine learning models like RF might fail to capture the intricate relationships, resulting in overfitting.

Technological advancement allows easy access to real-time water quality data via on-line sensors. The collected real-time data can be used to train predictive models and assist the plant operation and management. Despite the advantages of what on-line sensors are capable of, sensor calibration and maintenance are critical. The malfunctioned sensor can induce wrong decisions for plant operation, ultimately deteriorating treatment efficiency in WWTPs. Haimi et al. (2015) suggested that reliable and moderately-priced on-line sensors are not always available; in addition, sensor malfunctions (i.e., fouling or erroneous measurement) can cause the down-time of the sensors. For the unavailable sensors (i.e., "hard-to-measure" or expensive sensors), many research works have proposed building "soft sensors." Instead of using hardware sensors to measure the water parameters, the soft sensor generates real-time values through a machine learning model, which is trained by other easy-to-measure water quality data. In the works of Wang et al. (2019), easy-to-measure variables such as pH, flow rate, TSS, and ammonium nitrate (NH_4-N) are input to machine learning models to predict hard-to-measure water quality parameters of COD and total phosphate (TP). Pattnaik et al. (2021) also used DO, pH, conductivity, turbidity, and temperature to train a model to predict BOD. It is believed that both research works can solve the issues of the unavailability of specific water quality sensors.

The automated treatment operation and management heavily relies on the reliability of the on-line sensors, thus, preventing and the early detection of when the sensors are malfunctioned is the upmost concern to the plant operators. Sensor fault detections can be catogorized into three groups, which are (1) individual faults—an outlier data which can be distinguished with the respect to others data points; (2) contextual faults—an anomalous instance in a specific context and normal in another; (3) collective faults—a cluster of irregular intances with respect to other data trends (Chandola). Many research papers have proposed using machine learning models to help identify the sensor fouling.

Two main types algorithms, which is regression and classification can be used for finding fouling signals. A regression algorithm can identify fouling signals by comparing model predicted outputs (e.g., ammonium or COD concentration) to the actual signals; a classification algorithm can distinguish fouling signals through the direct outputs of the model (i.e., the model outputs 2 class labels, one can be assigned as normal and the other is abnormal signal). Cecconi and Rosso (2021) proposed a ammonium fault detection mechanism, utilizing a regression ANN model, along with principal component analysis (PCA) and Shewhart monitoring charts (i.e., statistical control chart). The remarkable idea from this study is to analyze the residaul between the predicted ammonium and the real ammonium snesor signal and identify the individual and contextual faults with the help of statistical tools. Despite the accuracy of fault detection mechanism can reach R^2 value of 0.87, the method comes with great limitations. The author points out to maintain the high accuracy of the predictive model, the quality of the input data needs to be carefully attended by performing manual cleaning procedures on a weekly basis.

Research has tended to focus on solving collective faults in sensor fault detection (ref of soft sensor solving individual faults) rather than collective faults. The major reason is collectives faults are hidden in regular signals, and only by identifing a combination of signals by experts can spot the irregularity. Thus classification technique using deep learnig is proposed to address collective faults in the works of Mamandipoor et al. (2020). It is believed that this is the first research paper using a LSTM network to achieve a fully automatic fault detection method in WWTPs. Contrast to others works, input variables for model training heavily relies on the manual selection of the experts before inputing into models like PCA and fuzzy nerual networks. The significance of using a deep learning network is it's capability of capturing long-term temperol dependencies from a large dataset compared to machine learning models (i.e., PCA-SVM model). The results showed that the accuracy (i.e., F1-score) from LSTM model is 92%, outperformed the PCA-SVM model of 87%. This finding suggests using DL models in classification problems is promising for solving collective faults.

2.2.2 Water reclamation system

The increasing demands of water in cities is mainly attributed to the rapid urbanization and the population moving from rural to urban centers. In many major cities, the evergrowing water usage and wastewater discharge drive the development of water reclamation (Lyu et al., 2016). In WWTPs, the technologies applied in water resue include disinfecting with chlorine addition, ultra-violet (UV) irradiation, biological treatment, and membrane filtration, etc (Norton-Brandão et al., 2013). However, even with the most advanced water treatment technology, the treated reclaimed water quality is still subject to the variability and varations of pollutant contents in wastewater effluent (Chen et al., 2003), and can potentially fail to meet the reclaimed water standard. The research studies propose to apply machine learning techniques to assist the disinfection process in water reclamation can be catogorized into three groups (1) optimize the treatment management in WWTPs to alleviate the loadings of water reclamation process (Al-Ghazawi and Alawneh, 2021; Viet et al., 2021); (2) actively branch out the desired and undesired wastewater effluent for subsequnt disinfection process of water resue or direct disposal into water body (Chen et al., 2003); (3) adapt process control methods to stablize the disinfection performance in the reclaimed water system (Demir and Woo, 2014).

The technology advancement and research studies of water reuse have been discussed for more than two decades. However the reseach publications aim at improving the reclaimed water system as a whole in recent years are not too many. The economic reasons behind constructing water reuse facilities universally could be the major obsticle for the government sectors. The economic burden of both building new reclaimed water institution on new locations or retrofit existed WWTPs is deterrent (Adewumi et al., 2010). To discover more values and resuable resources from water reuse, Chojnacka et al. (2020) takes the circular economy perpective into accelearting the process of adopting water reuse system for agriculture production. The author introduces the potential of gradually replacing chemical fertilizers with partially treated wastewater for sustainable crops production despite there are many limitations to be overcome. In Italy, the circular concept is also studied by Colella et al. (2021). Four different resource recovery senarios were brought up and two of the senarios include the nutrients recovery turned into nitrogen and phosphorus fertilizers. Several researchers in recent years have provided the overall potential and challenges of treated wastewater reuses in the world, it is believed the day of using reuse water universally will soon advant with the collaboration across different disciplines.

Reclaimed water for non-potable reuses can serve for irrigation for agricultures, toilet flushing and irrigation for landscaping, etc. Water Supply Department (WSD) will soon implement a reclaimed water supply system in SWHEPP by disinfecting the teriary treated sewage (i.e., MBR permeate). The produced reclaimed water will be served for non-potable reuses and is required to satisfy the water quality standards, shown in Table. 2.1.

Table 2.1: Endorsed Reclaimed Water Quality Standards from Water Supply Department.

Parameter	Unit	Requirement [a]
E. coli	cfu/100 mL	Not detectable
Colour	Hazen Unit	≤ 20
Ammoniacal Nitrogen (NH_3-N)	mg/L as N	≤ 1
Total Residual Chlorine	mg/L	≥ 0.2
Dissolved Oxygen	mg/L	≥ 0.2
Turbidity	NTU	≤ 5
5-day Biochemical Oxygen Demand	mg/L	≤ 1
pH	-	6-9
Threshold Odour Number	-	≤ 100
Synthetic detergents	mg/L	≤ 5

[a] The water quality standards for all parameters are applicable at the point-of-use of the system.

2.3 Tools and techniques for enchancing the performance of machine learning modeling

2.3.1 Programming languages

Matrix Laboratory (Matlab) is a propreitary programming and numeric computing platform used across industries and academia for data analysis, algorithm developments and model buildings. In wastewater treatment industry, Matlab is known for using with an add-on software called Simulink for modeling, simulating, and analyzing the dynamic system (i.e., chemically enhanced primary clarifier (Bachis et al., 2015). The use of Matlab-Simulink in wastewater treatment industry is known for the development control strategies of WWTP automations. In 1987, International Water Association (IWA) developed the first mathematical model for simulation-based evaluation, which is Activated Sludge Model 1 (ASM 1), and the modified activated sludge models and Benchmark Simulation Models (BSM) were further developed in the following years (bin Talib, 2011). The difference between the two is, ASM is designed for developing control strategies exclusively in activated suldge treatment process, and BSM 1 is to develop the automation in the entire WWTP (Ballhysa et al., 2020).

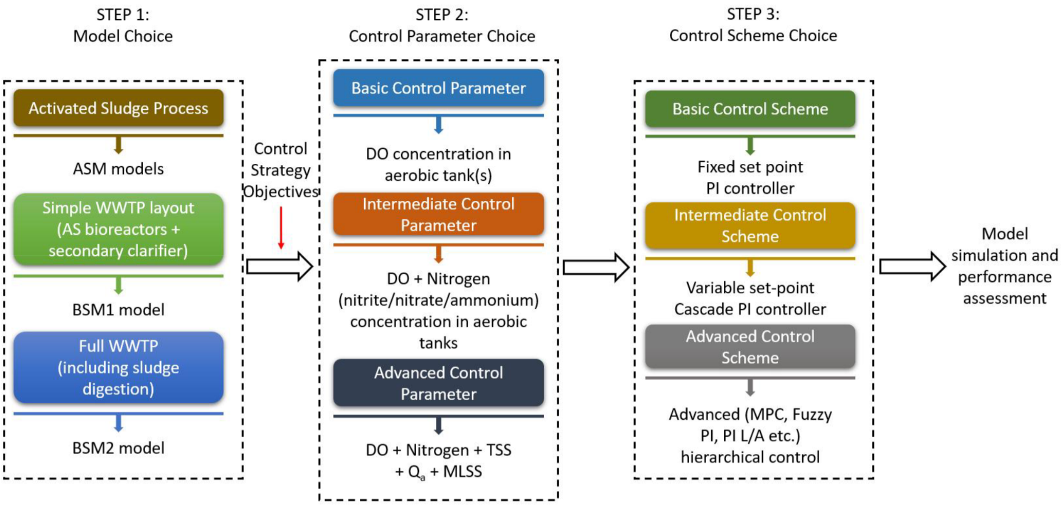


Figure 2.1: Proposed framework for control strategy design by Ballhysa et al. (2020).

In recent year, many publications present an interesting way to demonstrate how machine learning based model predicitve control (MPC) can outperfrom the conventional PID controller in WWTPs using BSM. The researchers use Matlab-Simulink to simulate the treatment processes in WWTPs while the block of PID controllers are swapped to machine learning models, and the effluent quality or treatment system performance can be differentiated via BSM simulated results. Wang et al. (2020) compared the stability of chlorinated water quality in the effluent of a DWTP with two control strategies, which are PID feedback controls and a predictive model based support vector machine (SVM). The BSM simulated results showed the SVM model required 21 minutes less to reach the residaul chlorine setpoint compared to PID feedback controls. A proposed neuro-fuzzy PID controller (i.e., a hybrid machine learning model consisted of nerual networks and fuzzy logic) also showed a superior performance in optimizing the chlorine dosing rate and to minimize the chance of errors (Hong et al., 2012). The significance of using BSM in Matlab-Simulink enables the performance of traditional and machine learning based control strategies can be compared in objective and fair senarios, also providing the practicability of machine learning to the experts in the field. Matlab is a powerful and resourceful platform providing various machine learning functions, including point-and-click apps for training and evaluation, available algorithms of classification and regression algorithms, and Automatic machine learning (AutoML), etc (MathWorks, 2022c). The direct access to the abundant features along with the integration of Simulink makes Matlab an appealing option for many researchers in wastewater treatment industry, especially in the research domain in machine learning and control strategy simulation. Despite the countless benefits of using Matlab, Python programming language stands out in different ways.

Python is a high-level, interpreted, and object-oriented programming language, and features with simple and easy to learn syntax providing good readability (Wha). The large developer community (e.g., GitHub and Stackoverflow) and open-source access (i.e., free of charge) have made Python an ideal tool for machine learning starters. The most cutting-edge research in the field of Artificial Intelligence is often led by the Tech Giants like Google and Amazon, which conduct research on Python (e.g., machine learning frameworks of TensorFlow (Google)in Python), as well as the big research community using Python. All the lasted updates and developments relating to machine learning architectures and techniques are usually accessible in open-source Python community, including the example codes. Contrary to Python, users on commercial software Matlab need to wait for the software engineers working in Matlab to update the lastest machine learning applications onto Matlab plaform, which is a time consuming process and create a delay of time and accessibilities to many resources (Castro, 2018). Machine learning developers in wastewater treament industry can freely choose between the programming methods based on the research need. For those looking for mature machine learning algorithms can simple use Matlab and be satisfied with the functionalities, on the other hand, for those intend to incoporate more new techniques and architecutures in machine learning model can consider using Python as the programming language. Interestingly, MathWorks recently announced using Python functions in Simulink Model (MathWorks, 2022a), despite the update from Matlab, to the best of my knowledge, there is no research papers develop machine learning on Python and run on Matlab-Simulink.

2.3.2 Data pre-processing

The ubiquitous sensors installed in WWTPs for treatment automation generate a massive amount of data on daily basis. Before being used for any purposes, the data must be understandable for explanation and relevant enough for water experts to extract valuable information (Kehrein et al., 2020). Without the help of Artificial Intelligence, data manipulation before training machine learning models can be time-consuming and challenging. The specific designed algorithms can perform data evaluation and augmentation, thus the quality of data can be improved. Any statistical or machine leranign algorithms which can complete these tasks are known as the data pre-processing methods. The causes of sensors rendering undesired data with low quality are from the limitations of the hardware sensors and the dynamics of the sampling locations. In general, the fouing data generated by sensors can be described in eight distinct states (Rosen et al., 2008; Newhart et al., 2019):

1) Operational: Sensor is working properly with normal measurement noise.
2) Excessive drift: When a sensor outputs a value progressively further from the true-value.
3) Shift: When the output of the sensor is a constant amount away from its true value.
4) Fixed value: When the sensor is stuck and keeps repeating the same value.
5) Complete failure: Similar to a fixed value fault, but the sensors either give offthemaximum or minimum, value, zero or no value at all.
6) Wrong gain: When signals away from the calibration point are under- orover-amplified bythe sensor.
7) Calibration: The sharp change in sensor output directly following a calibration.
8) Isolated fault: When a single point in a series shows an incorrect value.

The researchers and experts have been proposing solutions for filling the data gaps created from sensor faults and maintenance operations, but number and length of missing values are largely subject to the dynamics of the system being monitored and other factors. In their open-source wastewater data treatment toolkit,De Mulder et al. (2018) has recommended five data inputation strategies aimed at data generated from water resource recovery facilities:

1) Interpolate.

2) Use a correlation with other available measurement signals.

3) Replace with a corresponding value in an average daily profile.

4) Repeat the values obtained on the preceding day.

5) Replace with the output of a model.

The efficient monitoring of sensors and proper use of the data for developing control strategies in wastewater treatment industry rely on careful data quality control. In recent years, the automated data evaluation has drawn attentions of experts and reseraches in this field while manually detection of sesor fouling is unrealistic due to the tasks are labor-intensive and laborious. Alferes et al. (2013) presented three practical approaches for data quality validation, which are capable of automated calculate single abnormal vaules and collective faults over a long period of time. The author claimed that the significance of the research work is performing data quality validation scheme on multivariate dataset. The pitfalls of the study is despite the promising approaches proposed in the study, the validity still depend on the thresholds or acceptability limits in the actaull WWTPs. Similar to the data inputation strategies, the real situation differs tremendously across different WWTPs. That being said, instead of providing general guidance of how to munipulate data, the focus should be emphasized on how to use algorithms to help users understand, analyze, and process the fouling data.

2.3.3 Feature engineering

The purpose of feature engineering aims at enriching the raw dataset through selecting, manipulating, and transforming data, which forms better dataset relating to the underlying targets to be learning by the machine learning model. Feature engineering and data pre-processing are easily confused with each other, the fundamental difference between the two is the former creates actual features which are not included in the raw data, while the latter is a data noise removing and cleaning process. In the study of Mamandipoor et al. (2020), feature engineering was performed to generate five extra features, which are the statistical metrics of mean, maximum, minimum, variance and standard deviation of a specific input feature. However, in the comparisons of the final results, the author only emphasized on evaluating model accuracies across varied machine learning models (i.e, PCA-SVM and LSTM models). Another interesting technique used by Zaghloul et al.

(2021) is to create the gradient values of an input variable to assist the model to better learn the trend of the historical removal rate of water parameters in aerobic granular sludge reactors. Similar to the results showed in the work of Mamandipoor et al. (2020), the influence of how engineered features affects the ultimate model accuracy is excluded in the results and discussion part. This raises many questions like how significant the feature engineered inputs are to the model accuray, and which techniques can be used upon which senarios.

There is still a considerable ambiguity with regard to the neccessity of using feature engineered inputs in traning predictive model in WWTPs. In the prediction of total nitrogen (TN) in the effluent, the author input nine features and performed feature sensitivity analysis, which can capture the change of the output values attributed to the change input. The result showed that the top three most significant inputs, which are temperature, TN flow and pH share significant effectiveness to the prediction of TN. The author claimed physical related cause-and-effect relationships bewteen the effluent TN and those top three effecitve features can be elucidated by machine learning model (Guo et al., 2015). In another work of predicting influent BOD concentration, the study clearly stated using five inputs instead of three inputs will cause model overfitting, and three inputs for model training was considered sufficient citepAlsulaili. Varaibles that are created from feature engineering have no physical properties, leading to extra unexplainable essence in addition to the black box nature of machine learning models. Besides, extra model inputs from feature engineering can also cause overfitting if the data quality is not carefully evaluated. Said by Andrew Ng, "Coming up with features is difficult, time-consuming, requires expert knowledge. Applied machine learning is basically feature engineering". From the quote and the recent studies we are uncertain to how feature engineering techniques can practically help the development of machine learning models in wastewater treatment industry, more research is required to futher elucidate the effectiveness of performing feature engineering.

CHAPTER 3

METHODS AND MATERIALS

3.1 Wastewater treatment plant description

3.1.1 Process and data sources in SWHEPP

Shek Wu Hui Effluent Polish Plant (SWHEPP) is a secondary sewage treatment plant, which treats the municipal wastewater of the Sheung Shui, Fanling Districts and adjacent areas, and treated leachate effluent from North East New Territories (NENT) leachate treatment plant. The plant is designed for 300,000 population equivalents (PE) in 2001, and in 2009, the daily treatment capacity has been expanded from 80,000 m^3/day to 93,000 m^3/day. SHWEPP is operated and maintained by Drainage Services Department (DSD), and the plant will be upgraded to teritary treatment level to increase the treatment capacity of 190,000 m^3/day by the end of 2025. As shown in Fig. 3.1, the treatment plant is mainly comprised of primary sedimentation, secondary biological treatment, and final sedimentation followed by a membrane bioreactor (MBR), which provides an advanced level of organic and suspended solids removal. To monitor the effluent quality in real-time, low volume of the MBR effluent is pumped to an effluent container near by the MBR location. Two on-line meters, ammoniacal nitrogen on-line sensor and colour level on-line analyzer are installed in the effluent container, which are indicated as (a) and (b) in Fig. 3.1.

3.2 Data collection and preparation

3.2.1 On-line data monitoring and collection

To enable us to perform on-line monitoring of ammonium concentration (NH_3-N) in the MBR effluent, a Ammonium and Potassium Probe, AmmoLyt®Plus 700 IQ (Xylem Company) is installed as in Fig. 3.3a in the effluent container, as shown in Fig. 3.2. The operation was commenced on 27 April 2021 and completed on 27 March 2022. The

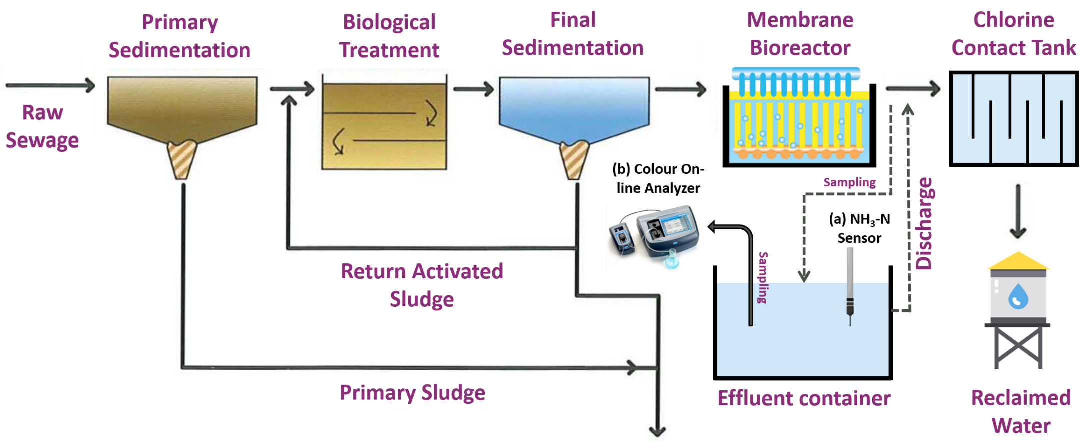


Figure 3.1: Sewage treatment process flowchart at SWHEPP (adapted from Drainage Services Department 2020)

ion-selective electrode (ISE) probe provides continuous and reagentless monitoring of ammonium and potassium at the configured interval of one measurement per minute. Due to the ISE probe cannot differentiate the potentials difference cause by ammonium and potassium ions in the electrodes, the on-line monitoring of ammonium concentration requires the continuous calibration using potassium concentration.

The instrument records ammonium concentration as NH_4-N mg/L, a form to express the sum of nitrogen found in reduced nitrogen (III) form. Ammonia has a reported pKa of 9.25 (National Center for Biotechnology Information, 2022), meaning ammonium is a primary species under the pH of 9.25 in water. In WWTPs, the pH in water normally ranges from pH of 7–8, making the NH_4-N concentration the dominant species. Both ammonia and ammonium contain one nitrogen atom, 1 mg/L NH_3-N is the same as 1 mg/L NH_4-N. Thus, to prevent confusion, in the following paragraph the unit of NH_4-N will be expressed by NH_3-N, which is the unit used in the water quality standard. The collection of on-line ammonia data is achieved through downloading csv files from the website connected to the IQ Sensor Controller (Xylem Comapny), as shown in Fig. 3.3b.

An hourly monitoring of the colour levels of MBR effluent was conducted from 5 October 2021 to 26 February 2022 by using a custom-made on-line colour analysis system. Originally, the spectrophotometer as Fig. 3.4a and a peristaltic pump as Fig. 3.4b can only initiate a single measurement of colour level by pressing the "READ" buttom on the DR3900 panel. To realize continuously sampling and analyzing colour level without human intervention, an actuator with programmable time function was mounted on the panel of DR3900, as shown in Fig. 3.4c.

Figure 3.2: Colour levels and ammonia concentration are measure in the effluent container (i.e., on the right of the image.) A water pump transports MBR effluent to the effluent container continuously at real-time. The black vault on the left of the image contains a laptop and a colour spectrophotometer.

The automatic sampling and analzying of the colour level begins with the action of the actuator, by clicking on the "READ" button to initiate the colour analysis at a fixed interval of 30 minutes. 3 mL of sample was collected from the effluent container and delivered to the spectrophotometer cell. Then, the sample was subsequentially analysed by the spectrophotometer with the data transmitted to an automatic data acquisition and storage software pre-installed in the laptop. The DR3900 device is connected to a laptop, which receives the real-time data and stores on a data management software from Hach company. To access the real-time data from the laptop, Google Remote Desktop is used to operate the laptop via Internet cloud services using any devices having access to the Internet. The entire process is illustrated in Fig. 3.5. After the measurement, the sample will be discharged to the effluent container and the online colour monitoring system is left idle until the next measurement.

The maintenance and calibration of the DR3900 spectrophotometer is performed on a weekly basis. During the maintenance, the DR3900 device was shut off, and chlorine solution at the concentration of 100 mg/L was pumped into the sampling tubes and the plastic cuvette for disinfection and cleansing. The cleanse of the tubes and cuvette were

(a) AmmoLyt®Plus 700 IQ, Xylem.

(b) DIQ/S 284-EF controller, Xylem.

Figure 3.3: Instrument of on-line ammonium monitoring system.

manually inspected with eyes to make sure no foreign objects were stuck inside. Deionized water was brought to the site to perform the spectrophotometer calibration after the reboot of DR3900.

Based on the proposed model training methods, which ammonia and colour data are used as the second features of training colour and ammonia forecasting models, the size and time of the ammonia and colour datasets should be the same. In addition, abnormal data caused by sensor downtime should also be excluded. Thus, we chose the ammonia and colour data from 23 December 2021 to 22 January, as shown in Fig. 3.6.

3.2.2 Loss function for model evaluation

Loss functions are used to determine the error between the model outputs (i.e., prediction or forecasting values) and the given target value (DeepAI, 2022). The bigger the difference between the ground truth $\boldsymbol{y}$ and the model outputs $\hat{\boldsymbol{y}}$, the higher the value of the loss function is, meaning the model perfomred poorer. A low value for the loss means the modle perfomred well. The selection of the types of the loss function is essential for training the model to perform specific tasks. In this study, Mean Squared Error (MSE) is used for evaluating the regression models. The values of MSE will never be negative, and is formally defined by the following equation:

$$MSE = \frac{\sum(y_i - \hat{y}_i)^2}{n} \tag{3.2.1}$$

(a) SIP10 peristaltic pump, Hach

(b) DR3900 spectrophotometer, Hach

(c) Customized clicker/actuator

Figure 3.4: Instruments of on-line colour analysis system.

3.2.3 Data cleaning and pre-processing

In this study, ammonia concentration and colour level forecasting models will be trained, and the model training steps are shown in Fig. 3.7. The training processes are split into two sections, one is the baseline model training steps, the other is proposed model training steps. The training steps of the first section used cleaned data to train forecasting models and generated baseline model performance, which will be further compared with the model perfromance generated from the second section. The second section includes using pre-processed datasets (i.e., data smoothing) and feature engineering enhanced datasets to train the forecasting model. In machine learning, the data used for training models is refered to model inputs, features and variables.

The raw data embedded in the original csv files exists many issues, such as missing values, having extreme low or high values, and unreadable texts, etc. Thus, the data cleaning and pre-processing are necessary for more effective process of model training. Python programming language and related modules of Numpy and Pandas were used

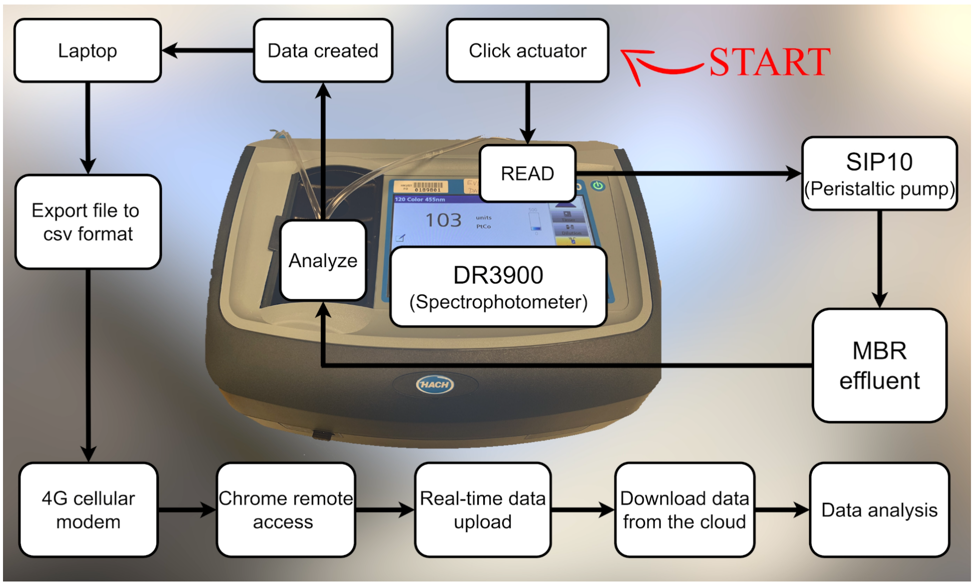


Figure 3.5: Schematic diagram of the custom-made on-line colour anlaysis system.

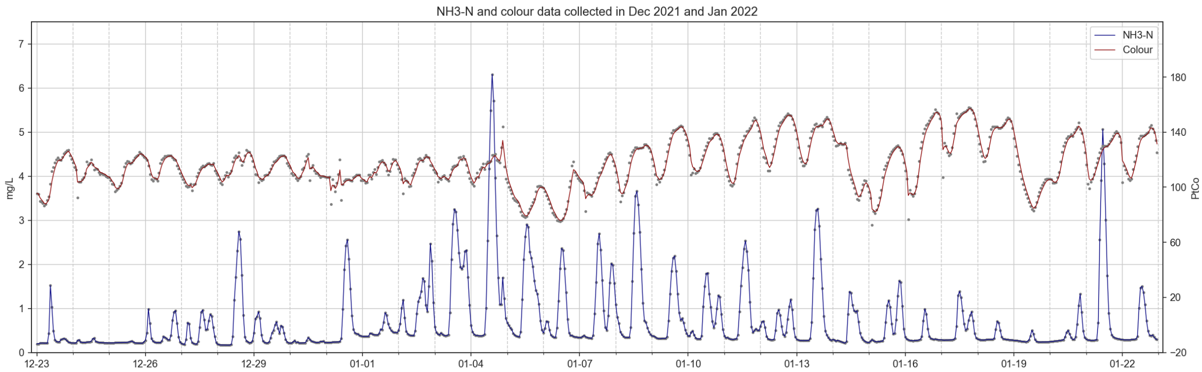


Figure 3.6: Ammonia and colour data collected from 23 December 2021 to 22 January 2022.

to clean and pre-process the raw dataset for further usage. The ammonia raw dataset contained 44,640 samples (data points) with 8 variables, giving a matrix size of 44,640 x 8, and the samples were collected in time series at 1 minute interval. The colour level raw dataset contained 1488 samples with 34 variables, giving a matrix size of 1488 x 34, and the samples were collected in time series at 30 minute interval.

Before the high-resolution data from colour and ammonia datasets were compressed into time series data at 1 hour interval via averaging, extreme values were manually removed. For ammonia dataset, we replaced the values higher than 7.0 mg/L with NaN (i.e., Not a number), and futher use interpolation to fill up the NaN along with the missing values in the dataset. For colour dataset, we manually took out the relatively low data points on the days when the maintenance and calibration tasks were performed;

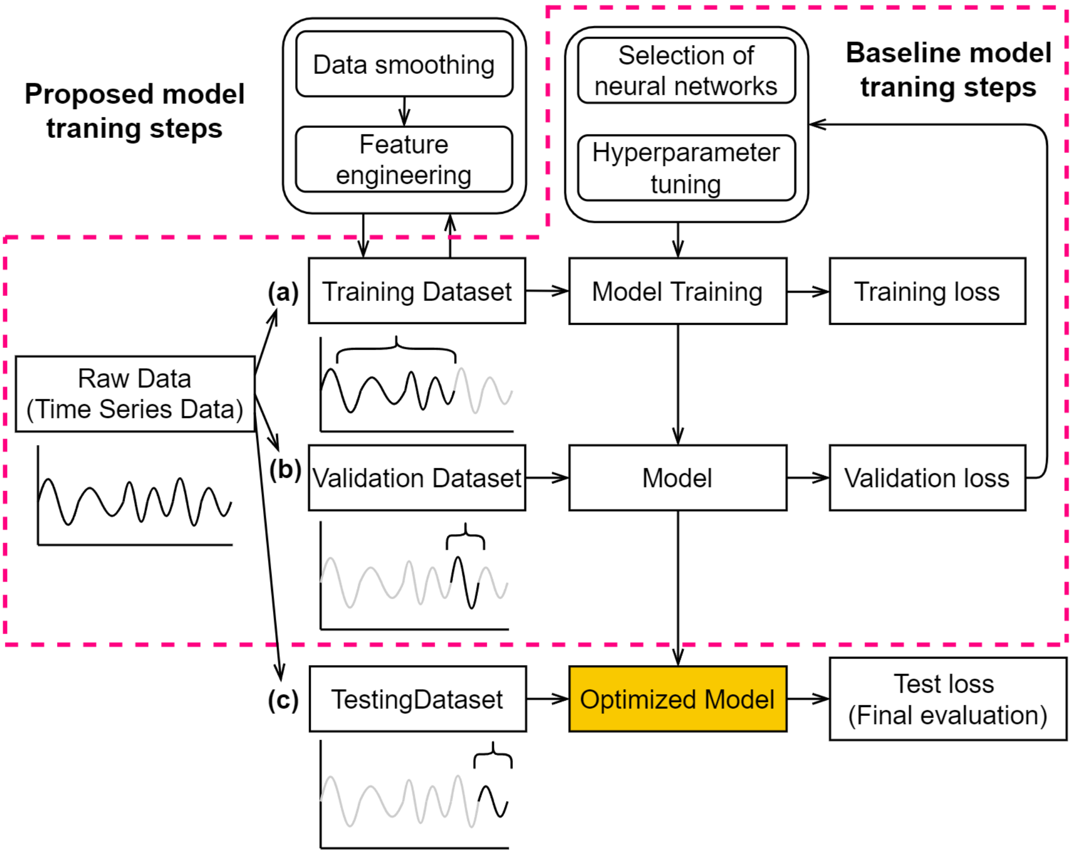


Figure 3.7: Machine learning model training steps.

extremely values higher than 300 Hazen Unit were also replaced by NaN. Same as the data cleaning method used for ammonia dataset, the missing values and NaN were filled up via interpolation.

3.2.3.1 Data smoothing with Savitzky-Golay and EWMA filter

Data smoothing was performed on both ammonia and colour datasets using the same method. One of the effective ways to remove the noise from the dataset is to apply data smoothing filters. Two filteres were applied in this study, Savitzky-Golay (SG) and Exponentially Weighted Moving Average (EWMA) filters.

A SG filter is a digital filter that can be applied to a set of digital data points for the purpose of smoothing the data without distorting the data tendency. This is achieved via convolution, by fitting successive sub-sets of adjacent data points with a low-degree polynomial by the method of linear least squares (Wikipedia, 2022b). The illustration is shown in Fig. 3.8a and the procedures of how data points are smoothed is presented in the following steps:

1) Extract short-time window (i.e., blue dots in Fig.3.8a)

2) Determine polynomial degree (e.g., different polynomial degree is compared in Fig. 3.8a).

3) Find the smoothed data point (i.e., at center of the window).

4) Repeat for shifted window (e.g., similar to moving average).

The equation to decribed the smoothed value of $\boldsymbol{Y_j}$ can be expressed in Eq. 3.2.2:

$$Y_j = (C \otimes y)_j = \sum_{i=\frac{1-m}{2}}^{\frac{m-1}{2}} C_i y_{j+i}, \; \frac{m+1}{2} \leq j \leq n - \frac{m-1}{2} \tag{3.2.2}$$

where Y_j corresponds to the j^{th} smoothed data point, m to the window size (i.e., numer of data points intended to smooth out) and C_i to the convolution coefficients (i.e., determined by Savitzky and Golay (1964)).

Exponentially weighted moving average (EWMA), also known as auto-regressive (AR) filtering, is a technique that filters measurements. An EWMA filter smoothes a measured data point by exponentially averaging that particular point with all previous measurements. The EWMA equation can be expressed in Eq. 3.2.3:

$$\begin{aligned} \alpha &= \frac{2}{span + 1} \\ y_0 &= x_0 \\ y_t &= (1-\alpha) y_{t-1} + \alpha x_t \end{aligned} \tag{3.2.3}$$

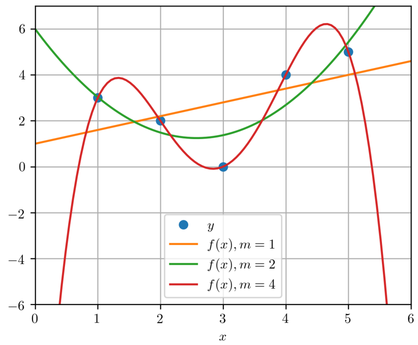
where α corresponds to the decay paratmeter, x_t to the value at a time period, y_t to the value of the EWMA at any time period t, span to the window size.

Both SG and EWMA filters are required to select the hyperparamters, the selected values are presented in Table. 3.1.

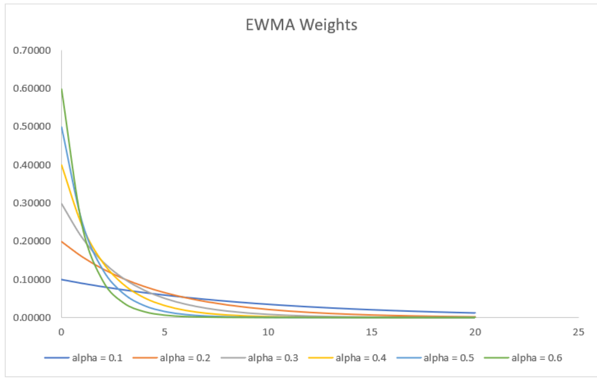
Fig. 3.9 shows the influences of different windows sizes on SG filters as in Fig. 3.9a and on EWMA filters as in Fig. **??**.

3.2.3.2 Outlier Removal

Despite the extreme values in the ammonia raw dataset were removed based on simple conditions (i.e., concentration higher than 7.0 mg/L), the ammonia sensor can still capture



(a) SG filter with different polynomial degree (Taal, 2017).



(b) Examples of weights with exponential decay at varied alpha values (CFI, 2022).

Figure 3.8: Illustration of the influence of different polynomial degrees in the fitting of SG filter and the weigth decay with varied alpha values in EWMA filter.

Table 3.1: The selected hyperparameters for SG and EWMA filters.

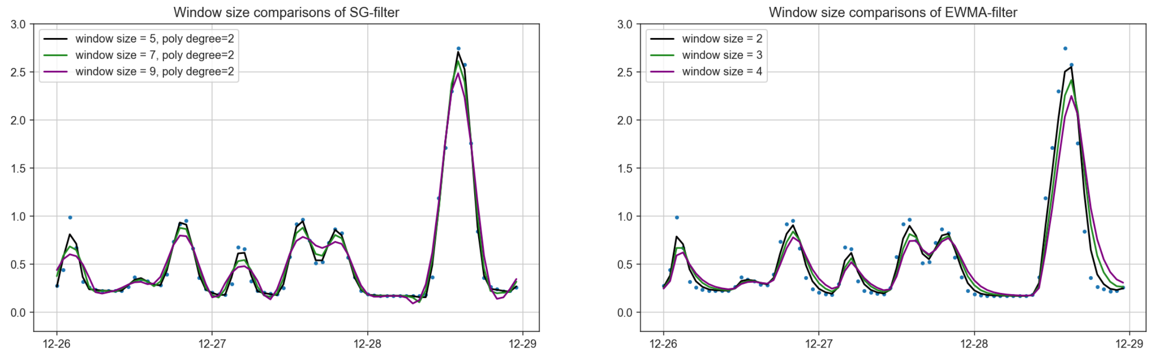
Group Name	Window size	Polynomial degree
SG-5	5	2
SG-7	7	2
SG-9	9	2
EWMA-2	2	-
EWMA-3	3	-
EWMA-4	4	-

unideal data points collectively. In the outlier removal process, we intended to identify the collective faults of ammonia data in the unit of an entire day. To determine whether the ammonia data on a specific day shows collective fault, two abnormal conditions are defined:

1) NH_3-N fluctuation ≤ 0.1 (i.e., lower than the sensor resolution).

2) No diurnal fluctuation (i.e., Fluctuation = peak value – bottom line value).

To automiatically realize the identification of noraml or abnormal signals, peak analysis was performed on the daily ammonia data. The analysis takes a one-dimension array (i.e., the data form of ammonia in a day) and finds all local maximum values by simple comparison of neighboring values. This function will also provide information such as width and prominence, as in Fig. 3.10 to help us identify whether the diurnal fluctuation is existed.



(a) (b)

Figure 3.9: Illustration of the influence of different polynomial degrees in the fitting of SG filter and the weigth decay with varied alpha values in EWMA filter.

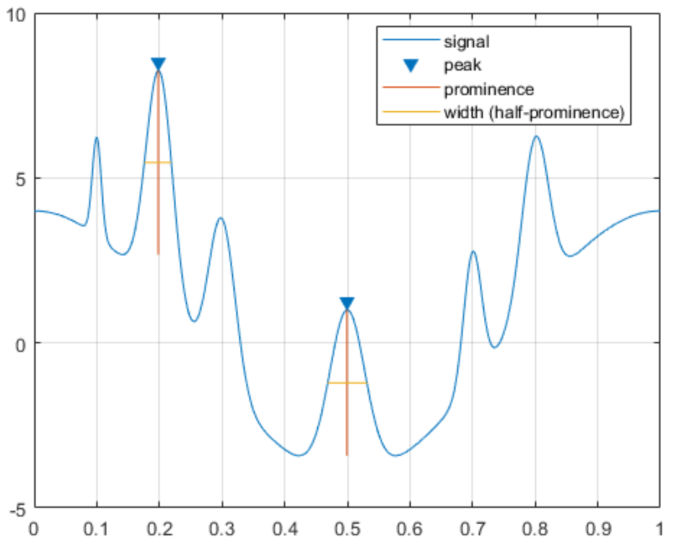


Figure 3.10: Illustration of peak analysis. Four important elements are automatic caculated by the function (MathWorks, 2022b).

3.2.3.3 Feature Engineering

To create addition features from the raw datasets, we have carefully observed and analyzed the SWHEPP influent. We discovered that the SWHEPP influent is consisted of treated landfill effluent from NENT landfill leachate site and municipal wastewater, as shown in Fig. 3.11. We observed that with higher blending ratio, which is calculated from the daily volume of treated leachate effluent divided by the daily inflow volume of SHWEPP, the colour level is also higher, as shown in Fig 3.13a. With the the Pearson coefficient of 0.68, the increased volume of treated leachate effluent in public sewege system is proportional to the increase of the colour levels in the SHWEPP influent, while the ammonia concentration is mostly from the municipal wastewater. During the mixing of both type of the wastewater as in Fig. 3.12a, pollutants contribute to colour levels will be diluted by the municipal wastewater, same as the opposite for the dilution of the ammonia concentration. In Fig. 3.13b, we can observe the time when the lowest colour level of the day occured is close to when the highest of ammonia concentration was observed. The changes of colour levels and ammonia concentration are interative, thus, in feature engineering, colour level data was selected for training ammonia forecasting model; ammonia data was selected for training colour forecasting model, as shown in Fig. 3.17.

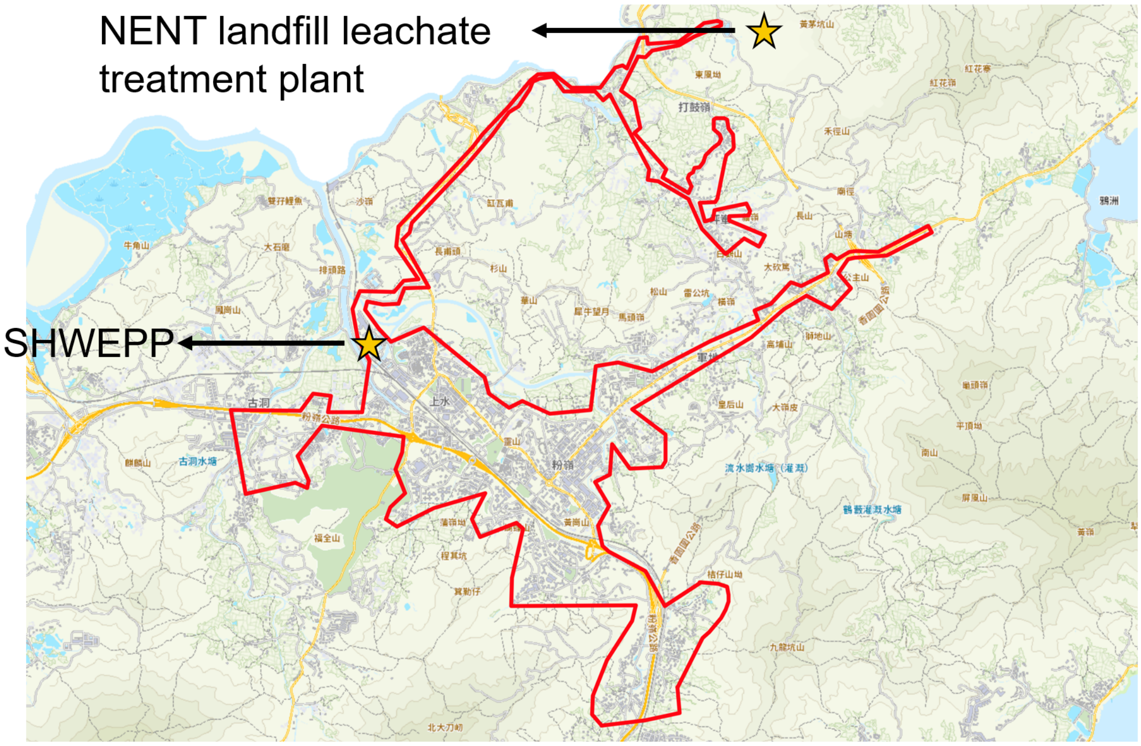
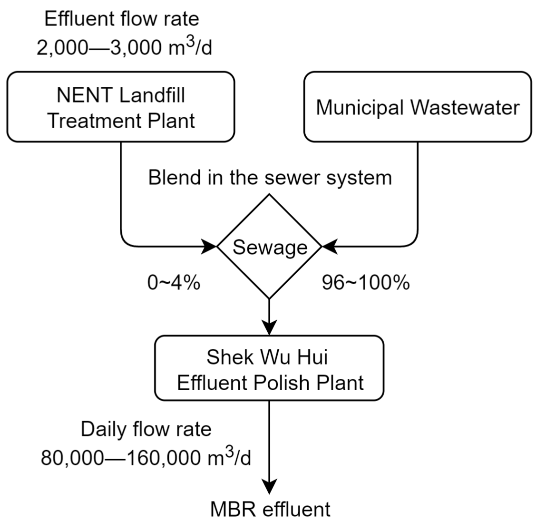
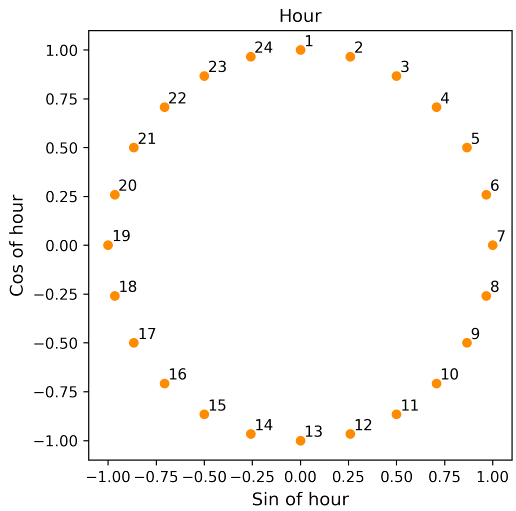


Figure 3.11: Sewer system coverage of SHWEPP. The covered areas (i.e., area circled in red boundary) include Fanling/Sheung-Shui new towns and NENT landfill leachate treament plant.

The new features are inspired from the research work of Abu-Bakar et al. (2021). The author pointed out the four types of hourly household water consumption patterns as in Fig. 3.14, which correlates the specific time of the day to the volume of the water consumed in households. In other words, as fresh water is consumed, wastewater is generated at the same time, the wastewater then enters the public sewage system and result in the increase of ammonia concentration. As shown in Fig. 3.15, the peak analysis tool helped us to identify the peak hour of the ammonia concentration, which occured at around 13:00 to 14:00 o'clock at noon, and 20:00 to 21:00 o'clock at evening. Thus, it is convinced that



(a) Flowchart showing the blending of treated leachate effluent with municipal wastewater.



(b) Positional encoding of hour components.

Figure 3.12: Analysis of influent quality composition and the illustration of the positional encoding.

time features will be able to help the machine learning models to better correlate and predict the change of ammonia concentration in the wastewater.

Time feature is realized through a technique called positional encoding (POS). The positioanl encoded feature was achieved as the following steps:

1) The timestamp are represented as three elements—hour, day and month.

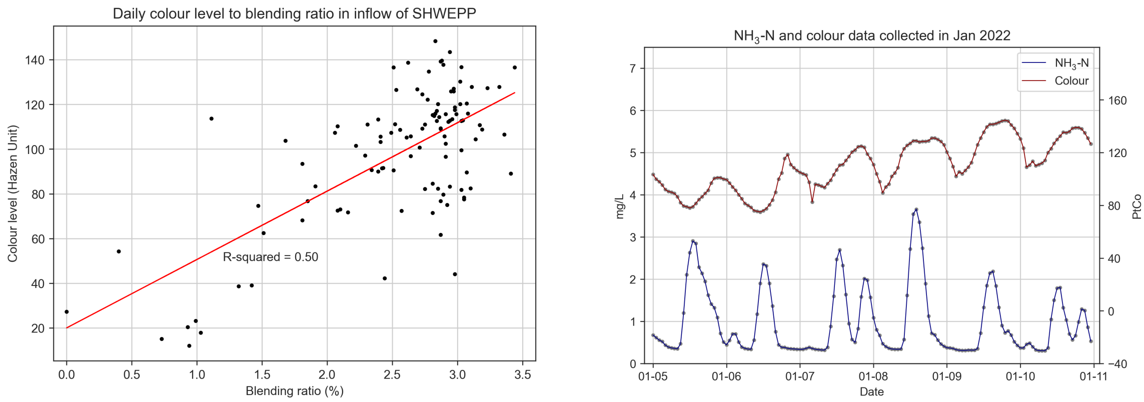
2) Each element will bed decomposed into sine and cosine components.

3) Last step is applied to hours and days to make all elements represented cyclically.

Due to the size of the datasets used in this study for training ammonia and colour forecasting model is 31 days, only hour element was transformed into sine and cosine components as in Fig. 3.12b.

3.2.4 Data transformation

Before the pre-processed data is fed into the models for training, we need to split the data into three clusters, which are training (60%), validation (20%), and testing dataset (20%). Among each training dataset, the data will be further split into input variables $\boldsymbol{X}$ and output variable $\boldsymbol{Y}$ (i.e., training X/training Y, testing X/testing Y). During the



(a) Coefficienct between blending ratio and colour levles.

(b) Trend comparison of ammonia concentration and colour levels.

Figure 3.13: Observatios of ammonia concentration and colour levels in SHWEPP influent.

training process, machine learning algorithms will learn a target function $\boldsymbol{f}$ to best map $\boldsymbol{X}$ to $\boldsymbol{Y}$.

A taining dataset is a set of examples (e.g., historical data) for models to learn the hidden trends and information in the data, shown in (a) in Fig. 3.7, and the training loss is calculated by taking the sum of loss for each example in the training dataset after each epoch. Since it is impossible to have the optimized hyperparameters in the first try of the training, a validation dataset as in (b) in Fig. 3.7 is used to assess the model performance until we obtain the optimzed settings. The validation loss plays an important role during the model training, the adjustments of the hyperparameters will directly reflect on the change of the validation loss, the lower the values, the better the model performance is. As the optimzed model is obtained, testing dataset is used to evaluate the performance of the forecasting model, as shown in (c) in Fig. 3.7. To the forecasting Models, testing dataset has never been seen by the models. If the model tuning process was performed on the testing dataset, the model performance would be a biased result since the hyperparameters are revised in favor to the evalution of the testing dataset.

In Fig. 3.7, the hyperparameters will remained the same once the optimzed values are found, thus generating a baseline model perfromance of a specific machine learning model. The baseline results will be further compared with the results from the model trained by the proposed model trianing steps, which include datasets that have been performed data smoothing and feature engineering techniques.

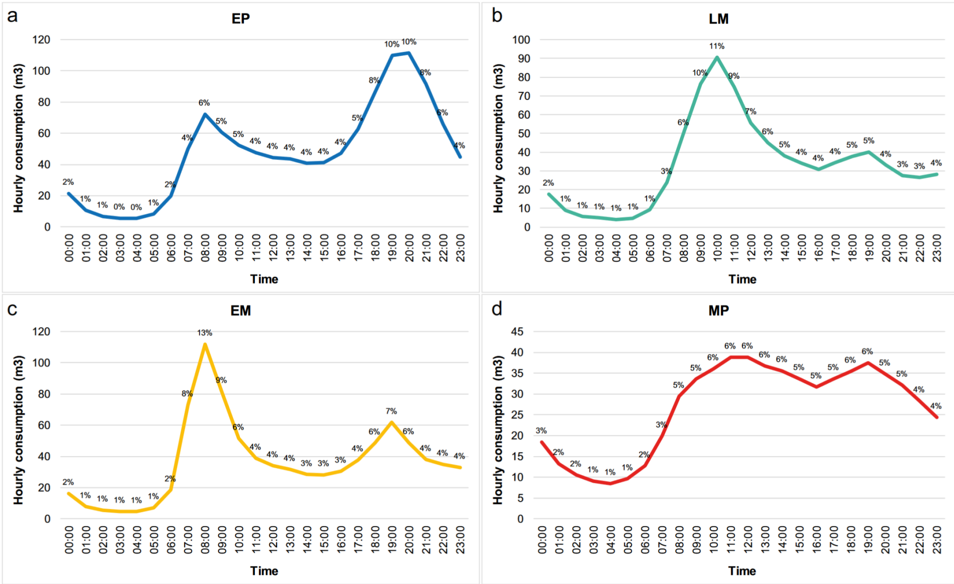


Figure 3.14: Hourly water consumption patterns in households (Abu-Bakar et al., 2021). (a) Cumulative pattern and percentage of hourly consumption for households in the "Evening Peak (EP)" cluster (b) Cumulative pattern and percentage of hourly consumption for households in the "Late Morning Peak Peak (LM)" cluster. (c) Cumulative pattern and percentage of hourly consumption for households in the "Early Morning Peak (EM)" cluster. (d) Cummulative pattern and percentage of hourly consumption for households in the "Multiple Peak (MP)" cluster. Consumption is in (m3).

3.2.5 Feature selection

Fig. 3.17 illustrates which features are selected during the model training processes. In baseline model trianing steps, for both ammonia and colour forecasting model, only one feature is used for training for each model, which is ammonia and colour data, respectively. The model trained by a single feature, followed the baseline model training steps, will generate baseline models. The results from the final evaluation will be defined as the baseline model performance, which will be compared with the model evaluated results from proposed model training steps. Once the baseline model performance is obtained, more features will be input to the model training processes in the order of 2 inputs, 3 inputs, and 4 inputs.

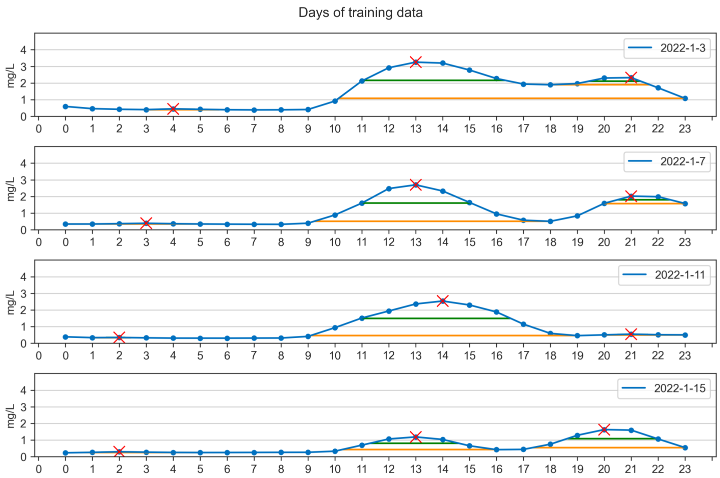


Figure 3.15: The daily patterns of ammonia concentration on 3, 7, 11, 15 Janurary 2022.

3.3 Machine learning models

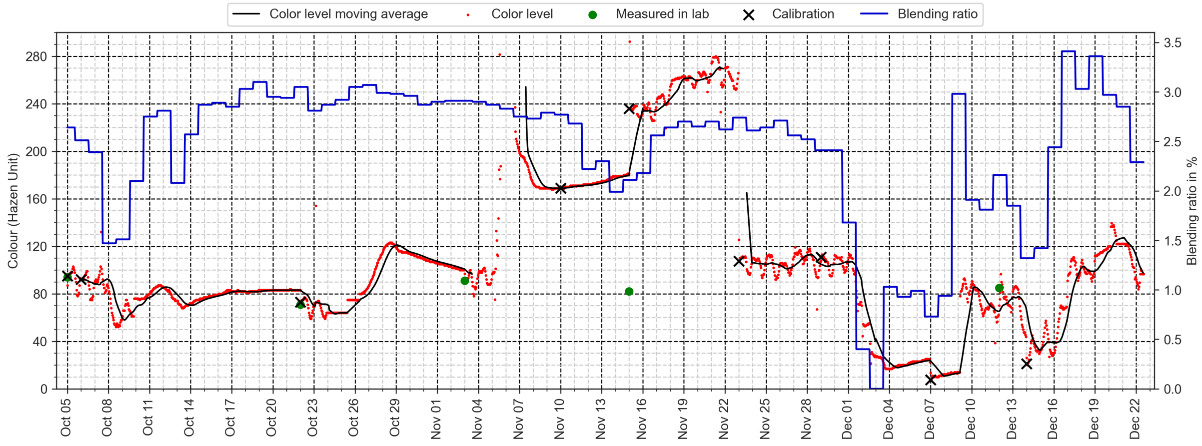
3.3.1 Random Forest

The machine learning model used in this study (i.e., not deep learning models) is random forest (RF). It is an ensemble method which the final output is obtained by averaging the results from multiple tree learners (Wang et al., 2021), as shown in Fig. 3.18a. The training algorithm applies the general technique of bootstrap aggregating, also known as bagging, to tree learners. Given a training set $X = x_1, ..., x_n$ with targets $Y = y_1, ..., y_n$, bagging repeatedly (B times) selects a random sample with replacement (i.e., not putting the samples back to the population) of the training set and fits trees to these samples (Wikipedia, 2022a), RF generate an output through the following steps:

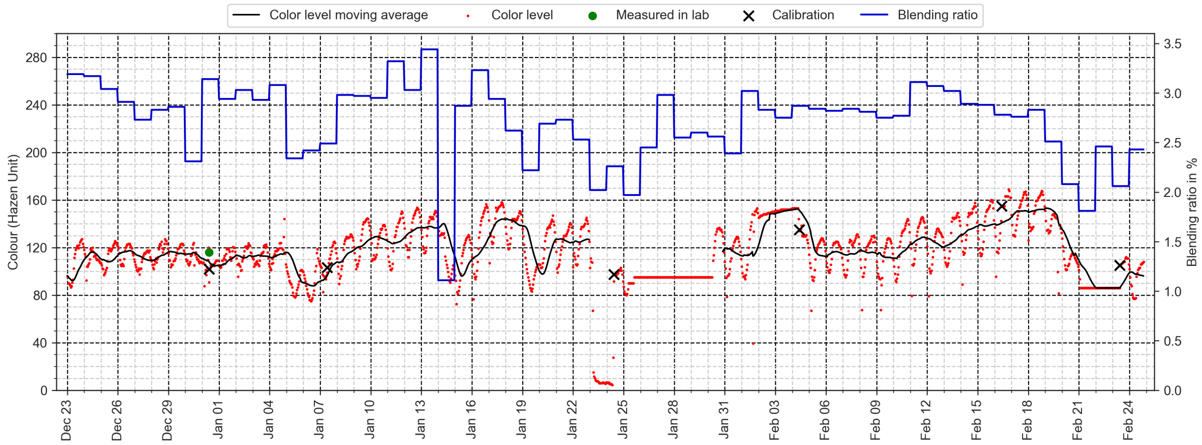
For $b = 1, ..., B$:

1) Sample (with replacement) n training examples from X, Y, call these X_b, Y_b.
2) Train a regression tree f_b on X_b, Y_b.
3) Predict unseen samples $x^{'}$ by averaging the predicdtions from all the regression tree learners on $x^{'}$ as in Eq. 3.3.1:

$$\hat{f} = \frac{1}{B}\sum_{b=1}^{B} f_b(x^{'}) \tag{3.3.1}$$



(a) Data collected from 5 October 2021 to 22 December 2021.



(b) Data collected from 23 December 2021 to 24 February 2022.

Figure 3.16: Monitored colour level in MBR effluent and the change of blending ratio (v/v) of treated leachate effluent to municipal wastewater in the inflow of SWHEPP during December 2021–January 2022. Date of manually calibration and colour level measured in laboratory is also provided as black cross and green dot. The moving average of colour level is calculated by averaging the colour level in the past 24 hours. Note: The colour levels analysed by the on-line colour monitoring system were compared to the manually measured data obtained from the laboratory, which showed errors of 2.08%, 4.05%, 1.11%, 65.25%, 4.94% and 11.0% in the TSE samples collected 5 Oct, 22 Oct, 3 Nov, 15 Nov, 12 Dec, and 31 Dec 2021, respectively.

3.3.2 Deep Neural Networks

Artificial Neural Network (ANN) is a very broad term that encompasses any form of Deep Learning model. A typical ANN consists with input, hidden and output layers, and each layer comprises multiple neurons (i.e., nodes). The connected neurons are to simulate the human brain by process and transmit input signals to the next nodes (Mohseni-Dargah et al., 2022) . What sets apart from a ANN model to a DNN model is that the former

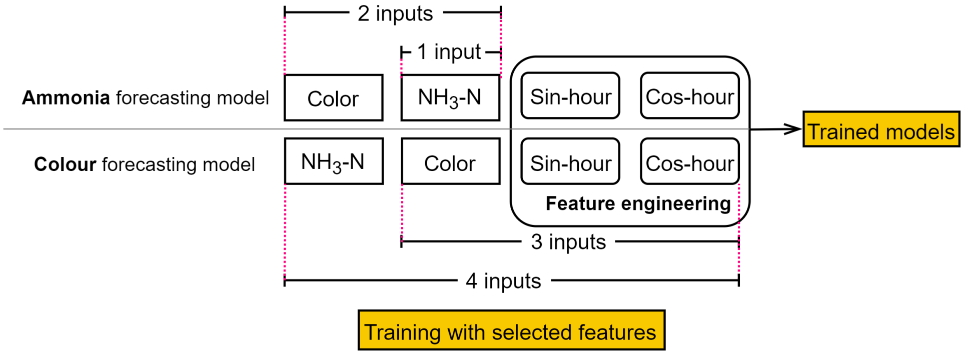
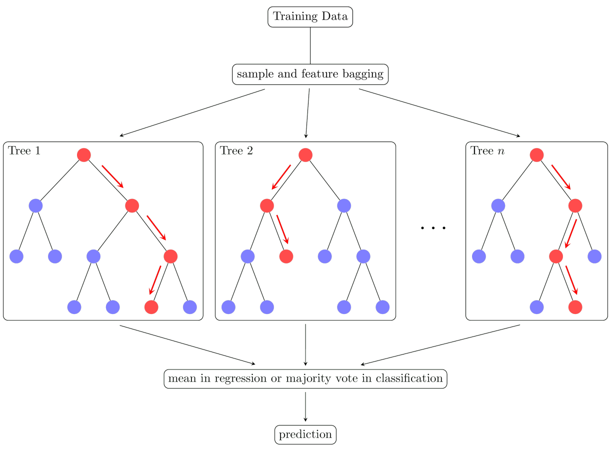
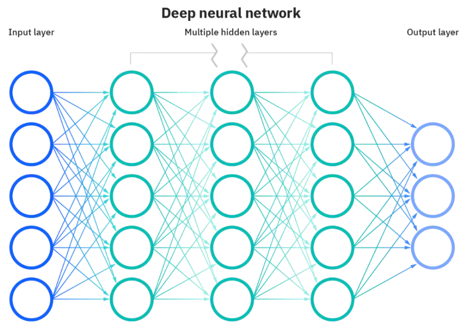


Figure 3.17: Illustration of feature selections for model training.

contains only one hidden layer while the latter has more than one, as shown in Fig. 3.18b. The DNN models are nonlinear, which finds the correct mathematical manipulation to turn the input into the output (Bangaloreai, 2018).



(a) Random Forest (RF) (Riebesell, 2022).



(b) Deep Neural Network (DNN) (IBM, 2022).

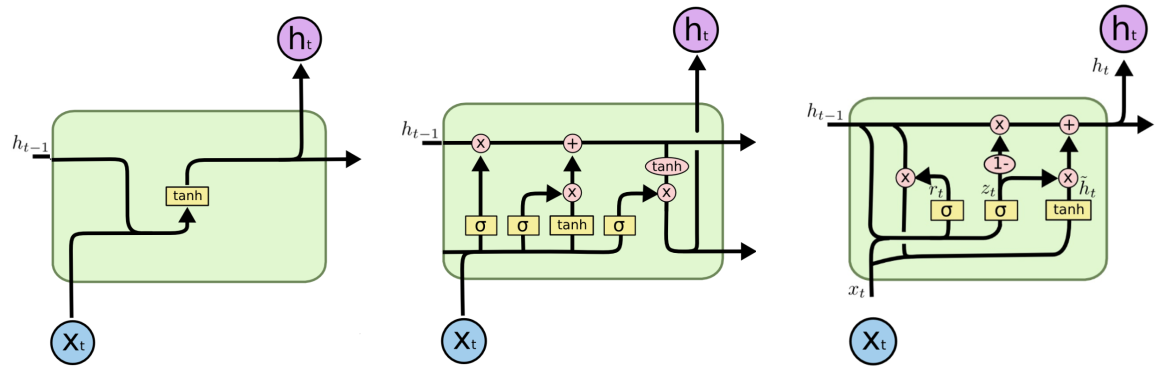
Figure 3.18: Illustration of RF and DNN model structure.

3.3.3 Recurrent Neural Network

A recurrent neural network (RNN) is a type of Artificial Neural Network which designed to work with sequence data. For instance, sequence data are time series, DNA, language, speech and sequences of user actions data, etc. The ammonia concentration and colour level data are time series data, which is a series of data points listed in minute orders (Donges, 2021). A distinguished characteristic of RNN is that they share parameters across each layer of the network by allowing information to be passed from last step of the network to the next. Unlike RNN, feedforward networks like DNN have different weights across each node. The reuse of previous information for making decision on RNN makes it capable of "learning" from the previous inputs. The realization of the memorizing function is through a memory unit called hidden state (i.e., a vector contains weights) in RNN architecture, which enable RNN to presist data, thus capture short term dependencies. The RNN architecture is presented in Fig. 3.19a. The general formulation of a RNN is expressed in Eq. 3.3.2 (Mamandipoor et al., 2020):

$$h_t = \sigma(W^h h_{t-1} + W^x x_t + b) \tag{3.3.2}$$

where x_t is the current input, h_t is the current hidden state (output), h_{t-1} is the previous output, W^x is the weights of the hidden state, W^h is the weight of the input, b is the bias, σ is the sigmoid activation function.



(a) Recurrent Neural Network (RNN).

(b) Long Short-term Memory (LSTM).

(c) Gate Recurrent Unit (GRU).

Figure 3.19: Variant architectures of Recurrent Neural Networks (adapted from Olah (2015)). x_t corresponds to the current input, h_{t-1} to the last hidden state (output), h_t to the current output, tanh is the tangent activation function, σ is the sigmoid activation function,$\times$ is the vector pointwise multiplication, $+$ is the vector pointwise addition.

3.3.4 Long Short-term Memory

Long Short-term Memory (LSTM) is a deep recurrent neural networks (RNN), an advanced and improved version of RNN. The advent of LSTM is to solve problems requiring learning long-term temporal dependencies which cannot be learned by RNN due to the simple model architecture. The fundmental of LSTM network is built on memory blocks called "cells", which are responsible for tranferring and receiving the states (i.e., vectors) recording the information from the previous cells. In a cell block, there are input gate, forget gate and the output gate. The function of these three gates is to control the movement of the information into and out of the cell via the sigmoid function. The inputs of the cell will first go through a forget gate (f_t) as Eq. 3.3.3a, where the function will mutiply each element in the input states by values ranging from 0 to 1 to realize the effect of "forget". Next, a input gate (i_t) as in Eq. 3.3.3b will decide whether the new information should be updated or ignored by sigmoid function (i.e., 0 or 1), followed by a tangent function giving weight of importance (i.e., -1 to 1) to the values which passed by as in Eq. 3.3.3c. New memory then is appended to the previous memory C_{t-1} resulting a new C_t. Lastly, output values (h_t) is obtained based on output cell state (O_t) as in Eq. 3.3.3e and Eq. 3.3.3f (Le et al., 2019). The equations for LSTM structure are shown in Eq. 3.3.3:

$$f_t = \sigma(W_f[h_{t-1}, X_t] + b_f) \tag{3.3.3a}$$

$$i_t = \sigma(W_i[h_{t-1}, X_t] + b_i) \tag{3.3.3b}$$

$$\tilde{C_t} = tanh(W_n[h_{t-1}, X_t] + b_n) \tag{3.3.3c}$$

$$C_t = C_{t-1}f_t + \tilde{C_t}i_t \tag{3.3.3d}$$

$$O_t = \sigma(W_o[h_{t-1}, X_t] + b_o) \tag{3.3.3e}$$

$$h_t = O_t tanh(C_t) \tag{3.3.3f}$$

where f_t corresponds to the forget gate, i_t to the input gate, $\tilde{C_t}$ to the candidate cell state, C_t to the current cell state, O_t to the output cell state, h_t to the output values, σ to the sigmoid function, X_t to the current input, tanh to the tangent function, W and b are the weight matrices and bias of the corresponding output gate, respectively.

3.3.5 Gate Recurrent Unit

Gated Recurrent Unit (GRU) model is a variant of LSTM model, by combining the forget gate and input gate into an update gate as in Fig. 3.19c, GRU has less parameters compared to LSTM. The advantage of GRU over LSTM is less computing power required while maintaining a similar model performance compared to LSTM. The inputs of GRU model first enter the update gate (z_t) as in Eq. 3.3.4a, where the function will help the model to determine how much of the past information needs to be passed along to the future via sigmoid functions. Followed by the reset gate (r_t) as in Eq. 3.3.4b, which is used to decide how much of the past information to forget. Althogh Eq. 3.3.4a and Eq. 3.3.4b have the same inputs of X_t and h_{t-1}, the usages of the gates are different. The outputs of reset gate will be used to determine the candidate hidden state ($]tildeh$) as in Eq. 3.3.4c, where the tangent fucntion will determine the importance of current input (X_t), reset gate output, and previous hidden state (h_t). At the last step, the output values (h_t) is calculated from the candidate hidden state ($\tilde{h_t}$), previous hidden state (h_{t-1}), and the outputs of update gate as in Eq. 3.3.4d. The equations of GRU structures are presented in Eq. 3.3.4 (Cheng et al., 2020):

$$z_t = \sigma(X_t W_{xz} + h_{t-1} W_{hz} + b_z) \tag{3.3.4a}$$

$$r_t = \sigma(X_t W_{xr} + h_{t-1} W_{hr} + b_r) \tag{3.3.4b}$$

$$\tilde{h_t} = tanh(X_t W_{xh} + (r_t \circ h_{t-1}) W_{hh} + b_h) \tag{3.3.4c}$$

$$h_t = z_t \circ h_{t-1} + (1 - z_t) \circ \tilde{h_t} \tag{3.3.4d}$$

where z_t corresponds to the update gate, r_t to the reset gate, $\tilde{h_t}$ to the candidate hidden state, h_t to the output values, σ to the sigmoid function, tanh to the tangent function, X_t to the current input, W and the b are the weight matrices and bias of the corresponding output gate, respectively.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Baseline performance of the forecasting models

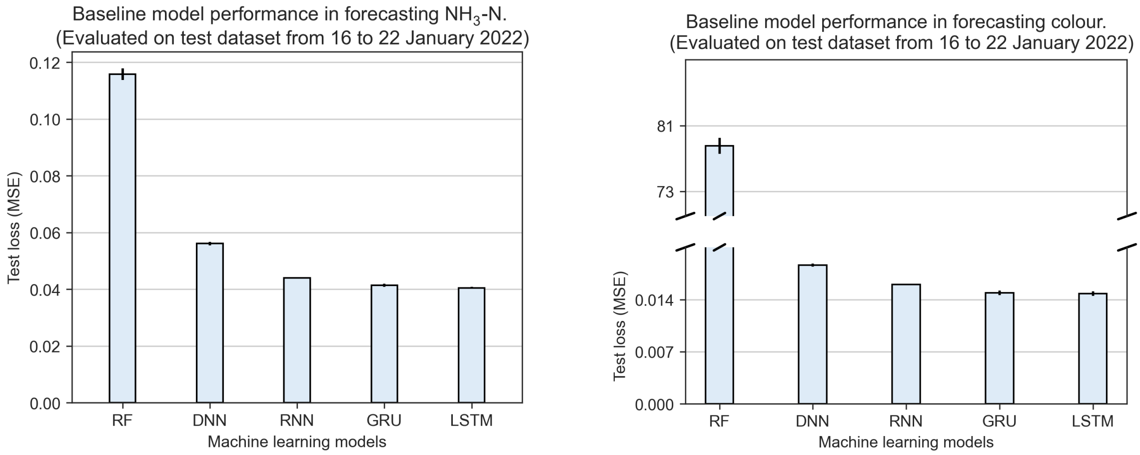
In this study, five machine leanring algorithms were trained with univariate datasets to predict the ammonia concentrations and colour levels in reclaimed water system. The forecasting model performance is presented in Fig. 4.1. The performance of RF models in Fig. 4.1a and Fig. 4.1b showed much higher test loss values compared to DNN, RNN, GRU and LSTM models. During the processes of hyperparameter turning, we discovered that the RF model performance didn't improve much when the models were trained with a varied number of estimators, while test loss values of all the other deep learning models decreased quite much toward the optimum settings of the hyperparameters.

The significant higher test loss of RF models compared to other models can be visualized by plotting the forecasted values with the ground truths (i.e., observed values). In Fig. 4.2, one-step-ahead forecast horizon of ammonia concentration and colour level is plotted by RF as in Fig. 4.2a and Fig. 4.2c and LSTM models as in Fig. 4.2b and Fig. 4.2d. It's easier to observe that the RF models are less capable of predicting the water quality paratmers.

4.2 Improved performance on forecasting models using data pre-processing techniques

4.2.1 Models trained by pre-processed datasets

In this study, we investigate whether the datasets treated by the proposed data pre-processing methods can improve the baseline model performance using the same hyperparameter settings. As shown in Table. 4.1 and Table. 4.3, we listed all the test loss values of five machine learning algorithms trained with each proposed pre-processed methods for ammonia concentrations and colour levels forecasting. The machine learning algorithm



(a) Test loss values from five ammonia forecasting models.

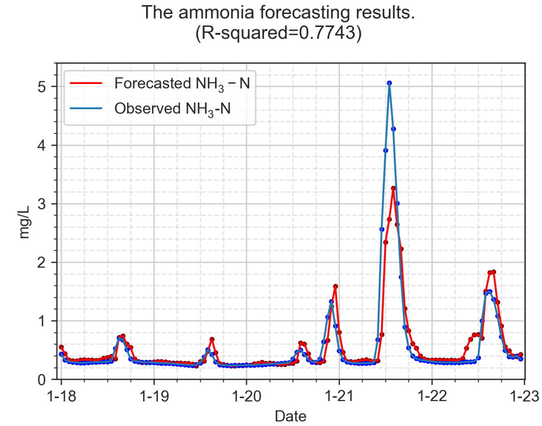
(b) Test loss values from five colour forecasting models.

Figure 4.1: Baseline performance of ammonia and colour forecasting models.

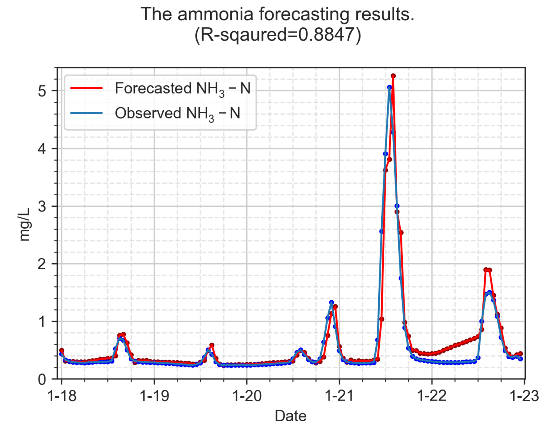
trained by datasets which were applied with SG filters at different window sizes are denoted as model-sg5, model-sg7, model-sg9; the naming rule applies the same to datasets applied with EWMA filters; for the method of outlier removal for ammonia data is denoted as model-or; models trained with the raw datasets are denote as model-obs (i.e., observed dataset).

The improvements on the performance of ammonia forecasting models are most significant with the use of SG filters. GRU-sg5 and GRU-sg7 reduced 7.0% and 7.4% in the test loss compared with GRU-obs, while LSTM-sg5 and LSTM-sg7 reduced 4.2% of the test loss compared to LSTM-obs. Both data smoothing filters reduced the test loss and the improvements can be attributed to the modified relationships bewteen each datapoints. The SG filters modified the original datapoints by covoluting with both previous and the following datapoints, which resembles the working mechanisms of recurrent neural networks, while the EWMA filter modified the datapoints by averaging the value of current datapoint with previous ones. The performance of RF models was the poorest in the baseline model performance compared to other models. The results presented in Table. 4.1 indicate despite RF models were trained with data pre-processing methods, the model performance in test loss was still much higher than the poorest deep learning model, which is DNN-sg9 in this case.

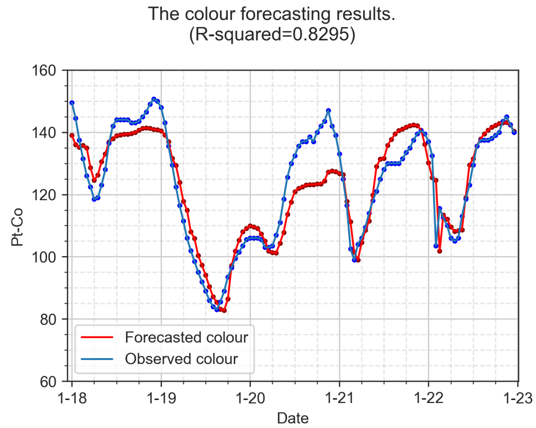
Empirically, when different models are evaluated by the same testing dataset, the best Model-Dataset combination shold have both the lowest values of test and validation loss. For instance, GRU-sg7 model in forecasting ammonia has the lowest test loss of 0.0383,



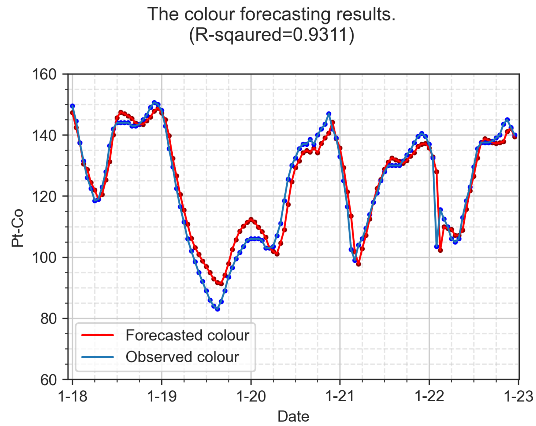
(a) Baseline RF model forecasting ammonia concentration.



(b) Baseline LSTM model forecasting ammonia concentration.



(c) Baseline RF model forecasting colour levels.



(d) Baseline LSTM model forecasting colour levels.

Figure 4.2: Visulization of the model forecasting results.

yet the validation loss of 1.2508 only ranks the tenth from the smallest validation loss vlaues. The models with top three lowest values of the validation loss are LSTM-ew3, LSTM-ew2 and LSTM-ew4. This finding points to the potential of the heterogeneity between the trianing and testing datasets. This hypothesis was the explanation with the highest likelihood when no overfitting was observed in the training datasets. Further tests were carried out using testing dataset from October to examine how the Model-Dataset ranks of test and validation loss values will change into. To the best of my understanding, the comparisons between testing and validation loss are not discussed on the currently available research papers in modelling of wastewater treatment industry.

As shown in Table. 4.2, the top three ranks of Model-Dataset in the lowest validation loss is the same to the top three ranks in the test loss values. This is in good agreement with how the heterogeneity of the datasets can impact on the model performance. The

Table 4.1: Baseline performance of ammonia forecasting model, evaluated on test dataset from **16 to 22 Janurary 2022**. Loss values are calculated by MSE.

Model-Dataset	Test loss	Valid loss	Model-Dataset	Test loss	Valid loss
GRU-sg7	0.0383	1.2508	RNN-or	0.0432	1.6345
GRU-sg5	0.0385	1.2644	RNN-ew3	0.0434	1.6041
LSTM-ew3	0.0388	1.0796	RNN-obs	0.0440	1.6734
LSTM-sg5	0.0388	1.2346	RNN-sg9	0.0442	1.7046
LSTM-sg7	0.0388	1.1804	DNN-obs	0.0561	3.2383
GRU-ew2	0.0389	1.1891	DNN-sg5	0.0562	3.2170
GRU-ew4	0.0391	1.2390	DNN-ew2	0.0563	3.1677
GRU-ew3	0.0392	1.2199	DNN-ew3	0.0569	3.2317
LSTM-ew2	0.0392	1.0969	DNN-sg7	0.0570	3.2014
LSTM-ew4	0.0395	1.1219	DNN-ew4	0.0571	3.2188
GRU-sg9	0.0396	1.3097	DNN-or	0.0572	3.1972
LSTM-or	0.0398	1.2612	DNN-sg9	0.0574	3.2484
LSTM-obs	0.0405	1.3993	RF-obs	0.1158	-
GRU-or	0.0405	1.2366	RF-sg9	0.1196	-
LSTM-sg9	0.0410	1.3076	RF-ew2	0.1286	-
GRU-obs	0.0414	1.3638	RF-or	0.1294	-
RNN-sg5	0.0415	1.5088	RF-sg5	0.1298	-
RNN-ew2	0.0421	1.5425	RF-ew3	0.1313	-
RNN-sg7	0.0423	1.6267	RF-sg7	0.1409	-
RNN-ew4	0.0432	1.5992	RF-ew4	0.1441	-

evluations of the ammonia forecasting models in October 2021 showed a complete different outcomes compared to the one in January 2022. Surpirsingly, the top three ranks of Model-Dataset in the lowest validation loss are the same of the lowest test loss, which are 0.0158 from LSTM-ew3, 0.0161 from LSTM-ew2, and 0.0163 from LSTM-ew4. Instead of GRU, LSTM becomes the best model for training ammonia forecasting model. The most remarkable results in Table. 4.2 is that EWMA filter seems to be the most ideal pre-processing methods for traning deep learning models as LSTM-ew3, GRU-ew3, RNN-ew4 and DNN-ew3 models showed the best model performance in test loss compared to the same models trained by other data pre-processing methods.

The test loss values of the colour forecasting models are presented in Table. 4.3. The best performed colour forecasting models are the LSTM models trained by EWMA filters, which are 0.0136 from LSTM-ew4, 0.0138 from LSTM-ew2 and LSTM-ew3. Interestingly, LSTM models trained by EWMA also showed the best performance in ammonia forecasting models. The top three ranks of Model-Dataset in the lowest validation loss ranks the

Table 4.2: Baseline performance of ammonia forecasting model, evaluated on test dataset from **10 to 16 October 2021**. Loss values are calculated by MSE.

Model-Dataset	Test loss	Valid loss	Model-Dataset	Test loss	Valid loss
LSTM-ew3	0.0158	1.0796	RNN-or	0.0197	1.6345
LSTM-ew2	0.0161	1.0969	RNN-sg7	0.0201	1.6267
LSTM-ew4	0.0163	1.1219	RNN-sg9	0.0205	1.7046
LSTM-sg5	0.0166	1.2346	RNN-obs	0.0206	1.6734
GRU-ew3	0.0167	1.2199	DNN-ew3	0.0316	3.2317
GRU-ew4	0.0169	1.2390	DNN-or	0.0316	3.1972
GRU-ew2	0.0170	1.1891	DNN-sg7	0.0316	3.2014
GRU-sg9	0.0174	1.3097	DNN-ew2	0.0318	3.1677
LSTM-obs	0.0175	1.2366	DNN-ew4	0.0319	3.2188
LSTM-or	0.0177	1.2612	DNN-obs	0.0319	3.2383
GRU-sg5	0.0178	1.2644	DNN-sg5	0.0319	3.2170
GRU-sg7	0.0180	1.2508	DNN-sg9	0.0319	3.2484
LSTM-sg7	0.0180	1.1804	RF-sg9	0.1307	-
GRU-or	0.0187	1.3993	RF-sg7	0.1311	-
LSTM-sg9	0.0188	1.3076	RF-sg5	0.1343	-
GRU-obs	0.0189	1.3638	RF-ew2	0.1346	-
RNN-ew4	0.0190	1.5992	RF-ew3	0.1368	-
RNN-ew2	0.0191	1.5425	RF-obs	0.1443	-
RNN-ew3	0.0193	1.6041	RF-ew4	0.1451	-
RNN-sg5	0.0195	1.5088	RF-or	0.1477	-

6th, 20th, and 1st from the lowest test loss values. However, we don't have extra testing datasets for re-evaluating the colour forecasting models. Compromises have to be made during the analysis of colour forecasting models.

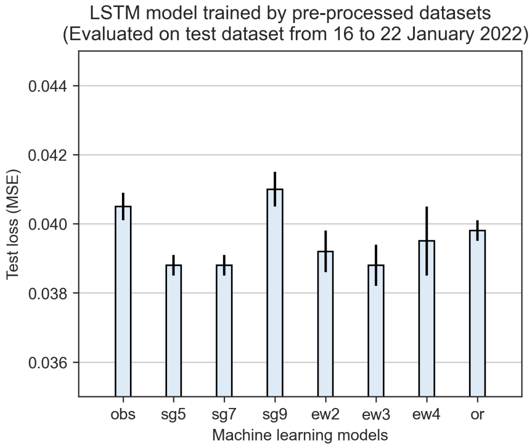
By comparing the baseline performance and the influences of data pre-processing methods on machine learning models, our findings appear to be well substantiated the use of LSTM models for training ammonia and colour forecasting models due to it's outstanding model performance evaluated by test loss values. Although EWMA filters showed surprising effects on improving the performance of most models, the influence of pre-processing methods are still not consistant across different models and training datasets. Thus, in the testings of the proposed model training processes will include all the pre-processing methods for model training, and LSTM will be used as the only machine learning model.

Table 4.3: Baseline performance of colour forecasting model, evaluated on test dataset from **16 to 22 Janurary 2022**. Loss values are calculated by MSE.

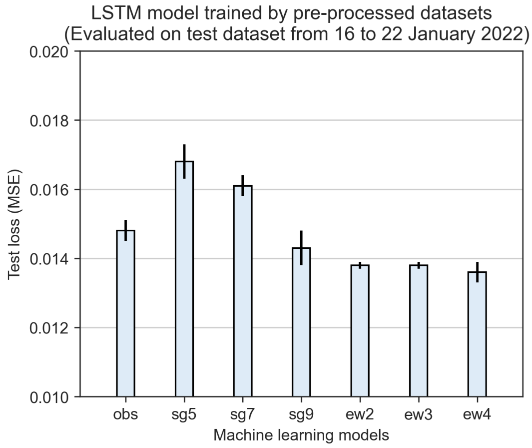
Model-Dataset	Test loss	Valid loss	Model-Dataset	Test loss	Valid loss
LSTM-ew4	0.0136	0.7515	RNN-obs	0.0160	1.0623
LSTM-ew2	0.0138	0.8011	LSTM-sg7	0.0161	0.7439
LSTM-ew3	0.0138	0.7547	LSTM-sg5	0.0168	0.8355
GRU-ew3	0.0140	0.8068	DNN-sg5	0.0180	1.4702
GRU-ew2	0.0142	0.8330	DNN-sg7	0.0180	1.4823
GRU-ew4	0.0143	0.7694	DNN-sg9	0.0180	1.4574
LSTM-sg9	0.0143	0.7137	DNN-ew4	0.0181	1.4632
RNN-ew3	0.0144	0.8492	DNN-ew3	0.0182	1.4716
RNN-ew4	0.0147	0.8476	DNN-ew2	0.0183	1.4946
RNN-sg9	0.0147	0.8363	DNN-obs	0.0186	1.5397
LSTM-obs	0.0148	0.9744	RF-sg9	63.6847	
GRU-obs	0.0149	0.9927	RF-sg7	73.8263	
RNN-ew2	0.0150	0.9083	RF-ew3	75.1974	-
GRU-sg9	0.0151	0.7575	RF-ew4	77.8829	-
RNN-sg5	0.0158	0.8846	RF-obs	78.5296	-
RNN-sg7	0.0158	0.8755	RF-ew2	78.8753	-
GRU-sg7	0.0159	0.7791	RF-sg5	81.0696	-
GRU-sg5	0.0160	0.8080	-	-	-

4.2.2 The effect of window size of data smoothing filters

The influences of window sizes in data smoothing process are investigated using LSTM models and illustrated in Fig. 4.3. SG window sizes of higher and lower have different impacts on ammonia and colour forecasting models. For instance, LSTM-sg5 performed better than LSTM-sg9 in forecasting ammonia, LSTM-sg9 outperformed LSTM-sg5 in forecasting colour. The similar pattern can be observed in models trained by EWMA filters as well For ammonia forecasting model, LSTM-ew3 is better, while for colour forecasting model, LSTM-ew3 is better. Therefore, the window sizes of the data smoothing filters needs to be carefully selected. The unpredictable influences of applying data smoothing filters on forecasting models impedes the determination of the optimal data smoothing method in the subsequent experiments. For the futher studies, all the pre-processing methods will be applied on the LSTM models.



(a) Baseline performance of ammonia forecasting models trained by LSTM.



(b) Baseline performance of colour forecasting models trained by LSTM.

Figure 4.3: Baseline performance of ammonia and colour forecasting models.

4.3 Exploit hidden patterns in MBR effluent water quality to enhance model performance

4.3.1 Ammonia forecasting models

In the section of feature engineering, we have introduced the selection and creation of the extra input features for training forecasting models as shown in Fig. 3.17. In this study, a forecasting model trained by 1 input is called an univariate model and denoted as LSTM-1; a forecasting model trained by 2 inputs is called a multivariate model and denoted as LSTM-2. For models trained by 3 and 4 inputs are denoted as LSTM-3 and LSTM-4. In Fig. 4.4, the performance of ammonia forecasting models trained by 2 to 4 inputs (i.e., LSTM-2, LSTM-3, LSTM-4) are compared with the baseline performance (i.e., LSTM-1-obs) to demonstrate how the feature engineered features influenced on the model outputs.

Leaving out the potential influences of heterogeneity between training and testing datasets on comparing the model performance, interesting resutls were still observed. As shown in Fig. 4.4, LSTM-4-obs showed the highest test loss, followed by LSTM-3-obs, LSTM-2-obs and LSTM-1-obs. This result indicate that for LSTM models trained with more input featues can result in a poorer model performance. Based on our understandings to the extra features such as color levels and sine/cosine features, models trained with more inputs are expected lower test values. The model performance from LSTM-sg7 and

LSTM-sg9 fits well with what we hypothesized. The results showed the test loss values of the LSTM models trained by datasets applied with sg7 and sg9 filters followed the trend of LSTM-4<LSTM-3<LSTM-2<LSTM-1. The most remarkable results are from LSTM models trained by datasets applied with SG filters at window size of 7. Comparing to the baseline model performance (i.e., LSTM-1-obs), the test loss values of LSTM-1-sg7, LSTM-2-sg7, LSTM-3-sg7 and LSTM-4-sg7 reduced by 4.2%, 6.4%, 7.9%, and 8.9%, respectively.

Our findings in the results of ammonia forecasting models suggests that colour level is an indispensible input for improving the model performance. LSTM-2 models trained by datasets applied with any pre-processing methods showed lower test loss compared to LSTM-1, except LSTM-2 trained by dataset without applying any methods. There is a strong probability leads us to believe that the flucturation of ammonia concentration is highly correlated with the colour level in SHWEPP influent even without the direct evidence.

The methods of training LSTM models on pre-processed datasets have proved it's benefits in improving baseline model performance, yet the test loss values were only reduced slightly for those models trained with EWMA filtered datasets. As shown in Fig. 4.4, LSTM-3-ew2, LSTM-4-ew2, LSTM-3-ew4 and LSTM-4-ew4 shared very similar test loss values to LSTM-1-obs, indicating the advantages of enhanced quality in training dataset were not fully reflected on the model performance when LSTM models were trained by EWMA filtered datasets.

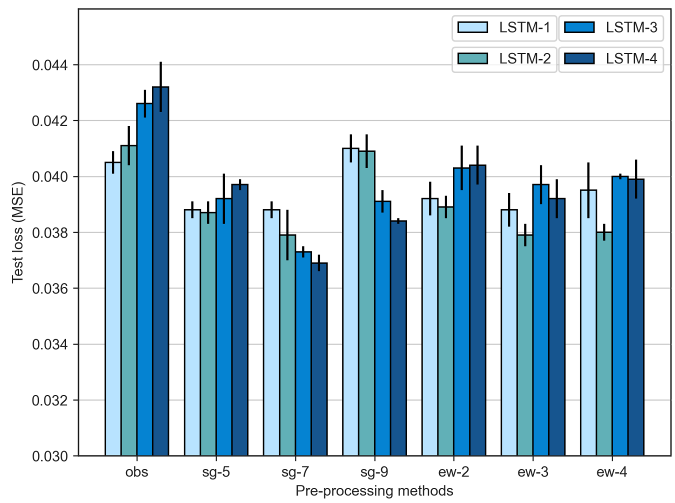


Figure 4.4: Comparisons of the model performance in forecasitng ammonia concentrations.

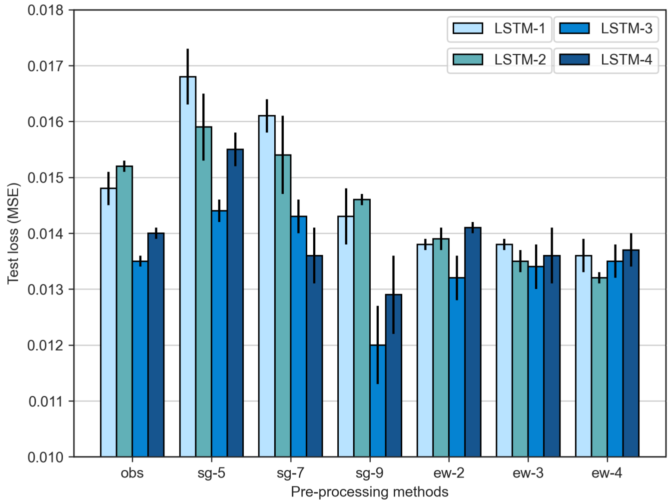


Figure 4.5: Comparisons of model performance in forecasting colour levels.

4.3.2 Colour forecasting models

As shown in Fig. 4.5, most of the proposed pre-processing methods improved the performance of colour forecasting models. All the LSTM models trained by EWMA filtered datasets have lower test loss compared to the baseline model performance, while part of the LSTM models trained by SG filtered datasets showed improvement on the model performance. The performance of models trained by SG filtered datasets was rather disappointing. We observed that the test loss of LSTM-sg5, LSTM-sg7 and LSTM-sg9 showed much higher values of standard deviations, and this was probably as a result of the poor quality of the raw colour data.

From the results of ammonia forecasting models, we thought that LSTM models trained by datasets applied with sg7 will generate the lowest test loss in LSTM-4, however, the results in the colour forecasting models revealed that the lowest test loss was generated from LSTM-3-sg9, with test values of 0.0121, a 28.6% improvement in model performance compared to the baseline model performance. Contrary to expectations, datasets trained by four inputs failed to generate the lowest test loss. The fact of having higher test loss in LSTM-4 compared to LSTM-3 is evident and can be found in Fig. 4.5 except LSTM-4-sg7. It is very likely that including ammonia concentrations as an input features worsened the quality of the training dataset and resulted in a poorer performance for colour forecasing models.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATION

5.1 Conclusions

5.1.1 Machine learning models vs deep learning models

The selection of using which machine learning and deep learning models was not widely discussed to the best of our knowledge in the modelling of wastewater treatment industry. This study has investigated on the model performance of machine learning model of RF, and four other deep learning models of DNN, RNN, GRU and LSTM on forecasting ammonia concentrations and colour levels in reclaimed water system for assisting treatment operation and management. The evidence from this study suggests deep learning models are much capable in learning from the historical data and generate more accurate forecasting results. In both ammonia and colour forecasting models, the test loss values of RF are much higher than the values from the least performanced deep learning model of DNN. Among all the deep learning models, the results indicate LSTM and GRU models have the lowest test loss of 0.0405 and 0.0414, respectively. However, the further research works suggest LSTM models trained with pre-processing methods generate the lowest test loss compared to GRU, making the LSTM model the most promising recurrent neural network model for training forecasting models.

5.1.2 Data pre-processing techniques

Our research also highlighted the importance of how the model performance can be improved from applying data pre-processing and feature engineering techniques. Generally speaking, all the proposed data smoothing and outlier removal methods reduced the test loss values compared to the baseline model performance (i.e., the window sizes of the filters need to be carefully selected), as showin in Fig. 4.3. It is believed that the convoluted datapoints generated from data smoothing filters enable the recurrent neural networks to predict the future values more easily.

5.1.3 Feature engineering

This study is the first step towards enhancing our understanding to the potential benefits of using created features for model training. The thorough examinations of the Geomap nearby the SHWEPP and the investigation of water composition in the public sewege system helped us to hypothesize that the change of ammonia concentrations and colour levels are dependent to each other. With the help of additional colour/ammonia data for ammonia/colour forecasting model, the test loss reduced by 6.4% (i.e., LSTM-2-sg7 compared to LSTM-1-obs) and 10.8% (i.e., LSTM-2-ew4 compared to LSTM-1-obs), respectively.

Moreover, the similarity between the household consumption patterns and the daily fluctuation of ammonia concentrations have unexpectedly helped us to formulate the time features via positional encoding. The influence of the sine and cosine hour features on the model perfromance showed tremendous improvements on both ammonia and colour forecasting models. In the former, test loss dropped by 8.9% (i.e., LSTM-1-obs compared with LSTM-4-sg7) while the latter reduced by 28.6% (i.e., LSTM-1-obs compared with LSTM-3-sg9). The remarkable use of positional encoding features is it is not limited to just ammonia and colour forecasting models. Any time series data characterized with daily fluctuation patterns can adopt the use of the features of sine and cosine hour as long as the patterns are based on actaul events. In addition, the positional encoding features are not limited to hour, we can encode features into from seconds to weeks, and even years, the application of it is infinite. However, the feature engineering method clearly has some limitations. In the results of ammonia forecasting models, LSTM-2-obs, LSTM-3-obs and LSTM-4-obs showed higher tess loss compared to LSTM-1-obs, indicating when the models were trained by any features other than ammonia, the model performance worsened. In addition to that, when extra features were train with EWMA filters, the test loss increased, and the worsening of model performance also occured on colour forecasting models trained by EWMA filters. Our results suggest that feature engineering needs to be carefully evaluated and experimented before the real use. Despite the limitations, the combination use of feature engineering in building ammonia and colour forecasting models in this study has fully proved it's advantages.

5.2 Recommendations for future research

Due to the insufficient ammonia and colour data, we cannot differentiate whether the undesired model performance was caused by the heterogeneity of the training and testing datasets or caused by the pre-processing and feature engineering methods we applied on the datasets. It is recommended a larger dataset (e.g., dataset with the size of 2 months or longer) should be used in the future study when evaluating the proposed methods in this study. The insufficient amount of data could also lead to the unstable performance of different models trained by the same data smoothing methods. For instance, LSTM-4-sg7 and LSTM-3-sg7 have the lowest test loss among LSTM-4 and LSTM-3 models, however, LSTM-2-ew4 has the lower test loss than LSTM-4-sg7. We failed to explain what has caused such outcome.

All the forecasting models in this study only focus on predicting ammonia concentration and colour levles, and in the futher study, more water quality parameters should be included. In reclaimed water system, the concentration of water quality parameters such as turbidity and E. coli are also regulated by Water Supply Department. The violation of any water quality parameter will directly lead to the disqualification of being used as reclaimed water. Moreover, The hidden correlations reside between each water quality parameter will most likely be helpful in building any water quality forecasting models.

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