Development of a Novel Water Quality Index Model Using Data Science Approaches

By

Md Galal Uddin

Supervisors: Dr. Agnieszka I. Olbert, Dr. Stephen Nash,

University Of Galway, Ireland

And

Dr. Azizur Rahman

Charles Sturt University, Wagga Wagga, Australia

OLLSCOIL NA GAILLIMHE
UNIVERSITY OF GALWAY

A thesis submitted to the University of Galway as fulfilment of the requirements for the Degree of Doctor of Philosophy, in the College of Science and Engineering.

Department of Civil Engineering, School of Engineering,

College of Science and Engineering,

University of Galway, Ireland

February 2023

Table of Contents

Declarations

I hereby declare that the presented thesis, in whole or in part, has not been submitted to any university for the purpose of pursuing any degree. I further declare that, with the exception of where reference is provided, the work is entirely my own.

Signed:

____

Md Galal Uddin February 2023

Dedication

This research work is dedicated to my beloved wife Kazi Shama Ferdous Tania and my daughter Sabiqunnahar Jafira, especially Jafira devoted much more of her childhood time without her father than could be captured in a few fantastic and memorable times with him.

Abstract

Surface water quality management is an essential task to acheive "good" water quality across all states. A number of tools and techniques are widely used to assess water quality, the water quality index (WQI) model is one of them. Commonly, the WQI model is used to convert various water quality indicator data into a single numerical value and its use has increased tremendously due to its simple mathematical operation and the fact that its results are easy to interpret by both professionals and non-experts. Most WQI application to date have focused on freshwaters - lakes, river, and ground waters, with just a small number focused on coastal water quality assessment. Despite their advantages, WQI models have received criticism with respect to their reliability, validity, and inconsistency of results. In addition, several studies have revealed that the existing WQI model results contain a lot of uncertainty due to eclipsing and ambiguity problems associated with their architecture.

The research focuses on the development of a novel WQI model for coastal and transitional coastal (TrC) waters. A comprehensive WQI model was developed for assessing TrC waters, with significant improvements over existing WQI models. The model consists of five identical components, including: (i) indicator selection technique—a random forest machine learning algorithm was used to select the crucial water quality indicator; (ii) sub-index (SI) functions—three brand new linear interpolation functions were developed for rescaling various water quality indicators' information into a uniform scale; (iii) indicators' weight method—a novel approach was developed using the random forest machine learning (ML) algorithm and mathematical rank sum weighting technique for estimating the weight values based on the relative significance of real-time information on water quality; (iii) aggregation function—the weighted quadratic mean (WQM) function was utilized for computing the water quality index (WQI) score; and (v) score interpretation scheme - a brand new classification scheme was proposed by analysing a range of classification techniques for assessing the state of water quality.

Model performance was evaluated and validated across four Irish TrC waterbodies using the EPA’s water quality monitoring data. Model performance was tested and evaluated using state-of-the-art machine learning (ML) and artificial intelligence (AI)

techniques in terms of reducing the eclipsing and ambiguity problems as well as model uncertainty. The key findings from the applications results are as follows:

- The sensitivity results of model indicate that the model outputs could be explained by more than 95% of the input entities, including less than 2% uncertainty with a 95% confidence interval at $p < 0.0001$.
- The model performance validation results of NSE and MEF show that the developed model is superior for computing WQI scores at most monitoring sites across four application domains through the summer and winter periods.
- In addition, most statistical measures of performance metrics also indicate that the model is more effective for the prediction of WQI score in TrC waters.
- The assessment results of water quality proved that the developed model is reliable for optimizing the model ambiguity and eclipsing problems.
- Moreover, the performance of model applications reveals that suggested indicators: dissolved oxygen (DOX), biological oxygen demand (BOD_5), pH, water temperature (TEMP), transparency (TRAN), and three nutrient enrichment indicators included total oxidized nitrogen (TON), dissolved inorganic nitrogen (DIN), and molybdate reactive phosphorus (MRP)O might be adequate and reliable to monitor the transitional and coastal waters with the proposed model.
- Overall, the model's results (applications, sensitivity, eclipsing, ambiguity, and uncertainty) indicate that the proposed model is more robust than other WQI approaches.

The developed model could be useful for further improvement of the existing WQI system and effective in improving the typical monitoring program for managing TrC waters in the world. Although the present model was developed for transitional and coastal water quality, the approach could also be utilized to assess water quality in other waterbody types, e.g. rivers or lakes, and geographical locations.

Acknowledgements

First, I would like to express my sincere gratitude to my honorable supervisor, Dr Agnieszka I. Olbert for her technical advice, encouragement and outstanding supervision during the research period. I sincerely thank to my co-supervisor, Dr Stephen Nash, for providing excellent supervision through his expertise and guidelines over the research work. I also would like to express my sincere gratitude to Prof. Dr Azizur Rahman of Charles Sturt University in Wagga Wagga, Australia, for his excellent international co-supervision, support, guidelines, and extraordinary effort to carry out computational analysis through the present research.

I wish to thank and sincerely acknowledge the members of my Graduate Research Committee, Prof. Padraic O'Donoghue, Prof. Michael Hartnett, Prof. Mark Healy, and Dr. Guangxue Wu, as well as all faculty staff, and researchers at the College of Science and Engineering, University of Galway (UoG), who have provided constructive and effective advice and supports through the project period to complete this research.

I would like to acknowledge the Hardiman Research Scholarship of the UoG, which funded this research. I also acknowledge the Environmental Protection Agency of Ireland for providing water quality data that has been used in this research to develop and validate the model. I sincerely acknowledge the Eco HydroInformatics Research Group (EHIRG), School of Engineering, CoEI, UoG, Ireland, for providing computational laboratory facilities to complete this research. I would like to express my thanks to the staff and all research associates of the EHIRG, for their support during the long journey, especially, Mir Talas Mahammad Diganta for providing numerous supports over the research period.

My wife Kazi Shama Ferdous Tania and my daughter Sabiqunnahar Jafira deserve special thanks and recognition for their patience and invaluable support over the past four years. Especially, I would like to thank my parents in-law, Kazi Muzammal Haque and Kazi Sahana Begum, for their numerous crucial supports and priceless counsel throughout my life.

I'd like to sincerely thank my father, Al Hazz Abul Kalam, who has served as my life coach and future shaper and has always been an inspiration to me, telling me things like, "You have to go forward with your own excellence; I am a poor farmer; I did not have the chance to get a good education, but I will always try to provide my best for achieving your dream if you want to reach the top level of higher education in the world." But I am aware that my father lacked the necessary means to do that. However, when I lost my confidence, I used to talk with him to boost my strength. I sincerely acknowledge my beloved mother, Payara Begum, for her contribution to my life.

I would like to cordial thanks my uncle, Rahamat Ullah Miazi, who taught me how to write and read the alphabet initially in my childhood with a lot of love.

A special thanks to my mentors, Dr. Md. Moniruzzaman, Professor of Geography and Environment at Jagnanath University in Dhaka, and Md. Abu Hasan, Scientific Officer at the Bangladesh Reference Institute for Chemical Measurments in Dhaka, who constantly inspire me to do research.

Finally, my thanks to all of my family’s members, friends, and colleagues for their friendship and support throughout the years.

List of Publications

The research work presented in this thesis has resulted in the following 8 journal publications which are included as thesis chapters:

Chapter 2: Uddin, M.G., Nash, S., Olbert, A.I., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol Indic 122, 107218. https://doi.org/10.1016/j.ecolind.2020.107218

Chapter 3: Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022d. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment. Water Res 219, 118532. https://doi.org/10.1016/j.watres.2022.118532

Chapter 4: Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2023a. A novel approach for estimating and predicting uncertainty in water quality index model using machine learning approaches. Water Res 229, 119422. https://doi.org/10.1016/j.watres.2022.119422

Chapter 5: Performance analysis of the water quality index model for predicting water state using machine learning techniques. Process Safety and Environmental Protection 169, 808–828. https://doi.org/10.1016/j.psep.2022.11.073

Chapter 6: Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022b. Assessing optimization techniques for improving water quality model. Journal of Cleaner Production. https://doi.org/10.1016/j.jclepro.2022.135671

Chapter 7: Uddin, M.G., Nash, S., Talas, M., Diganta, M., Rahman, A., Olbert, A.I., 2022b. Robust machine learning algorithms for predicting coastal water quality index, Journal of Environmental Management. https://doi.org/10.1016/j.jenvman.2022.115923

Chapter 8: Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022b. A sophisticated model for rating water quality. Science of The Total Environment.

https://doi.org/10.1016/j.scitotenv.2023.161614

Chapter 9: Uddin, M.G., Nash, S., **Rahman**, A., Olbert, A.I., 2022d. An improved methodology for the assessment of trophic status for coastal and transitional waters using machine learning and artificial intelligence approaches. Water Res. Under Review.

The research work was also disseminated at various national and international conferences resulting in the 7 publications listed below:

1) **Uddin, M.G.,** Stephen Nash, Olbert, A.I., 2020b. Application of Water Quality Index Models to an Irish Estuary, in: Civil and Environmental Research. Civil Engineering Research Association of Ireland (CERAI), pp. 576–581.

2) **Uddin, M.G.,** Olbert, A.I., Nash, S., 2020a. Assessment of water quality using Water Quality Index (WQI) models and advanced geostatistical technique, in: Civil Engineering Research Association of Ireland (CERAI). Civil Engineering Research Association of Ireland (CERAI), Cork Institute of Technology, Cork, pp. 594–599.

3) **Uddin, G.,** Nash, S., Olbert, A.I., 2022a. Optimization of Parameters in a Water Quality Index Model using Principal Component Analysis, in: Proceedings of the 39th IAHR World Congress. Proceedings of the 39th IAHR World Congress. https://doi.org/10.3850/IAHR-39WC2521711920221326

4) **Uddin, M.G.,** Nash, S., Rahman, A., Olbert, A.I., 2022c. Development of a water quality index model - a comparative analysis of various weighting methods, in: Çiner, Prof.Dr.A. (Ed.), Mediterranean Geosciences Union Annual Meeting (MedGU-21). Spinger, Istanbul, pp. 1–6.

5) **Uddin, M.G.,** Nash, S., Diganta, M.T.M., Rahman, A., Olbert, A.I., 2022a. A comparison of geocomputational models for validating geospatial distribution of water quality index, in: Priyanka, H., Rahman, A., Basant agarwal, Binita Tiwari (Eds.), Computational Statistical Methodologies and Modeling for Artificial Intelligence. CRC Press, Taylor & Francis Publisher, USA

6) **Uddin, M.G.,** Nash, S., Rahman, A., Olbert, A.I., 2022c. Development of an efficient water quality model using cutting-edge artificial intelligence techniques,

Australia and New Zealand Regional Science Association International 45th Annual Conference. Charles Sturt University, Wagga Wagga, 286 Pine Gully Rd, Charles Sturt University NSW 2678 , Australia, pp. 19.

7) **Uddin, M.G.,** Nash, S., Rahman, A., Olbert, A.I.. Sensitivity of indicator weights in the water quality index model for assessing coastal water quality [Abstract]. In: The 18th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES), 2023 September 24-30; Dubrovnik, Croatia. 2023. Abstract no SDEWES2023.0019.

“Water is a global issue; we have to address it globally.”

Roger A. Falconer

1. Introduction

1.1 Research background

Surface water quality poses significant environmental, sociological, and economic risks in many parts of the world. As such, sustainable management of water resources has become a challenge of critical importance (Fu et al., 2022; Liu et al., 2017; Rogers et al., 2020). Due to population growth, industrialisation and urbanisation over many decades, freshwater usage and wastewater production have significantly increased (Hartnett et al., 2012; Hartnett and Nash, 2004; Javed et al., 2017; Uddin et al., 2018). Both human activities and natural processes have caused a continuous degradation of surface water quality in recent decades, many countries have adopted a range of policies and guidelines to manage surface water quality and provide more effective water resource management to reverse this negative trend (Hering et al., 2010; Kallis, 2001; Lenton and Muller, 2012). Member states of the European Union (EU), for example, adopted the Water Framework Directive (WFD) in 2000 and it has been an effective instrument for the management of the quality of water and its ecosystem (Carsten Von Der Ohe et al., 2007; Hering et al., 2010; Kallis, 2001; Zotou et al., 2019). The WFD envisaged the achievement of at least a "good environmental status" of all waterbodies such as coastal and transitional (TrC) water, rivers and lakes by 2015 (Brack et al., 2017; Carsten Von Der Ohe et al., 2007; EPA, 2001; Hering et al., 2018; Santos et al., 2021). The WFD and other similar frameworks rely on assessment of water quality.

Monitoring programmes are one of the most widely used techniques for assessing water quality, but it has some drawbacks. Several studies have reported that the traditional monitoring program is not affordable for developing (and even some developed) countries due to some of its specific requirements, such as the need for highly equipped and advanced laboratory facilities, skilled manpower, sufficient funding etc. (Dimri et al., 2021; Hartnett et al., 2011; Sutadian et al., 2016; Telci et al., 2009; Zhu et al., 2019). Moreover, it is also very time-consuming (Jiang et al., 2020; Strobl and Robillard, 2008), it is limited in its spatial extents, and it has received some criticism of its technical aspects, and data accuracy (Strobl and Robillard, 2008).

In recent years, a range of tools and techniques have been developed to assess the quality of surface waters and diagnose the health of aquatic ecosystems. Water quality index (WQI) models are an excellent example. They use mathematical techniques to express multiple water quality characteristics with a single dimensionless number and have been shown to be a useful tool for assessing surface water quality and their ecological status (Gupta and Gupta, 2021; Smith, 1990; Sutadian et al., 2016a). Compared to other hydrological/water quality models, WQI models are relatively easy to apply and their results are easy to interpret by both professionals and non-experts (Abbasi and Abbasi, 2012; Bai Varadharajan et al., 2009; Nives, 1999; Sutadian et al., 2018).

Based on initial investigation, the WQI model(s) consists of five sequential components, including:

(i) the indicators selection process used to select the crucial water quality indicators in terms of their relative significance;
(ii) sub-index (SI) functions that transfer water quality measurements into dimensionless form, ideally without hiding any real information about the indicators;
(iii) a weighting generation technique, used for assigning the importance of indicators based on their relative influence on water quality;
(iv) the aggregation function that uses the SI and weighting values to calculate a single numerical number (overall index score) called the "WQI score", and
(v) the classification scheme that is used to interpret/translate the WQI score in order to classify the water quality as "good", "fair", "marginal" etc.

Since their first development, applications of WQI models have greatly increased because, in contrast to traditional hydrological or water quality models which require highly developed mathematical and analytical skills as well as a complex computational architecture, the WQI is based on very basic mathematical operations, is simple to use, and is cost effective. Many different WQI models have been developed by various organizations/countries/researchers for assessing water quality.

These have been focused on specific domains or waterbodies like lakes, rivers, groundwater, mine waters, wastewater etc. Recently, the WQI model has received criticism of it reliability, validity, and inconsistency of results (Abbasi and Abbasi, 2012; Gupta and Gupta, 2021b; Juwana et al., 2016a; Sutadian et al., 2016). Several studies have revealed that WQI models can produce a significant amount of uncertainty from various sources within the model components (Abbasi and Abbasi, 2012; Chakravarty and Gupta, 2021; Effendi et al., 2015; Gradilla-Hernández et al., 2020; Gupta et al., 2003; Gupta and Gupta, 2021b; Juwana et al., 2016b; Sutadian et al., 2018; Verma et al., 2019). Researchers have argued that a considerable amount of uncertainty is contributed to the WQI model by the indicators' selection process, SI functions, and using inappropriate aggregation functions (Abbasi and Abbasi, 2012; Gupta et al., 2003; Gupta and Gupta, 2021b; Juwana et al., 2016a, 2016b; Lumb et al., 2011; Sutadian et al., 2016).

In developing a WQI model, indicator selection is one of the crucial stages. In order to select important water quality indicators, existing WQI models used various techniques such as principal components analysis (Chakravarty and Gupta, 2021; Dezfooli et al., 2018; Fadel et al., 2021; Hou et al., 2016; Islam Khan et al., 2022; Ma et al., 2020; Parween et al., 2022; Tripathi and Singal, 2019; Zeinalzadeh and Rezaei, 2017), correlation technique (Heydari et al., 2013; Ibrahim et al., 2021; Kothari et al., 2021a, 2021b; Michalak and Kwasnicka, 2006), expert opinions (Grbić et al., 2013; Medeiros et al., 2017; Sutadian et al., 2017), analytical hierarchy process (Juwana et al., 2016b; Sutadian et al., 2017), Delphi technique (Horton, 1965; Kullar et al., 2019; Taylor and Ryder, 2003), and simple data availability (Sutadian et al., 2017). Recently, these techniques have criticism in terms of reliability and appropriateness for selecting indicators. They can lead to inclusion of irrelevant indicators or omission of important ones and to the attribution of weightings that are not truly reflective of real-world indicator importance. Several recent studies have revealed that traditional indicator selection techniques contributed a significant amount of uncertainty in the final assessment due to inappropriate indicator selection (Cheng et al., 2018; Jiang et al., 2018; Pan et al., 2022).

Another important component of a WQI model is the SI function, which allows conversion of indicator concentrations into dimensionless values. The SI generation has been reported in several studies to be one of the main sources of uncertainty (Abbasi and Abbasi, 2012; Uddin et al., 2021) as the process can conceal the integral information of water quality (Lumb et al., 2011; Sutadian et al., 2016; Uddin et al., 2021). A range of techniques have been used to calculate the SI values. For example, the Oregon WQI model applied logarithmic transformations and a nonlinear regression technique to obtain its SI values (Cude, 2001; Dunnette, 1979) and several, such as the Almeida index (2012), the House index (1989), and the Hanh surface WQI model, applied a rating curve technique to obtain the SI value. Several WQI models used standard guideline values (Abbasi and Abbasi, 2012; Hoseinzadeh et al., 2015; Liou et al., 2004; Lobato et al., 2015; Medeiros et al., 2017; Misaghi et al., 2017; Sutadian et al., 2016) while a few studies used water concentrations directly as SI values (Dojlido et al., 1994). In addition, a few models such as the Dojildo model omit the step altogether to avoid inconsistence in WQI measurement (Cash et al., 2001). Several recent studies have revealed that SI techniques can produce a significant amount of uncertainty due to the eclipsing problem of SI function(s) which is an overestimating/underestimating problem of the SI functions (Abbasi and Abbasi, 2012; Sutadian et al., 2016).

Indicator weighting is another important component of the WQI model. Commonly, the indicator weight value is estimated based on the relative importance of the water quality parameter and/or the appropriate guidelines for water quality (Sarkar and Abbasi, 2006). The majority of existing WQI models applied unequal weighting techniques where the sum of all of the parameter weight values was equal to 1 (Gupta and Gupta, 2021; Lumb et al., 2011; Sutadian et al., 2016). A few WQI models (for example the Horton, Bascaron and Ameida index) used unequal weighting but the weightings were integers and their totals were greater than 1. Some models, such as the Oregon model, used an equal weighting approach where all parameters were assigned an equal weighting. On the other hand, a few widely used models like the CCME index, the Smith index, and the Dojildo index do not require weight values for estimating the final score (Dojlido et al., 1994; Hansda et al., 2018; Saffran et al., 2001; Smith, 1990). The most common techniques used to determine the indicator weight values include the analytical hierarchy process, expert judgement, or simple literature recommendations (Abbasi and Abbasi, 2012; Gupta and Gupta, 2021; Sutadian et al., 2017). Most WQI models frequently used the expert judgement approach (Gazzaz et al., 2012; Ocampo-Duque et al., 2006; Sutadian et al., 2016) which is particularly open to error; while an expert may be quite comfortable ranking indicators based on their relative importance; they will likely struggle with the precision imposed by the eliciting of exact weights. This is true even for a group of experts who may struggle to agree on a ranking of indicators never mind precise weightings. A number of recent studies have reported that a considerable amount of uncertainty in WQI scores is generted from using inappropriate weightings (Juwana et al., 2016; Smith, 1990; Sutadian et al., 2018, 2016).

The aggregation function, which determines the overall water quality index, is the most crucial component of a WQI model. Various WQI aggregation functions have been intercompared in the literature (Mladenović-Ranisavljević and Žerajić, 2018; Zotou et al., 2018), and significant variations in formulations has been found (Gupta et al., 2003; Zotou et al., 2018). To date, most models have used either additive functions or multiplicative functions or a combination of the both techniques. Several studies report that the aggregation function is another crucial source of model uncertainty due to the ambiguity problem (Abbasi and Abbasi, 2012; Sutadian et al., 2016). Like the eclipsing problem of the SI functions, ambiguity is a similar type problem that occurs due to the use of inappropriate aggregation function(s) (Abbasi and Abbasi, 2012; Gupta et al., 2003).

The final WQI model component is the classification scheme which is used to translate WQI scores into qualitative water quality classifications like “good”, “fair”, “marginal”, “poor”, “bad” etc. Existing WQI models have used a range of classification schemes (Chadli and Boufala, 2021; Effendi et al., 2015b; Gupta and Gupta, 2021b; Lumb et al., 2011a; Verma et al., 2019); consequently, different models may provide different interpretations for the same water quality. The contributes to considerable uncertainty in the correct classification of water quality which has led to observations in the literature that WQI models do not express the actual state of water quality (Gupta and Gupta, 2021; Sutadian et al., 2016; Uddin et al., 2021).

As WQI models are becoming more widely used globally, the concerns about their various issues and weaknesses outlined above are also growing. According to recent studies, existing WQI model can provide ambiguous information to the water resources manager as a result of these issues, causing the responsible persons to fail to respond as quickly as required (Liou et al., 2004; Li et al., 2016; Sutadian et al., 2016; Uddin et al., 2021). Although, over the years, some components of WQI models have been modified and/or newly developed, far too little attention has been paid to improving the WQI model in terms of reducing model uncertainty or addressing existing concerns. There is a need for a significant improvement of each model component in terms of reducing eclipsing, ambiguity and uncertainty within the model.

To date, the WQI has primarily been applied to fresh waterbodies, i.e. lakes, rivers and reservoirs. To the best of the author's knowledge, there are no existing WQI models focused on coastal water quality, and there is no specific framework for developing a coastal water WQI model, with the exception of a few studies that have utilized common WQI models like the NSF index (Gupta et al., 2003; Jha et al., 2015), CCME index (de Rosemond et al., 2009), or modified NSF WQI (Ma et al. 2020) for assessing coastal water quality. The aim of this resreach was to develop a novel water quality index model for determination of water quality status of marine waters which are much more dynamic environments than fresh waterbodies. The model will provide an accurate, cost-effective and universal solution that will be applicable to any marine waterbody. Such a model will aid surface water monitoring and resource management as directed by the European Union Water Framework Directives (EU-WFD).

1.2 Research aims and objectives

The primary goal of the research was to develop a novel WQI model that can be widely used for efficient assessment of marine water quality and will improve existing water quality monitoring programs. The research goal was obtained by completing the following objectives:

1. Investigate the potential of WQI models as a tool for assessing the quality of marine waters (to include TrC waters and shallow shelf seas).
2. Investigate the sensitivity of WQI assessment to spatial and temporal resolution of input water quality data.
3. Development a new standardised WQI model for marine waters which can be applied to any marine waterbody in any geographical extent. This was a multi-step process as follows:

3.1 Develop an appropriate method for selecting the most important water quality indicators for inclusion in a model application in order to reduce the model uncertainty from this process.

3.2 Develop more robust SI function(s) for converting water quality indicator measurements into dimensionless forms without losing any crucial information about the indicators.

3.3 Develop a novel method for estimating indicators' weighted values based on their relative importance.

3.4 Determine the most appropriate aggregation function for calculating the overall water quality index/score.

3.5 Developing a generalized classification scheme for appropriate classification of marine waters.

4. Develop a novel approach for estimating WQI model uncertainty that can compute model uncertainty at each step of the modelling process.
5. Analyse the performance of the new WQI model in terms of correct classification of marine waters using the new classification scheme.
6. Test and validate the new WQI model by application to different case study sites.
7. Develop an ML algorithm for the new WQI model in order to accurately predict the WQI score at a monitoring site.
8. To develop a methodology for the assessment of the trophic status for coastal and transitional waters.

1.3 Description of the model development and application domain

Cork Harbour, an Irish estuary that is characterized by complex ecological interactions, was used as a case study to develop and test the new WQI model and demonstrate the model's capability. The harbour is heavily populated and industrialized. It is located on the southwest coast of Ireland. It is the largest natural harbour in Ireland and is a macro-tidal estuary with a typical spring tide range of 4.2 m at the entrance to the Harbour (Hartnett and Nash, 2015). Water depths are generally relatively shallow with much of the estuary having a depth of less than 5 m on spring tides. At low water, a major portion of the Harbour area is exposed to mudflats and sandflats.

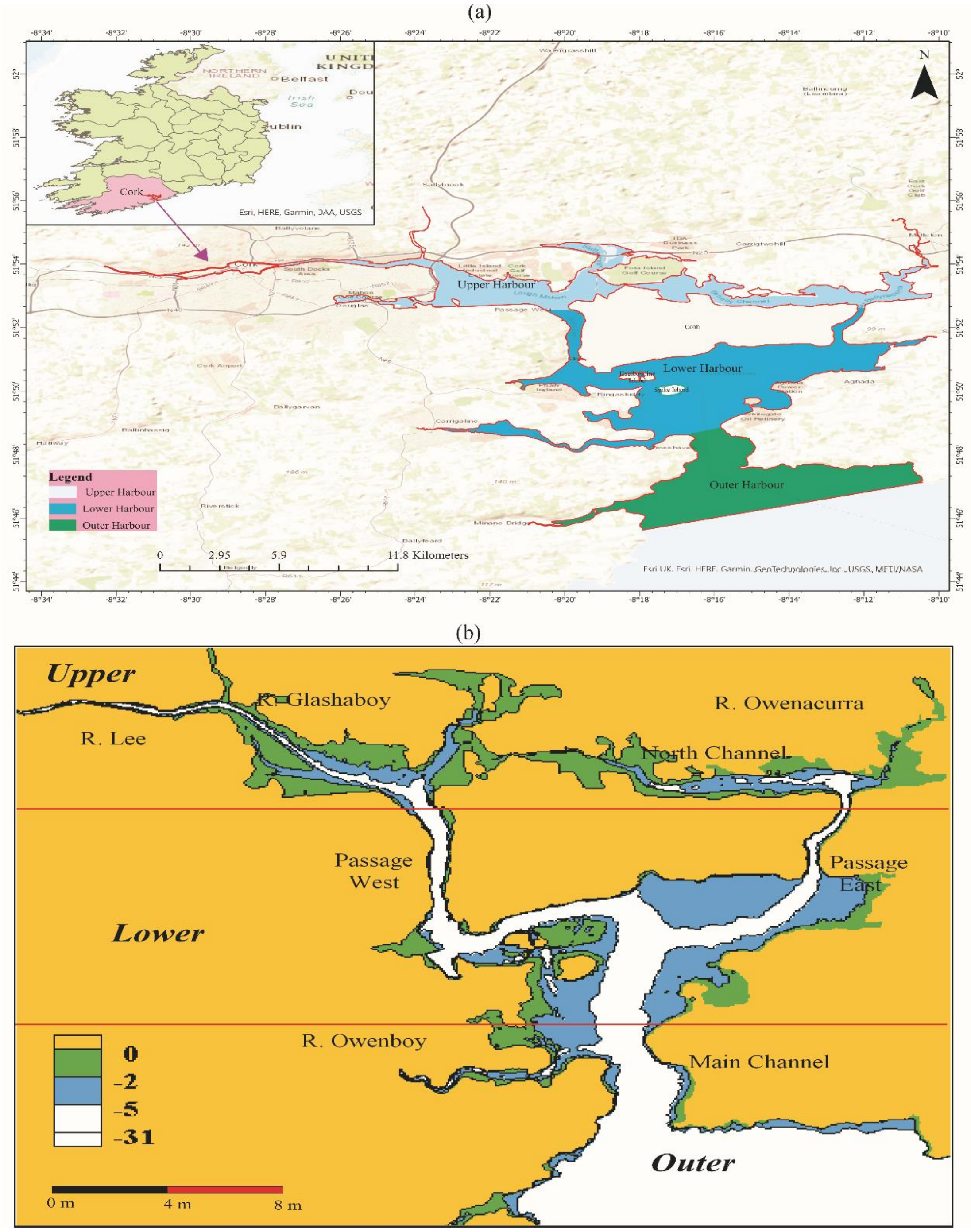


Figure 1.1. Model development domain: Cork Harbour, Cork, Ireland.

Cork Harbour deepens towards the mouth in the main Channel to depths of about 30 m. A number of rivers flow into the estuary, the largest being the River Lee which flows through Cork City and accounts for approximately 75% of the freshwater delivered to the estuary (Uddin et al., 2020). Cork City, located at the mouth of the River Lee, is home to a population of approximately 125,000. When its immediate suburbs are included, the population rises to approximately 200,000 (Hartnett and

Nash, 2015).

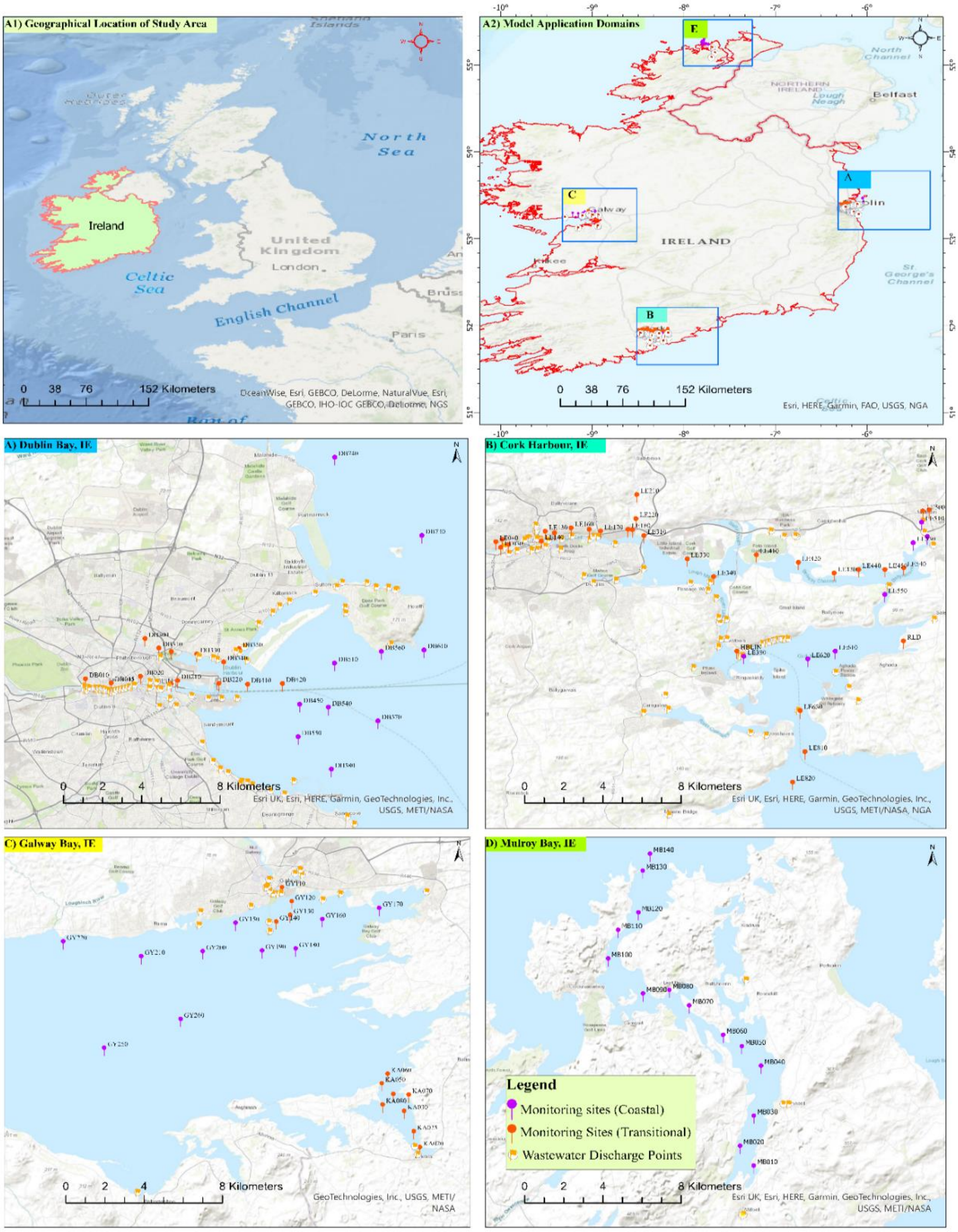


Figure 1.2. Model application domains and EPA monitoring sites for same.

The city is the industrial hub of the Irish southwest region and the surrounding hinterlands are subject to relatively intense agricultural activities which impact water quality in the region. Like much of Ireland, agriculture is widespread in the River Lee catchment, which covers an area of approximately 1,200 km^2. Additionally, effluent discharges (Figure. 1.2) from seven wastewater treatment plants (WWTPs) which further impact water quality in the Harbour (EPA, 2016).

For the purpose of regional evaluation, the Cork Harbour domain was divided into the three regions shown in Figure 1.1: (1) Upper Harbour (including River Lee, River Glashaboy, North Channel and River Owenacurra), (2) Lower Harbour (including Passage West and Passage East) and (3) Outer Harbour (including River Owenboy and the main channel of the Harbour).

After developing the model, it was tested across four coastal waterbodies including Cork Harbour, Dublin Bay, Galway Bay and Mulroy Bay for assessing water quality and evaluating sensitivity in terms of the spatio-temporal resolution. These bodies of water were chosen based on different geospatial settings which account for a wide range of different spatial attributes of Irish waterbodies. Figure 1.2 presents the four application domains in the research.

1.4 Research methodology

The research was completed using various water quality indexing models, tools, and techniques, a range of statistical and mathematical approaches, and state-of-the-art machine ML and AI techniques. The methodologies used to achieve each objective are briefly described here but are described in full detail in the various chapters.

1. **Investigate the potential of WQI models as a tool for assessing the quality of marine waters (to include TrC waters and shallow shelf seas).**
   A thorough literature review of existing WQI model architectures was carried out to identify (1) the various components of the WQI, (2) typical application sites, and (3) known limitations of the models.
2. **Investigate the sensitivity of WQI assessment to spatial and temporal resolution of input water quality data.**
   A range of WQI models were applied to a small number of different case study sites.

3. **Develop a new standardised WQI model for marine waters which can be applied to any marine waterbody in any geographical extent. This was a multi-step process as follows:**

3.1 Develop an appropriate method for selecting the most important water quality indicators for inclusion in a model application in order to reduce the model uncertainty from this process.

Indicator data were analyzed using a range of statistical and mathematical tools and techniques. State-of-the-art machine learning (ML) and artificial intelligence (AI) approaches were also used to optimize the limitations of existing techniques for selecting the crucial indicators.

3.2 Develop more robust SI function(s) for converting water quality indicator measurements into dimensionless forms without losing any crucial information about the indicators.

Various existing tools and techniques were analyzed and tested using different input datasets for various indicators in order to avoid the eclipsing problem.

3.3 Develop a novel method for estimating indicators' weighted values based on their relative importance.

A range of statistical, mathematical, and ML-AI approaches were utilized to identify the best technique that can significantly reduce the model uncertainty in terms of estimating weight value more accurately.

3.4 Determine the most appropriate aggregation function for calculating the overall water quality index/score.

The research was analyzed using various weighted and unweighted aggregation functions, including the existing WQI system, in order to identify the best function(s) that can reduce the ambiguity problem in the final assessment of water quality.

3.5 Developing a generalized classification scheme for appropriate classification of marine waters.

The present research was reviewed the existing available classification schemes, which are commonly used in the current WQI system, and developed a brand new, more generalized classification scheme, especially focused on marine waters.

4. Develop a novel approach for estimating WQI model uncertainty that can compute model uncertainty at each step of the modelling process.

For the computation of model uncertainty, various statistical, mathematical, and ML-AI approaches were utilized in this research, a method that could be broadly applied to comprehend the degree of uncertainty in the assessment of water quality. Additionally, tools could be also used to predict the degree of uncertainty in the assessment method.

5. **Analyse the performance of the new WQI model in terms of correct classification of marine waters using the new classification scheme.**

   The research was utilized a series of ML classifier algorithms to analyse the WQI model performance in order to correct multi-class classification of marine water incorporating new classification scheme.

6. **Test and validate the new WQI model by application to different case study sites.**

   The model was tested across four Irish marine waterbodies and validated using data from the EPA's water quality monitoring program; its performance was also tested using a variety of statistical metrics.

7. **Develop an ML algorithm for the new WQI model in order to accurately predict the WQI score at a monitoring site.**

   A range of ML algorithms were used and compared to identify the best algorithm(s) for predicting WQI using the new WQI approach. In addition, model hyperparameters were optimized for the developed WQI architecture in order to avoid the limitations of entire WQI system.

8. **To develop a methodology for the assessment of the trophic status for coastal and transitional waters.**

In order to achieve this objective, various statistical measures, ML and AI approaches were utilized. A number of statistical treatments were used to remove the multicollinearity problem from the assessment results. All required data analysis and graphical presentations were completed by using various programming languages: FORTRAN 2000, MATLAB R2022a, R 4.2,Python 3.11.1, and ArcGIS pro 3.0. The research used water quality data of Cork Harbour collected by the Irish Environmental Protection Agency (EPA). The EPA has been collecting water quality monitoring data from selected geospatial locations in Cork Harbour since 2007. The Irish Environmental Protection Agency (EPA) collects monthly water quality data from monitoring sites in Irish waterbodies. The relevant water quality indicator data for

Cork Harbour were obtained from https://www.catchments.ie/data/. Figure 1.2 presents the EPA designated water quality monitoring sites across Cork Harbour.

1.5 Outline of the thesis

In addition to this introduction, the thesis comprises eight research papers, seven of which have been published in high ranking international scientific journals and the remaining one of which is currently under review. The thesis closes with a general conclusions chapter. The following is a brief summary of each chapter:

- **Chapter 2** presents a comprehensive literature review of existing WQI models in order to achieve initial objective of the research. In particular, the WQI models' development history, existing available WQI models, classification of WQI models based on origin, structure, applications, etc., identification of major WQI model(s), architecture of different WQI models, procedures of the development of a WQI model, various mathematical or statistical tools and techniques for the determination of water quality indicators, the existing weight estimation process, various sub-indexing (SI) methods and limitations of the existing SI process, different aggregation functions, and their applications are described. Sources of model uncertainties, ambiguity, eclipsing problems, different classification schemes, etc. are also described. Based on the literature review, a conceptual research framework was developed in order to develop a novel WQI model for coastal waters.

- **Chapter 3** presents an improved WQI model for assessment of coastal water quality using Cork Harbour, Ireland, as the case study site, in order to obtain the second and third objectives of the research. A comprehensive framework for the development of a novel WQI model which reduces model uncertainty was developed. The extreme gradient boosting (XGBoost) machine learning technique was used to select crucial water quality indicators based on their relative importance, three SI functions, including a range of binary rules, were developed for transferring various WQ indicator information into dimensionless forms without losing or hiding any critical information about WQ. While these functions could be effective in optimizing the model ambiguity problem, a novel approach incorporating ML techniques with the rank order centroid method was developed for accurately estimating indicator weight values. The eclipsing and ambiguity problems were defined and discussed in terms of their nature. Two new aggregation functions - the weighted quadratic mean (weighted) and the arithmetic mean (unweighted) - were proposed to reduce model uncertainty and avoid the model ambiguity problem and were compared with the five most widely used aggregation processes. A new classification scheme was also developed for assessing coastal water quality to avoid the inconsistency of the final assessment results.

- **Chapter 4** describes a novel approach for estimating and predicting uncertainty in a WQI model using machine learning approaches in order to achieve research objective four. Based on the literature review (Chapter 2), it was noted that the various components of existing WQI models contribute a significant amount of uncertainty to the final WQI scores. To the best of the author's knowledge, there are no specific guidelines for estimating uncertainty in a WQI model. The present study developed novel techniques to calculate the uncertainty at each stage of the WQI model. Model uncertainty was calculated using the Monte Carlo simulation (MCS) technique, and the MCS results were compared and validated using ML prediction approaches. The new model approach of Chapter 3 was tested and validated in terms of the amount of contributing uncertainty.

- **Chapter 5** provides a novel approach for the performance analysis of the WQI model for predicting water state using machine learning techniques to obtain the research objective five. According to the review findings (Chapter 2), existing WQI models use a range of classification schemes for rating water quality. Consequently, different WQI techniques provides different interpretations for the same water quality attributes; this is called the "metaphoring problem" of the WQI model, and this is the first time that it is introduced and defined in this research. In order to remove the metaphoring problems from the entire WQI system, a new generalised classification scheme was developed (Chapter 3). In this research, the new WQI model(s) performance was tested using widely used ML multiclass classifiers, and the results were validated by comparing the EPA’s monitoring water quality data with the water quality status determined by adopting the new classification scheme for rating coastal waters. Details of the methodology for assessing model performance, the algorithms optimization processes, and the different evaluation metrics in order to correct multiclass classification are discussed. In addition, the XGBoost ML classifier algorithm was optimized for the new classification scheme, and a new algorithm for predicting multi-class water quality was developed.

- **Chapter 6** presents various important indicator selection algorithms/techniques that were tested and evaluated in this research to achieve the objective 3.1. In order to optimize the best subsets of indicators for the improved WQI model, a robust indicator optimization algorithm was developed, which can reduce the model's uncertainty in terms of the reliability of actual scenarios of water quality in the domain. Eighteen ML features selection algorithms were analysed and assessed using a range of statistical and mathematical approaches. In addition, a new evaluation metric, the absolute standardized residual estimate (ASRE), was introduced for assessing the indicator selection technique's reliability in terms of the actual information from monitoring sites. Details of the various feature selection algorithms, algorithm optimization processes, model validation techniques including new ASRE approach, and selection process for the best input for the improved WQI model are described.

- **Chapter 7** provides a sophisticated model for rating water quality that is here referred to as the "Irish Water Quality Index Model" or IEWQI in order to obtain the ultimate goal of the research, including objective six. Details of the IEWQI model development and validation process are presented. The proposed IEWQI model has five components with the following novelties: (i) for the optimization of model input the random forest algorithm used; (ii) three newly developed linear interpolation rescaling functions for computing the SI score, (iii) a comprehensive weighting approach combining the random forest technique with the mathematical function of rank sum technique, (iv) a new weighted quadratic mean (WQM) aggregation function to compute the WQI scores, and (v) a new classification scheme including four water classes ("good", "fair", "marginal", and "poor") to avoid the metaphoring problems.

- **Chapter 8** presents an ML algorithm for the IEWQI model that could be effective for predicting IEWQI scores at each monitoring point instead of repeatedly employing SI and weight values to reduce model uncertainty for achieving the objective seven of this research. A range of ML regression algorithms, configuration techniques, hyperparameters, and various evaluation metrics for assessing model performance are discussed a robust ML algorithm for predicting and assessing TrC waters is proposed.

- **Chapter 9** presents an enhanced assessment trophic status index (ATSI) model based on machine learning and artificial intelligence techniques for TrC waters in order to obtain research objective eight. Chlorophyll-a was not included in the new IEWQI model due to the multicollinearity problem. Since the IEWQI model cannot determine the trophic status of the TrC waters, it can only be used to evaluate the general state of the TrC waters in accordance with the WFD guidelines. As a result, an improved method for determining the trophic status of TrC waterbodies was developed. While the sensitivity was assessed in terms of the spatio-temporal resolution of various waterbodies, the developed ATSI model was tested and validated in four Irish TrC waterbodies. The model development process is described in detail.

- **Chapter 10** presents the key conclusions drawn from the research and recommendations for future research. In order to assess the TrC waters, bathing waters, and trophic status in the marine ecosystems, a comprehensive framework has also been proposed for the further development of this model for the assessment of surface water quality that could be helpful for the improvement of the traditional water quality monitoring approach in terms of reducing the limitation of the entire system.

1.6 References

Abbasi, T., Abbasi, S.A., 2012. Water Quality Indices, Statistical Accounting of Water Resources. Elsevier publications.

Bai Varadharajan, raman, Bai, raman v, Bouwmeester, reinier, 2009. Fuzzy logic Water Quality index and importance of Water Quality Parameters. Air, Soil and Water Research 2, 51–59. https://doi.org/10.4137/ASWR.S2156

Brack, W., Dulio, V., Ågerstrand, M., Allan, I., Altenburger, R., Brinkmann, M., Bunke, D., Burgess, R.M., Cousins, I., Escher, B.I., Hernández, F.J., Hewitt, L.M., Hilscherová, K., Hollender, J., Hollert, H., Kase, R., Klauer, B., Lindim, C., Herráez, D.L., Miège, C., Munthe, J., O'Toole, S., Posthuma, L., Rüdel, H., Schäfer, R.B., Sengl, M., Smedes, F., van de Meent, D., van den Brink, P.J., van Gils, J., van Wezel, A.P., Vethaak, A.D., Vermeirssen, E., von der Ohe, P.C., Vrana, B., 2017. Towards the review of the European Union Water Framework management of chemical

contamination in European surface water resources. Science of the Total Environment. https://doi.org/10.1016/j.scitotenv.2016.10.104
Carsten Von Der Ohe, P., Prüß, A., Schäfer, R.B., Liess, M., de Deckere, E., Brack, W., 2007. Water quality indices across Europe - A comparison of the good ecological status of five river basins. Journal of Environmental Monitoring 9, 970–978. https://doi.org/10.1039/b704699p
Cash, K., Neary, B., Hebert, S., Khan, H., Saffran, K., Williamson, D., 2001. Canadian Water Quality Guidelines for the Protection of Aquatic Life. Canadian Council of Ministers of the Environment.
Chadli, K., Boufala, M., 2021. Assessment of water quality using Moroccan WQI and multivariate statistics in the Sebou watershed (Morocco). Arabian Journal of Geosciences 14. https://doi.org/10.1007/s12517-020-06296-5
Chakravarty, T., Gupta, S., 2021. Assessment of water quality of a hilly river of south Assam, north east India using water quality index and multivariate statistical analysis. Environmental Challenges 5. https://doi.org/10.1016/j.envc.2021.100392
Cheng, Y., Li, Y., Ji, F., Wang, Y., 2018. Global sensitivity analysis of a water quality model in the three gorges reservoir. Water (Switzerland) 10. https://doi.org/10.3390/w10020153
Cude, C.G., 2001. Oregon water quality index: A tool for evaluating water quality management effectiveness. J Am Water Resour Assoc. https://doi.org/10.1111/j.1752-1688.2001.tb05480.x
de Rosemond, S., Duro, D.C., Dubé, M., 2009. Comparative analysis of regional water quality in Canada using the Water Quality Index. Environ Monit Assess 156, 223–240. https://doi.org/10.1007/s10661-008-0480-6
Dezfooli, D., Hosseini-Moghari, S.M., Ebrahimi, K., Araghinejad, S., 2018. Classification of water quality status based on minimum quality parameters: application of machine learning techniques. Model Earth Syst Environ 4, 311–324. https://doi.org/10.1007/s40808-017-0406-9
Dimri, D., Daverey, A., Kumar, A., Sharma, A., 2021. Monitoring water quality of River Ganga using multivariate techniques and WQI (Water Quality Index) in Western Himalayan region of Uttarakhand, India. Environ Nanotechnol Monit Manag 15, 100375. https://doi.org/10.1016/j.enmm.2020.100375
Dojlido, J., Raniszewski, J., Woyciechowska, J., 1994. Water quality index applied to rivers in the Vistula river basin in Poland. Environ Monit Assess. https://doi.org/10.1007/BF00546659
Dunnette, D.A., 1979. A Geographically Variable Water Quality Index Used in Oregon. Source Journal (Water Pollution Control Federation). https://doi.org/https://www.jstor.org/stable/pdf/25040240.pdf
Effendi, H., Romanto, Wardiatno, Y., 2015. Water Quality Status of Ciambulawung River, Banten Province, Based on Pollution Index and NSF-WQI. Procedia Environ Sci. https://doi.org/10.1016/j.proenv.2015.03.030
EPA, 2001. Parameters Of Water Quality: Interpretation and Standards, Environmental Protection AGENCY, Ireland. The Environmental Protection Agency, Ireland., Ireland. https://doi.org/10.1017/CBO9781107415324.004
Fadel, A., Kanj, M., Slim, K., 2021. Water Quality Index variations in a Mediterranean reservoir: a multivariate statistical analysis relating it to different variables over 8 years. Environ Earth Sci 80, 1–14. https://doi.org/10.1007/s12665-020-09364-x
Fu, G., Jin, Y., Sun, S., Yuan, Z., Butler, D., 2022. The role of deep learning in urban water management: A critical review. Water Res. https://doi.org/10.1016/j.watres.2022.118973
Gazzaz, N.M., Yusoff, M.K., Aris, A.Z., Juahir, H. and Ramli, M.F., 2012. Artificial neural network modeling of the water quality index for Kinta River (Malaysia) using water quality variables as predictors. Marine pollution bulletin, 64(11), pp.2409-2420.
Gradilla-Hernández, M.S., de Anda, J., Garcia-Gonzalez, A., Montes, C.Y., Barrios-Piña, H., Ruiz-Palomino, P., Díaz-Vázquez, D., 2020. Assessment of the water quality of a subtropical lake using the NSF-WQI and a newly proposed ecosystem specific water quality index. Environ Monit Assess 192. https://doi.org/10.1007/s10661-020-08265-7
Grbić, R., Kurtagić, D., Slišković, D., 2013. Stream water temperature prediction based on Gaussian process regression. Expert Syst Appl 40, 7407–7414. https://doi.org/10.1016/j.eswa.2013.06.077
Gupta, A.K., Gupta, S.K., Patil, R.S., 2003. A comparison of water quality indices for coastal water. J Environ Sci Health A Tox Hazard Subst Environ Eng 38, 2711–2725. https://doi.org/10.1081/ESE-120024458
Gupta, S., Gupta, S.K., 2021. A critical review on water quality index tool: Genesis, evolution and future directions. Ecol Inform 63, 101299. https://doi.org/10.1016/j.ecoinf.2021.101299
Hansda, S.K., Swain, K.K., Vaidya, S.P., Jagtap, R.S., 2018. Assessment of Water Quality Trends of Khadakwasla Reservoir Using CCME-WQI, in: Environmental Pollution. Springer Nature Singapore Pte Ltd.2018, pp. 381–401. https://doi.org/10.1007/978-981-10-5792-2_31

Hartnett, M., Nash, S., 2004. Modelling nutrient and chlorophyll_a dynamics in an Irish brackish waterbody. Environmental Modelling and Software 19, 47–56. https://doi.org/10.1016/S1364-8152(03)00109-9

Hartnett, M., Nash, S., Olbert, I., 2012. An integrated approach to trophic assessment of coastal waters incorporating measurement, modelling and water quality classification. Estuar Coast Shelf Sci 112, 126–138. https://doi.org/10.1016/j.ecss.2011.08.012

Hartnett, M., Wilson, J.G., Nash, S., 2011. Irish estuaries: Water quality status and monitoring implications under the water framework directive. Mar Policy 35, 810–818. https://doi.org/10.1016/j.marpol.2011.01.010

Hartnett, M. and Nash, S., 2015. An integrated measurement and modeling methodology for estuarine water quality management. Water Science and Engineering, 8(1), pp.9-19. https://doi.org/10.1016/j.wse.2014.10.001

Hering, D., Borja, A., Carstensen, J., Carvalho, L., Elliott, M., Feld, C.K., Heiskanen, A.-S., Johnson, R.K., Moe, J., Pont, D., 2010. The European Water Framework Directive at the age of 10: A critical review of the achievements with recommendations for the future. Science of The Total Environment 408, 4007–4019. https://doi.org/10.1016/j.scitotenv.2010.05.031

Hering, D., Borja, A., Jones, J.I., Pont, D., Boets, P., Bouchez, A., Bruce, K., Drakare, S., Hänfling, B., Kahlert, M., Leese, F., Meissner, K., Mergen, P., Reyjol, Y., Segurado, P., Vogler, A., Kelly, M., 2018. Implementation options for DNA-based identification into ecological status assessment under the European Water Framework Directive. Water Res. https://doi.org/10.1016/j.watres.2018.03.003

Heydari, M.M., Abbasi, A., Rohani, S.M., Hosseini, S.M.A., 2013. Correlation study and regression analysis of drinking water quality in Kashan City, Iran. Walailak J Sci Technol 10, 315–324. https://doi.org/10.5829/idosi.mejsr.2013.13.9.1027

Horton, R.K., 1965. An index-number system for rating water quality. J. Water Pollut. Control Fed. 37, 300–306. https://doi.org/10.2307/25035251

Hoseinzadeh, E., Khorsandi, H., Wei, C., Alipour, M., 2015. Evaluation of Aydughmush River water quality using the National Sanitation Foundation Water Quality Index (NSFWQI), River Pollution Index (RPI), and Forestry Water Quality Index (FWQI). Desalination Water Treat. https://doi.org/10.1080/19443994.2014.913206

Hou, W., Sun, S., Wang, M., Li, X., Zhang, N., Xin, X., Sun, L., Li, W., Jia, R., 2016. Assessing water quality of five typical reservoirs in lower reaches of Yellow River, China: Using a water quality index method. Ecol Indic 61. https://doi.org/10.1016/j.ecolind.2015.09.030

Ibrahim, S., Nazir, S., Velastin, S.A., 2021. Feature selection using correlation analysis and principal component analysis for accurate breast cancer diagnosis. J Imaging 7. https://doi.org/10.3390/jimaging7110225

Islam Khan, M.S., Islam, N., Uddin, J., Islam, S., Nasir, M.K., 2022. Water quality prediction and classification based on principal component regression and gradient boosting classifier approach. Journal of King Saud University - Computer and Information Sciences 34, 4773–4781. https://doi.org/10.1016/J.JKSUCI.2021.06.003

Javed, S., Ali, A., Ullah, S., 2017. Spatial assessment of water quality parameters in Jhelum city (Pakistan). Environ Monit Assess 189. https://doi.org/10.1007/s10661-017-5822-9

Jha, D.K., Devi, M.P., Vidyalakshmi, R., Brindha, B., Vinithkumar, N.V., Kirubagaran, R., 2015. Water quality assessment using water quality index and geographical information system methods in the coastal waters of Andaman Sea, India. Mar Pollut Bull. https://doi.org/10.1016/j.marpolbul.2015.08.032

Jiang, J., Tang, S., Han, D., Fu, G., Solomatine, D., Zheng, Y., 2020. A comprehensive review on the design and optimization of surface water quality monitoring networks. Environmental Modelling and Software 132, 104792. https://doi.org/10.1016/j.envsoft.2020.104792

Jiang, L., Li, Y., Zhao, X., Tillotson, M.R., Wang, W., Zhang, S., Sarpong, L., Asmaa, Q., Pan, B., 2018. Parameter uncertainty and sensitivity analysis of water quality model in Lake Taihu, China. Ecol Modell 375, 1–12. https://doi.org/10.1016/j.ecolmodel.2018.02.014

Juwana, I., Muttil, N., Perera, B.J.C., 2016a. Application of west Java water sustainability index to three water catchments in west Java, Indonesia. Ecol Indic 70, 401–408. https://doi.org/10.1016/j.ecolind.2016.06.017

Juwana, I., Muttil, N., Perera, B.J.C., 2016b. Uncertainty and sensitivity analysis of West Java Water Sustainability Index - A case study on Citarum catchment in Indonesia. Ecol Indic 61, 170–178. https://doi.org/10.1016/j.ecolind.2015.08.034

Kallis, G., 2001. The EU water framework directive: measures and implications. Water Policy 3, 125–142. https://doi.org/10.1016/S1366-7017(01)00007-1

Kothari, V., Vij, S., Sharma, S.K., Gupta, N., 2021a. Correlation of various water quality parameters and water quality index of districts of Uttarakhand. Environmental and Sustainability Indicators 9. https://doi.org/10.1016/j.indic.2020.100093

Kothari, V., Vij, S., Sharma, S.K., Gupta, N., 2021b. Correlation of various water quality parameters and water quality index of districts of Uttarakhand. Environmental and Sustainability Indicators 9, 100093. https://doi.org/10.1016/j.indic.2020.100093

Kullar, S.S., Shao, K., Surette, C., Foucher, D., Mergler, D., Cormier, P., Bellinger, D.C., Barbeau, B., Sauvé, S., Bouchard, M.F., 2019. A benchmark concentration analysis for manganese in drinking water and IQ deficits in children. Environ Int 130, 104889. https://doi.org/10.1016/j.envint.2019.05.083

Lenton, R., Muller, M., 2012. Integrated Water Resources Management in Practice. Routledge. https://doi.org/10.4324/9781849771740

Liou, S.M., Lo, S.L., Wang, S.H., 2004. A generalized water quality index for Taiwan. Environ Monit Assess 96, 35–52. https://doi.org/10.1023/B:EMAS.0000031715.83752.a1

Li, R., Zou, Z., An, Y., 2016. Water quality assessment in Qu River based on fuzzy water pollution index method. J Environ Sci (China) 50, 87–92. https://doi.org/10.1016/j.jes.2016.03.030

Lobato, T.C., Hauser-Davis, R.A., Oliveira, T.F., Silveira, A.M., Silva, H.A.N., Tavares, M.R.M., Saraiva, A.C.F., 2015. Construction of a novel water quality index and quality indicator for reservoir water quality evaluation: A case study in the Amazon region. J Hydrol (Amst) 522, 674–683. https://doi.org/10.1016/j.jhydrol.2015.01.021

Lumb, A., Sharma, T.C., Bibeault, J.-F., 2011. A Review of Genesis and Evolution of Water Quality Index (WQI) and Some Future Directions. Water Qual Expo Health. https://doi.org/10.1007/s12403-011-0040-0

Liu, J., Yang, H., Gosling, S.N., Kummu, M., Flörke, M., Pfister, S., Hanasaki, N., Wada, Y., Zhang, X., Zheng, C., Alcamo, J., Oki, T., 2017. Water scarcity assessments in the past, present, and future. Earths Future. https://doi.org/10.1002/2016EF000518

Ma, Z., Li, H., Ye, Z., Wen, J., Hu, Y., Liu, Y., 2020. Application of modified water quality index (WQI) in the assessment of coastal water quality in main aquaculture areas of Dalian, China. Mar Pollut Bull 157. https://doi.org/10.1016/j.marpolbul.2020.111285

Medeiros, A.C., Faial, K.R.F., do Carmo Freitas Faial, K., da Silva Lopes, I.D., de Oliveira Lima, M., Guimarães, R.M., Mendonça, N.M., 2017. Quality index of the surface water of Amazonian rivers in industrial areas in Pará Brazil. Mar Pollut Bull. https://doi.org/10.1016/j.marpolbul.2017.09.002

Michalak, K., Kwasnicka, H., 2006. Correlation-based feature selection strategy in neural classification. Proceedings - ISDA 2006: Sixth International Conference on Intelligent Systems Design and Applications 1, 741–746. https://doi.org/10.1109/ISDA.2006.128

Misaghi, F., Delgosha, F., Razzaghmanesh, M., Myers, B., 2017. Introducing a water quality index for assessing water for irrigation purposes: A case study of the Ghezel Ozan River. Science of the Total Environment 589, 107–116. https://doi.org/10.1016/j.scitotenv.2017.02.226

Mladenović-Ranisavljević, I.I., Žerajić, S.A., 2018. Comparison of different models of water quality index in the assessment of surface water quality. International Journal of Environmental Science and Technology 15, 665–674. https://doi.org/10.1007/s13762-017-1426-8

Nives, Š.-G., 1999. Water quality evaluation by index in Dalmatia. Water Res 33, 3423–3440. https://doi.org/10.1016/s0043-1354(99)00063-9

Ocampo-Duque, W., Ferre-Huguet, N., Domingo, J.L. and Schuhmacher, M., 2006. Assessing water quality in rivers with fuzzy inference systems: A case study. Environment International, 32(6), pp.733-742.

Pan, B., Han, X., Chen, Y., Wang, L., Zheng, X., 2022. Determination of key parameters in water quality monitoring of the most sediment-laden Yellow River based on water quality index. Process Safety and Environmental Protection 164, 249–259. https://doi.org/10.1016/J.PSEP.2022.05.067

Parween, S., Siddique, N.A., Diganta, M.T.M., Uddin, Md.G., 2022. Environmental and Sustainability Indicators Assessment of urban river water quality using modified NSF water quality index model. Environmental and Sustainability Indicators.

Rogers, B.C., Dunn, G., Hammer, K., Novalia, W., de Haan, F.J., Brown, L., Brown, R.R., Lloyd, S., Urich, C., Wong, T.H.F., Chesterfield, C., 2020. Water Sensitive Cities Index: A diagnostic tool to assess water sensitivity and guide management actions. Water Res 186. https://doi.org/10.1016/j.watres.2020.116411

Saffran, K., Cash, K., Hallard, K., 2001. CCME Water Quality Index 1.0 User's Manual. Canadian Water Quality Guidelines for the Protection of Aquatic Life 1–5.

Santos, J.I., Vidal, T., Gonçalves, F.J.M., Castro, B.B., Pereira, J.L., 2021. Challenges to water quality assessment in Europe – Is there scope for improvement of the current Water Framework Directive bioassessment scheme in rivers? Ecol Indic. https://doi.org/10.1016/j.ecolind.2020.107030

Smith, D.G., 1990. A better water quality indexing system for rivers and streams. Water Res. https://doi.org/10.1016/0043-1354(90)90047-A

Strobl, R.O., Robillard, P.D., 2008. Network design for water quality monitoring of surface freshwaters: A review. J Environ Manage 87, 639–648. https://doi.org/10.1016/j.jenvman.2007.03.001

Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2018. Development of a water quality index for rivers in West Java Province, Indonesia. Ecol Indic 85, 966–982. https://doi.org/10.1016/j.ecolind.2017.11.049

Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2017. Using the Analytic Hierarchy Process to identify parameter weights for developing a water quality index. Ecol Indic 75, 220–233. https://doi.org/10.1016/j.ecolind.2016.12.043

Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2016. Development of river water quality indices—a review. Environ Monit Assess. https://doi.org/10.1007/s10661-015-5050-0

Taylor, J.G., Ryder, S.D., 2003. Use of the Delphi method in resolving complex water resources issues. J Am Water Resour Assoc. https://doi.org/10.1111/j.1752-1688.2003.tb01570.x

Telci, I.T., Nam, K., Guan, J., Aral, M.M., 2009. Optimal water quality monitoring network design for river systems. J Environ Manage 90, 2987–2998. https://doi.org/10.1016/j.jenvman.2009.04.011

Tripathi, M., Singal, S.K., 2019. Use of Principal Component Analysis for parameter selection for development of a novel Water Quality Index: A case study of river Ganga India. Ecol Indic 96, 430–436. https://doi.org/10.1016/j.ecolind.2018.09.025

Uddin, M.G., Moniruzzaman, M., Quader, M.A., Hasan, M.A., 2018. Spatial variability in the distribution of trace metals in groundwater around the Rooppur nuclear power plant in Ishwardi, Bangladesh. Groundw Sustain Dev 7. https://doi.org/10.1016/j.gsd.2018.06.002

Uddin, M.G., Stephen Nash, Olbert, A.I., 2020. Application of Water Quality Index Models to an Irish Estuary, in: Civil and Environmental Research. pp. 576–581.

Uddin, M.G., Nash, S., Olbert, A.I., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol Indic 122, 107218. https://doi.org/10.1016/j.ecolind.2020.107218

Verma, R.K., Murthy, S., Tiwary, R.K., Verma, S., 2019. Development of simplified WQIs for assessment of spatial and temporal variations of surface water quality in upper Damodar river basin , eastern India. Appl Water Sci 0–15. https://doi.org/10.1007/s13201-019-0893-0

Zeinalzadeh, K., Rezaei, E., 2017. Determining spatial and temporal changes of surface water quality using principal component analysis. J Hydrol Reg Stud 13, 1–10. https://doi.org/10.1016/j.ejrh.2017.07.002

Zhu, X., Yue, Y., Wong, P.W.H., Zhang, Y., Ding, H., 2019. Designing an optimized water quality monitoring network with reserved monitoring locations. Water (Switzerland) 11, 1–25. https://doi.org/10.3390/w11040713

Zotou, I., Tsihrintzis, V.A., Gikas, G.D., 2019. Performance of Seven Water Quality Indices (WQIs) in a Mediterranean River. Environ Monit Assess 191. https://doi.org/10.1007/s10661-019-7652-4

Zotou, I., Tsihrintzis, V.A., Gikas, G.D., 2018. Comparative Assessment of Various Water Quality Indices (WQIs) in Polyphytos Reservoir-Aliakmon River, Greece. Proc West Mark Ed Assoc Conf 2, 611. https://doi.org/10.3390/proceedings2110611

2. A review of water quality index models and their use for assessing surface water quality

This chapter was published in the Journal of **"Ecological Indicators"** on November 17, 2020. Details can be found at the following web resource: https://doi.org/10.1016/j.ecolind.2020.107218

2.1 Chapter highlights

- Twenty-one different WQI models were identified and reviewed.
- Rivers are by far the most common application of WQI models.
- Most models comprised of four key components, the specifics of which varied significantly.
- There are two types of WQI models: weighted (which considers indicator weight values) and unweighted (which does not use indicator weight values).
- Importance parameters are selected using PCA, correlation, expert judgement, literature references, and data availability.
- Most WQI models used measured concentrations of indicators as SI values directly, whereas a few models utilized the rating curve technique.
- Indicators' weight values are determined using the AHP technique, whereas most rely on expert judgment/opinions.
- Three types of aggregation functions are widely used in the existing WQI system: (i) additive, (ii) multiplicative, and (iii) combined approaches.
- A range of classification schemes for rating water quality in literature.
- There is no specific guideline for developing a WQI model.
- Uncertainty, eclipsing, and ambiguity problems are key issues affecting model accuracy.

2.2 Abstract

The water quality index (WQI) model is a popular tool for evaluating surface water quality. It uses aggregation techniques that allow conversion of extensive water quality data into a single value or index. Globally, the WQI model has been applied to evaluate water quality (surface water and groundwater) based on local water quality criteria. Since its development in the 1960s, it has become a popular tool due to its generalised structure and ease-of-use. Commonly, WQI models involve four consecutive stages; these are (1) selection of the water quality parameters, (2) generation of sub-indices for each parameter (3) calculation of the parameter weighting values, and (4) aggregation of sub-indices to compute the overall water quality index. Several researchers have utilized a range of applications of WQI models to evaluate the water quality of rivers, lakes, reservoirs, and estuaries. Some problems of the WQI model are that they are usually developed based on site-specific guidelines for a particular region, and are therefore not generic. Moreover, they produce uncertainty in the conversion of large amounts of water quality data into a single index.

This paper presents a comparative discussion of the most commonly used WQI models, including the different model structures, components, and applications. Particular focus is placed on parameterization of the models, the techniques used to determine the sub-indices, parameter weighting values, index aggregation functions and the sources of uncertainty. Issues affecting model accuracy are also discussed.

Keywords: water quality index (WQI); surface water quality; water quality parameters; sub-index; aggregation function; model uncertainty and sensitivity

2.3 Introduction

Water is a crucial component of the environment; but surface water and groundwater quality have long been deteriorating due to both natural and human-related activities. Natural factors that influence water quality are hydrological, atmospheric, climatic, topographical and lithological factors (Magesh et al., 2013;Uddin et al., 2018). Examples of anthropogenic activities that adversely affect water quality are mining, livestock farming, production and disposal of waste (industrial, municipal and agricultural), increased sediment run-off or soil erosion due to land-use change (Lobato et al., 2015) and heavy metal pollution (Sánchez et al., 2007).

In recent times, developing countries have faced significant problems in protecting water quality when trying to improve water supply and sanitation (Debels et al., 2005; Kannel et al., 2007; Ortega et al. 2017; Carvalho et al., 2011). Even developed nations have been fighting to maintain or improve the status of their water quality in the face of problems such as nutrient enrichment and eutrophication of water resources (Abbasi and Abbasi, 2012; Debels et al., 2005) and the provision of water and wastewater services to increasing populations.

Management of water quality requires the collection and analysis of large water quality datasets that can be difficult to evaluate and synthesise. A range of tools have been developed to evaluate water quality data; the Water Quality Index (WQI) model is one such tool. WQI models are based on an aggregation functions which allow analysis of large temporally and spatially-varying water quality datasets to produce a single value, i.e. the water quality index, that indicates the quality of the waterbody. They are attractive to water management/supply agencies as they are relatively easy to use and convert complex water quality datasets into a single value measure of water quality that is easy to understand.

A WQI typically comprises four processes or components. First, the water quality parameters of interest are selected. Second, the water quality data are read and for each water quality parameter the concentrations are converted to a single-value dimensionless sub-index. The third step involves determining the weighting factor for each water quality parameter, and in the fourth step, an aggregation function is used to calculate a final single value water quality index by combining the sub-indices and weighting factors for all parameters. Many different WQI models have been developed with variations in model structure, the parameters included and their associated weightings, and the methods used for sub-indexing and aggregation (Debels et al., 2005; Kannel et al. 2007; Jha et al., 2015; Sun et al., 2016). Most of the WQI model components have been developed based on expert views and local guidelines (Hsu and Sandford 2007; Sutadian et al. 2016) and many models are therefore region-specific. Several researchers have highlighted the issue of uncertainty in WQI models (Kannel et al., 2007). Although uncertainty is inherent in any mathematical model (Lowe et al., 2017), all four stages of the WQI can be a potential source of uncertainty in the model.

The primary aim of this paper was to critically review the most commonly used WQI models and determine which were the most accurate. This involved a review of 110 published manuscripts from which we identified 21 WQI models used globally (see Figure 2.1), which were then individually and comparatively assessed. The review identified seven basic WQI models from which most other WQI models have been developed; these were subjected to a more thorough critical analysis. Section 2.4 of the paper presents a brief history of WQI model development. Section 2.5 presents an overview of the basic structure of WQI models and describes in detail the four major structural elements of most models, namely, (1) parameterisation, (2) parameter sub-indexing, (3) parameter weighting and (4) index aggregation. Section 2.6 describes the seven primary WQI models in detail while Section 2.7 presents and discusses the major findings of the review. Finally, Section 2.8 presents the main conclusions from the research.

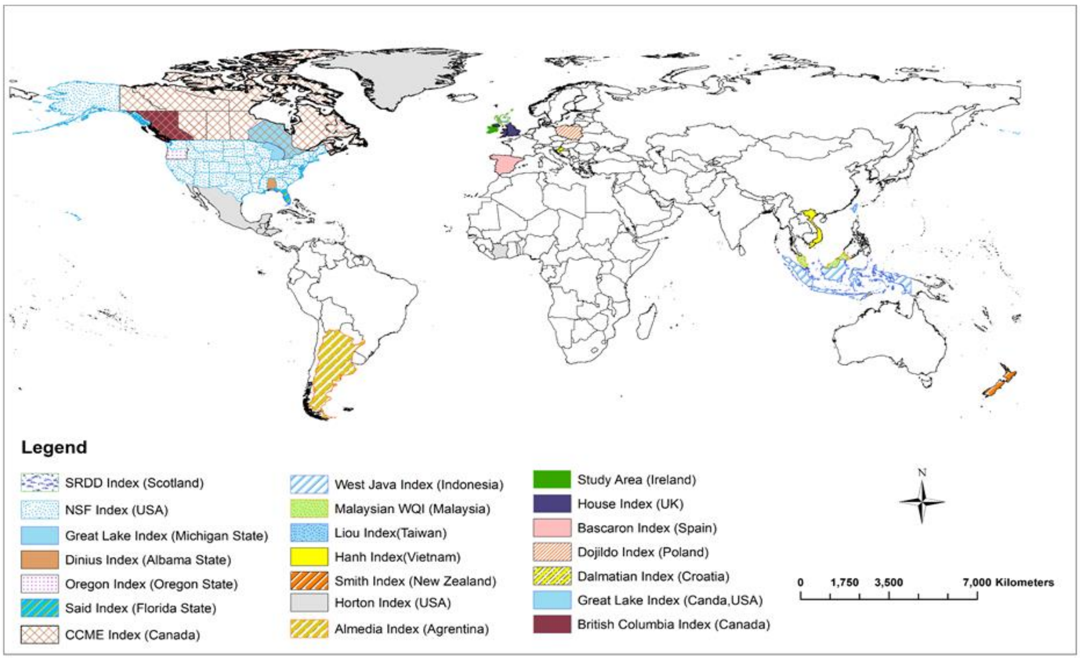


Figure 2.1. Most commonly used WQI models and regions of use (1960-2020).

2.4 A Brief history of WQI models

The development history of the WQI model is presented graphically in Figure 2.2. Although WQI models have only been developed over the last 50 years, water quality indices were being used for classification of water quality as far back as the mid-1800s (Abbasi and Abassi, 2012). Horton developed the first WQI model in the 1960s which is based on 10 water quality parameters deemed significant in most waterbodies

(Horton, 1965). Brown with support from the National Sanitation Foundation, developed a more rigorous version of Horton’s WQI model, the NSF-WQI, for which a panel of 142 water quality experts informed the parameter selection and weighting (Abbasi and Abbasi 2012). Several other WQI models have since been based on the NSF-WQI. In 1973, the Scottish Research Development Department (SRDD) developed their SRDD-WQI which was also somewhat based on Brown’s model and used it for assessment of river water quality (Brown et al., 1970). The Bascaron Index (Bascaron, 1979) , House Index (House, 1986) and Dalmatian Index (Štambuk-Giljanović, 2003) are all later derivatives of the SRDD-WQI. Steinhart et al. (1982) later developed the Environmental Quality Index model for the assessment of water quality in the Great Lakes ecosystems.

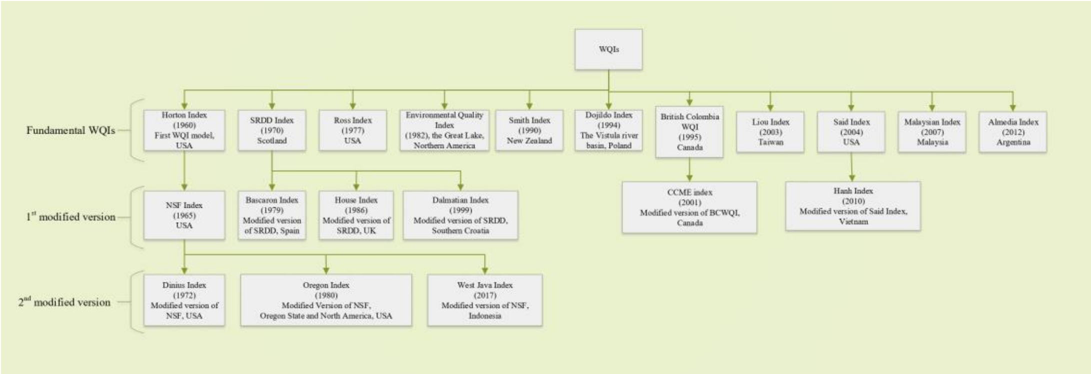


Figure 2.2. Historical development of the WQI model.

Another important development was the British Columbia WQI (BCWQI) which was developed by the British Colmubia Ministry for Environment, Lands and Parks in the mid-90’s and was used to evaluate the quality status of many waterbodies in the province of Britich Columbia, Canada (BCMOELP, 1996). Said et al. (2004) note that the BCWQI was fouind to have the highest sensitivity to sampling design and the highest dependency on the specific application of water quality objectives. The Water Quality Guidelines Task Group of the Canadian Council of Ministers of the Environment developed the CCME WQI in 2001 (CCME, 2001) following a review and revision of the BCWQI model (Ashok Lumb et al., 2011). The BCWQI model has been recognized since in 1990 by the CCME (Dunn 1995; H'ebert 1996; Rocchini and Swain 1995). In recent times models such as the Liou Index (Liou et al., 2004), the Malaysian Index (Gazzaz et al., 2012) and the Almeida Index (Almeida et al., 2012) have also been developed.

To date, more than 35 WQI models have been introduced by various countries and/or agencies to evaluate surface water quality around the world (Abbasi and Abbasi, 2012; Dadolahi-Sohrab et al. 2012; Stoner 1978; Sutadian et al., 2018; Kannel et al. 2007;). As shown in Figure 2.3, WQI models have been used in most parts of the world. Table 2.1 shows that, although WQI models have been applied to all major types of waterbodies, 82% of applications have been to assess river water quality. Additionally, the table shows that the CCME and NSF models have been used 50% of the reviewed studies.

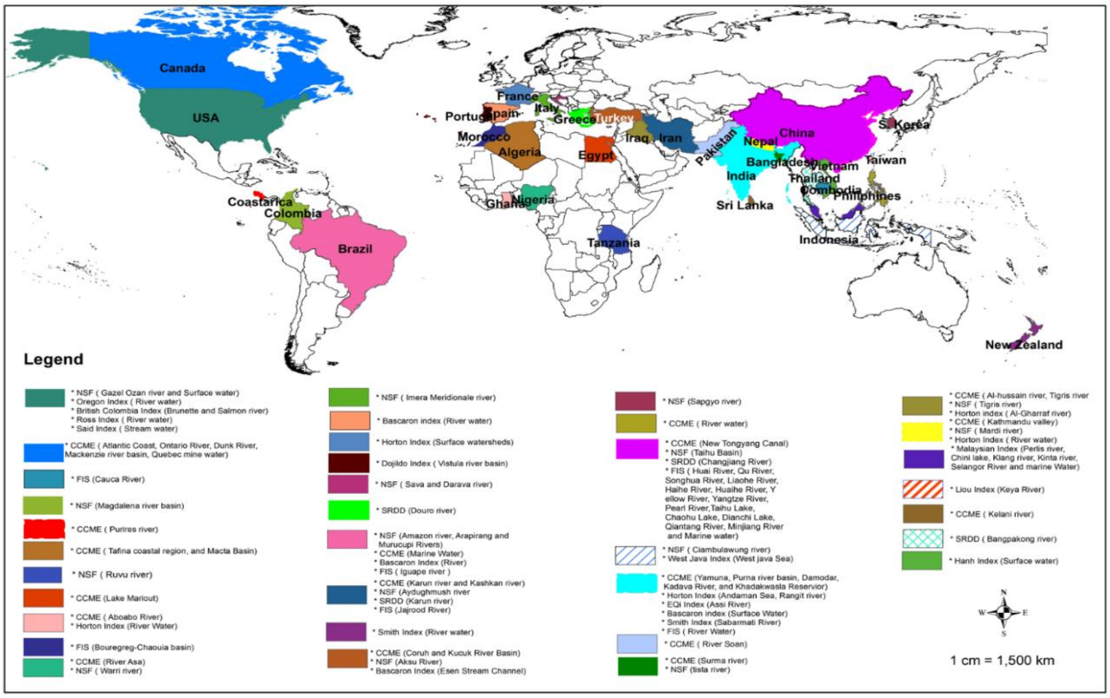


Figure 2.3. Countries and types of waterbodies in which WQIs have been applied globally.

2.5 WQI model structure

The general structure of WQI models is illustrated in Figure 2.4 and shows that most WQIs contain four main steps (Abbasi and Abbasi, 2012; Abrahão et al., 2007; Ashok Lumb et al., 2011; Sutadian et al., 2018), namely:

1) selection of the water quality parameters: one or more water quality parameters are selected for inclusion in the assessment
2) generation of the parameter sub-indices: parameter concentrations are converted to unitless sub-indices

3) assignment of the parameter weight values: parameters are assigned weightings depending on their significance to the assessment

4) computation of the water quality index using an aggregation function: the individual parameter sub-indices are combined using the weightings to give a single overall index. A rating scale is usually used to categorise/classify the water quality based on the overall index value.

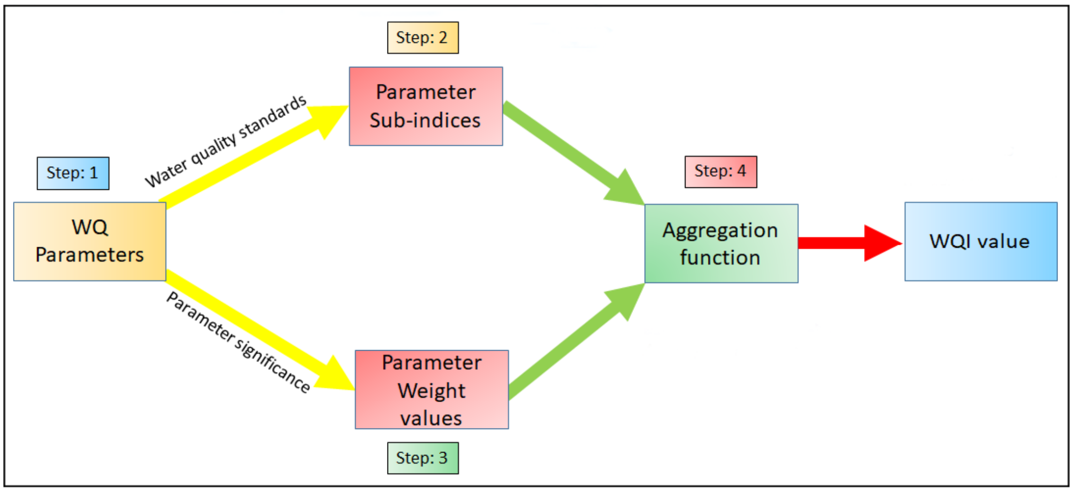


Figure 2.4. General structure of WQI model.

Table 2.1. Summary of WQI model applications (in total and by study area) found in literature published from 1960-2019.

WQI model	Number of Applications	Type of Study Area		
		River	Lake	Marine/coastal/sea
CCME	36	28	5	3
NSF	18	17	1	-
FIS	12	10	1	1
MWQI	8	6	1	1
Horton	7	6	-	1
SRDD	6	6	-	-
Bascaron	4	3	-	1
EQI	2	1	1	-
Oregon	2	2	-	-
Smith	2	2	-	-
Almedia	1	1	-	-
BCWQI	1	1	-	-
Dalmatian	1	-	-	1
Dojildo	1	1	-	-
Dinius	1	1	-	-
Hanh index	1	1	-	-
House index	1	1	-	-
Liou index	1	1	-	-
Said	1	-	-	1
WJWQI	1	-	-	1

The details of the components of the primary models are discussed in the following sections and a summary is presented in Table 2.2.

Table 2.2. Summary of structures of most common WQI models.

WQI model	Model Components				
	No of parameters and selection process	Sub-indexing procedure	Parameter Weighting	Aggregation techniques	Rating scale
Horton index (1960)[a]	• 8 parameters suggested • parameters significance and data availability	• parameters value used as sub-index value, and sub-index ranges from 0 to 100 assigned	• fixed and unequal system (4 for DO and 1 for other parameters) suggested	• used simple additive mathematical function (Eq. 9) • another modified function recommended (Eq. 10)	• Five categories - Very good (91 - 100) - Good (71 - 90) - Poor (51 - 70) - Bad (31 - 50) - Very bad (0 - 30) -
NSF index (1965)[b]	• 11 parameters • Used Delphi technique	• used water quality standard guideline and scale ranged from 0 to 1; When, Parameter value < standard = 1, Parameter value > standard = 0 modified	• the expert panel judgement, and sum of weight value is equal to 1 given	• used two mathematical functions • first one is additive formula (Eq. 4) • second one is multiplicative formula (Eq. 5)	• Five categories - excellent (90 - 100) - good (70 - 89) - medium (50 - 69) - bad (25 - 49) - very Bad (0 - 24)
SRDD Index (1970)[c]	• 10 parameters • Used Delphi	• Used expert opinion, and it ranged from 0 to 100 recommended by SRDD	• panel based and sum of weight value equal to 1 recommended by SRDD	• additive mathematical function adopted (Eq.11) • multiplicative formula that was used for NSF (Eq. 5),	• seven classification - clean (90 - 100) - good (80 - 89) - good with treatment (70 - 79) - tolerable (40 - 69) - polluted (30 -39) - several polluted (20 - 29) - piggery waste (0 - 19)

Dinius index (1972)[d] *modified version of NSF index	• 11 parameters • Delphi technique	• parameters value directly assigned as sub-index value	• used unequal weight • sum of Weighting value is equal to 10	• multiplicative function used (Eq.5)	• Five classification -Purification not required (90 - 100) - minor purification required (80-90) - treatment required (50 - 80) - doutful (40 -50)
Ross Index (1977)[e]	• 4 general WQ parameters • Delphi method	• Expert panel judgement based sub-index system •	• expert based and sum of weight value is equal to 1 given	• used additive mathematical equation, (Eq. 9)	Not specified
Bascaron Index (1979)[f]	• 26 parameters were suggested	• Parameters value directly transformed into sub-index value using liner transformation function • It ranges from 0 to 10	• Used unequal and fixed weighting technique • ranges from 1 to 4 • Sum of weight value is equal to 54	• Used two additive mathematical functions • Subjective based aggregation function (Eq. 19) • Objective WQI function (Eq. 20)	• Five classes - Excellent (90 -100) - Good (70 – 90) - Medium (50 - 70) - Bad (25 – 50) - Very bad (0 -25)

Oregon Index (1980)[g] *refined version of NSF index	• 8 parameters used Delphi process	• Sub-index were estimated using averaging mathematical functions. • Logarithmic transformation and non-liner regression were used for generating sub-index	• Sub-index values directly used as Weighting factors	• the weight arithmetic mean function was recommended by the Oregon department of environment (Eq. 9) • Dojlido et al., 1994, recommended the unweighted modified harmonic square mean formula as Eq. 6	• Five classes -excellent (90 - 100) -good (85 - 89) -fair (80 - 84) -poor (60 - 79) -very poor (< 60)
EQ index (1982)[h]	• 9 parameters recommended • Adopted Delphi method	• Fixed system, and used national-international water quality guideline • Used expert opinion	• fixed and unequal (0.1 for physical, chemical and biological parameters, and 0.15 for organic and inorganic r parameters)	• used simple additive mathematical function (Eq. 9)	• Five categories - excellent (90 - 100) - very good (80 - 89) - good (70 - 79) - fair (55 - 69) poor (<55)
House index (1986)[i] *refined version of SRDD index	• 9 parameters • Key personnel interview • Expert panel judgement process	• Parameters value directly used as a sub-index • Sub-index scale ranges from 10 to 100 •	• the expert panel judgement, and sum of weight value is equal to 1	• used SRDD aggregation technique, as (Eq. 11)	• recommended 4 classification - high quality (71 - 100) - reasonable quality (51 -70) - moderate quality (31 -50) - polluted (10 - 30)
Smith Index (1990)[j]	• 7 parameters • Used Delphi technique	• Fixed system and expert based	• Not required	• Used minimum operator function (Eq. 7) •	• Not specified

Dojildo Index (1994)[k]	• 26 parameters • Open (additional group) and close system (basic parameters group)	• Not required	• Not required	• Adopted square root of the harmonic mean function (Eq. 6)	• Four quality recommended by Dojildo - Very clean (75 – 100) - clean (50 -75) - polluted (25 - 50) - very polluted (0 - 25)
British Colombia Index (1995)[l]	• Used common monitoring parameters • Open choice system • At least 10 parameters	• Sub-index assigned based on expert opinion	• Unequal and expert based	• Simple specific mathematical formula	• Five classes - excellent (0 - 3) - good (4 - 17) - fair (18 - 43) - borderline (44 - 59) - poor (60 - 100)
Dalmatian Index (1999)[m] *modified version of SRDD index	• 8 parameters • Delphi technique	• Parameters value used directly as sub-index •	• Fixed and unequal weight fixed by expert panel • Sum of weight value equal to 1.	• Used automatic index formulas	• Categories not specified
CCME (2001)[n] *reformed version of BCWQI index	• 4 WQ parameters • Delphi technique	• Not required •	• Not required	• Used fixed mathematical functions (Eq. 12 - 18)	• Suggested 5 types of WQ - excellent (95 – 100) - Good (80 – 94) - fair (65 – 79) - marginal (45 – 65) - poor (0 – 44)

Liou Index (2003)[o]	• 13 parameters were used • Parameters were selected based on environmental and health significance	• Parameters actual concentration directly used as sub-index	• Equal Weighting system • Weighting factors were generated by the using rating curves that were illustrated based on the standard guideline of WQ variables	• Liou-WQI model proposed hybrid (additive and multiplicative) functions (Eq. 9, 10)	• Not specified
Said Index (2004)[p]	• 5 parameters • Based on environmental significance	• Parameters value used as sub-index	• Not required	• Used simple mathematical function (Eq. 8)	• Three WQ classification and index value ranges from 0 to 3. - highest purity (3) - marginal quality (< 2) - poor quality (<1)
Malaysian Index (2007)[q]	• 6 parameters used	• Parameters value directly used as sub-index, and it is ranged from 0 to 100	• Unequal and close system • Expert based • Sum of weight is 1	• Simple additive function used	• Parameter based individual rating scale used
Hanh Index (2010)[r]	• 8 parameters • Based on monitoring data availability	• Rating curve-based sun-indexing system • curve developed based on Vietnamese surface water quality standards	• not required	• Hanh suggested two aggregation techniques for evaluating overall water quality and as well as basic water quality (Eq.4, 5).	• five quality classification - Excellent (91 - 100) - good (76 - 90) - fair (51 - 75) - marginal (26 - 50) - poor (<25)

Almeida Index (2012)[s]	• 10 WQ parameters • Delphi technique	• Rating curve-based sun-indexing system • Parameters rating curve recommended by expert panel	• Close and unequal system • Weighting factors fixed by expert panel • Sum of weight value is 1	• Multiplicative mathematical function (NSF aggregation formula) used Eq. 5	• Four categories - Excellent (91 - 100) - good (81 - 90) - medium (71 - 80) - poor (< 70)
West Java Index (2017)[t]	• 13 parameters • Parameters were selected based on monitoring data availability and comparison of standards.	• Used straightforward mathematical function • Adopted guideline value for generating sub-indexing	• Multi decision making tools like as Analytic Hierarchy Process (AHP). • Fixed and unequal weight values • Expert based opinion • The sum of weight values is equal to 1	• Non equal geometric technique as Eq. 5	• Five classification - Excellent (90 - 100) - good (90 - 75) - Fair (75 - 50) - Marginal (50 - 25) - poor (25 - 5

Indices application Domains	References materials
[a]Focus based on the North America	*Alobaidy et al., tava, 2009; Ewaid and Abed, 2017; Gupta et al., 2017, 2016; Kannel et al., 2007; Oni and Fasakin, 2016; Panda et al., 2016; Sánchez et al., 2007; Shah and Joshi, 2017; Singh et al., 2018; Yidana and Yidana, 20092010; Banerjee and Srivastava, Sánchez et al., 2007; Shah and Joshi, 2017; Singh et al., 2018; Yidana and Yidana, 2009*
[b]Application domain in USA	*Babaei Semiromi et al., 2011; Bakan et al., 2010; denović-Ranisavljević and Žerajić, 2018; Mojahedi and Attari, 2009; Noori et al., 2018; Ortega et al., 2016; Rocha et al., 2015b; Sánchez et al., 2007; Tomas et al., 2017; Zeinalzadeh and Rezaei, 2017.*
[c]Surface water, Soctland	*Bordalo, 2001; Bordalo et al., 2006; Carvalho et al., 2011; Dadolahi-Sohrab et al., 2012; Ionuş, 2010*
[d]This model developed based on the cost-effective approaches	*Dinius, 1987*
[e]Evaluation of general water quality	*References missing*
[f]Model developed based on Spain	*Debels et al., 2005; Koçer and Sevgili, 2014; Pesce and Wunderlin, 2000; Sun et al., 2016*
[g]Oregon streams water, USA	*Cude, 2001; Dunnette, 1979*
[h]The Great lakes nearshore area, North America	*Schierow and Chesters, 1988; Steinhurt and Somogniz, 1982*
[i]The European community directives of specific uses purposes	*House, 1980*
[j]Surface water, New Zealand	*Shah and Joshi, 2015; Smith, 1990*

[k]*The Vistula river basin, Poland*	*References missing*
[l]*Surface water bodies, Colombia state, USA*	*Zandbergen and Hall, 1998*
[m]*River water, southern Croatia*	*Nives, 1999; Štambuk-Giljanović, 2003*
[n]*Surface water, Canada*	*CCME, 2001*
[o]*Keya river, Taiwan*	*Liou et al., 2004*
[p]*Streams water, USA*	*Said et al., 2004*
[q]*River water, Malaysia*	*Fulazzaky et al., 2010; Othman and Alaa Eldin, 2012; Amneera et al., 2013; Hasan et al., 2015; Naubi et al., 2016*
[r]*Surface water Vietnam*	*Pham et al., 2011*
[s]*The Potrero de los Funes river, Argentina*	*Almeida et al., 2012*
[t]*Java Sea, Indonesia*	*Sutadian et al.,2017*

2.5.1 Parameter selection

Parameter selection is the initial step of the WQI process and considerable variation was determined between models in the type and number of parameters selected and the reasons for selecting them. Table 2.2 gives a detailed overview of the parameters included in model studies on a model-by-model basis. The most commonly included parameters (see Figure 2.5) were temperature, turbidity, pH, suspended solids (SS), total dissolved solids (TDS), faecal coliforms (FC), dissolved oxygen (DO), biochemical oxygen demand (BOD) and ammonia nitrogen (NH_3-N). Most of the models employed eight to eleven water quality parameters (Table 2.3 and Figure 2.5). A few models used just four which were selected by the user, such as the CCME (2001), the Roos (1977) and the Said (2004) models (Ferreira et al., 2011; Khan et al., 2004; Lumb et al., 2006; Said et al., 2004), while the Bascaron model recommended twenty-six (26) parameters (Figure 2.5).

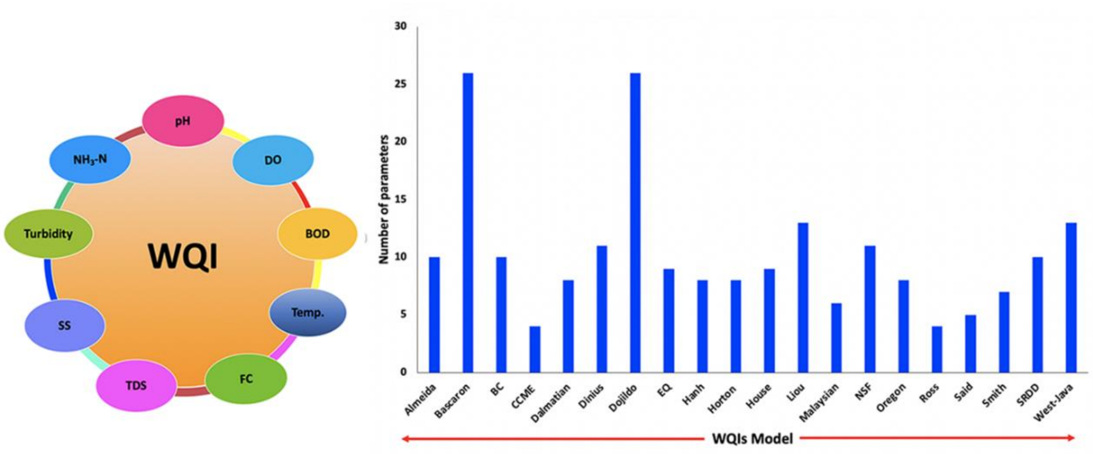


Figure 2.5. Most frequently used water quality parameters and number of parameters per model.

WQI model parameters were typically selected based on data availability, expert opinion or the environmental significance of a water quality parameter. Debels et al. (2005) reported that many WQI models employed only the basic water quality parameters due to lack of availability of other parameter measured data (Cude 2001; Debels et al., 2005; Banerjee and Srivastava 2009; Sutadian et al. 2018). Many researchers modified the model parameter lists based on data accessibility and obtainability and sometimes it is not possible to add the crucial water quality parameter into the model for this reason (Ma et al., 2020; Naubi et al., 2016). A number of WQI models did not include suspended solids, microbiological contamination and toxic compounds due to the high analytical cost and lack of modern analytical laboratory facilities (Debels et al., 2005). In several studies, the water quality parameters were selected based on the application type, e.g. drinking water quality assessment or urban environmental impact (Said et al., 2004; Kannel et al. 2007).

The Delphi technique was used for selecting water quality parameters in a number of WQI model applications (Abbasi and Abbasi, 2012; Dunnette, 1979). Here, the important parameters are selected based on gathering expert opinions through interviews or surveys (House, 1989). In general, there are no specific rules or guidelines for selecting the water quality parameter for inclusion in the WQI model. The traditional WQI model does not follow any systematic technique for setting their parameters. It seems that the WQI model parameters were generally chosen based on a few common water quality issues such as oxygen availability, eutrophication, health considerations, physical and chemical phenomena, and dissolved constituents. Even for several new WQI models it was found that they applied only general criteria and they did not employ any hazardous substances of water quality (Bayati et al., 2017; Bilgin, 2018; Ewaid, 2016; Mahmood, 2018; Noori et al., 2019; Ogbozige, F.J., Adie, D. E., Igboro, S.B., Giwa, 2017; Verma et al., 2019). Generally, WQI models did not consider any toxic or radioactive constituents to evaluate water quality (Said et al. 2004). A few models such as the Oregon index (1980), the Dojildo index (1994), the Liou index (2003), the Almeida index (2012) and the West-Java WQI (2017) recommended to include toxins (detergent, phenols), pesticides and trace variables (Pb, Cu, Zn, Cd, Hg. Mn, Fe, etc.) for evaluating water quality in a water body.

2.5.2 Sub-indexing

The primary goal of the sub-index process is to convert parameter concentrations into unitless values known as the parameter sub-indices (Abbasi and Abbasi, 2012). Several WQI models used standard guideline values of water quality to establish the sub-indices (Liou et al., 2004; Abbasi and Abbasi, 2012; Sutadian et al., 2016). While most of the reviewed models included this step, the CCME model (Cash et al., 2001) and the Dojildo model omitted the step and performed the final aggregation function using the parameter concentrations directly rather than sub-indices (Dojildo, 1994). The following sub-index rules were used by models (see Table 2.2).

Table 2.3. Water quality parameters included in WQI models.

	Common WQ parameters															Additional Parameters					Toxics, pesticides and trace metal								
	Physical					Chemical								Biological															
WQI	Temperature	Color or App.	Turbidity	SS	Total Solids	pH	DO	BOD	COD	Specific Conductivity	Alkalinity	Cl-	NH3-N	F. Coliforms	T. Coliforms	T. Phosphorus	T. Sulfate	Nitrates	T. hardness	Total Nitrogen	Cd	Mn	Zn	Cu	Hg	Pb	Phenols	Detergent	Others
Horton (8)						Y	Y			Y	Y	Y		Y															• Sewage treatment • carbon chloroforms extract
NSF (11)	Y		Y		Y	Y	Y	Y						Y		Y		Y											• Pesticides • Toxic components
SRDD (10)	Y			Y		Y	Y	Y		Y			Y	Y		Y				Y									
Dinius (11)	Y	Y				Y	Y	Y		Y	Y	Y		Y	Y				Y										
Ross (4)				Y			Y	Y					Y																
Bascaron (26)	Y	Y	Y			Y	Y	Y		Y		Y	Y		Y		Y	Y	Y									Y	• Permanganate reduction,

	Common WQ parameters															Additional Parameters					Toxics, pesticides and trace metal								
	Physical					Chemical								Biological															
WQI	Temperature	Color or App.	Turbidity	SS	Total Solids	pH	DO	BOD	COD	Specific Conductivity	Alkalinity	Cl-	NH3-N	F. Coliforms	T. Coliforms	T. Phosphorus	T. Sulfate	Nitrates	T. hardness	Total Nitrogen	Cd	Mn	Zn	Cu	Hg	Pb	Phenols	Detergent	Others
																													• Pesticides, oil and grease, • CN^-, Na^+, free CO2, • Mg^{2+}, P, NO_2^-, Ca^{2+} • visual appearance
Oregon (8)	Y				Y	Y	Y	Y					Y	Y		Y		Y		Y									
EQI (9)		Y		Y						Y		Y		Y		Y					Y				Y	Y	Y		• Chlorophyll a • Toxaphene, Polychlorinated Biphenyls, and Chloroform • Arsenic, Nickel
House (9)	Y			Y		Y	Y	Y				Y	Y		Y			Y											

	Common WQ parameters															Additional Parameters					Toxics, pesticides and trace metal								
	Physical					Chemical								Biological															
WQI	Temperature	Color or App.	Turbidity	SS	Total Solids	pH	DO	BOD	COD	Specific Conductivity	Alkalinity	Cl-	NH3-N	F. Coliforms	T. Coliforms	T. Phosphorus	T. Sulfate	Nitrates	T. hardness	Total Nitrogen	Cd	Mn	Zn	Cu	Hg	Pb	Phenols	Detergent	Others
Smith (7)	Y		Y	Y			Y	Y					Y	Y															
Dojildo (26)				Y		Y	Y	Y	Y			Y	Y			Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y		• Nickel • Free CN • Cr (VI) • Total Cr • Fe • COD-Cr • Dissolved solids
BCWQI																													• Parameters are not specified
Dalmatin (8)	Y						Y	Y							Y	Y				Y									• mineralization corrosion coefficient • protein nitrogen
CCME (4)																													• any four parameters

	Common WQ parameters															Additional Parameters					Toxics, pesticides and trace metal								
	Physical					Chemical								Biological															
WQI	Temperature	Color or App.	Turbidity	SS	Total Solids	pH	DO	BOD	COD	Specific Conductivity	Alkalinity	Cl-	NH3-N	F. Coliforms	T. Coliforms	T. Phosphorus	T. Sulfate	Nitrates	T. hardness	Total Nitrogen	Cd	Mn	Zn	Cu	Hg	Pb	Phenols	Detergent	Others
Liou (13)	Y		Y	Y		Y	Y	Y					Y	Y							Y		Y	Y		Y			• Cr
Said (5)			Y				Y			Y				Y		Y													
Malaysia (6)				Y		Y	Y	Y	Y				Y																
Hanh (8)			Y	Y			Y	Y	Y				Y		Y														• Orthophosphate
Almeida (10)			Y			Y			Y					Y	Y	Y		Y										Y	• enterococci, • *Escherichia coli*
WJWQI (13)	Y				Y		Y		Y			Y		Y		Y		Y					Y		Y	Y	Y	Y	

i. Parameter concentrations

The simplest sub-index process, used by the Horton index, the Dinius index, the Dalmatian Index, the Liou index and the Said index, used the measured parameter concentrations/values directly as the sub-index values without any conversion process.

ii. Linear interpolated functions

The NSF model used recommended parameter ranges from water quality standards to compute the sub-index values linearly (Effendi et al., 2015; Lobato et al., 2015; Tomas et al., 2017). The sub-index scale ranged between 0 to 100; when parameter concentrations were found below the recommended values, then the sub-index value was assigned 100, otherwise, 0 registered automatically (Hoseinzadeh et al., 2015; Lobato et al., 2015; Medeiros et al., 2017; Misaghi et al., 2017).The West Java WQI model used simple linear interpolation function. In this instance, the sub-index value was calculated using Eq. (2.1) and Eq. (2.2).

$$S_i = S_1 - \left[(S_1 - S_2)\left(\frac{X_i - X_1}{X_2 - X_1}\right)\right] \dots\dots\dots\dots\dots\dots\dots\dots\dots.. (2.1)$$

$$S_i = S_1 - \left[(S_1 - S_2)\left(\frac{X_1 - X_i}{X_1 - X_2}\right)\right] \dots\dots\dots\dots\dots\dots\dots..\dots\dots (2.2)$$

where S_i is the sub-index value for water quality parameter *i* computed for the measured value X_i. S_1 and S_2 are the maximum and minimum sub-index values for the maximum and minimum guideline values (X_1 and X_2) for parameter *i*. Eq. (2.1) is used when the measured parameter value is higher than the upper guideline value otherwise Eq. (2.2) is used (Dunnette 1979; Sutadian et al., 2016).

Liou et al. (2004) recommended equation (2.3) for obtaining the sub-index value for parameter *i*:

$$\boldsymbol{S_i = \frac{P_c}{M_{pl}}} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.3)$$

where P_c is the measured value and M_{pl} is the maximum permissible guideline limit (mg/L) of the water quality parameter.

iii. Rating curve functions

The environmental quality index (EQI) or Great Lakes Nearshore index (GLNI) (Schierow and Chesters, 1988), Malaysia river WQI (MRWQI) (Amneera et al., 2013; Fulazzaky et al., 2010; Gazzaz et al., 2012; Hasan et al., 2015; Naubi et al., 2016; Othman and Alaa Eldin, 2012; Shuhaimi-Othman et al., 2007; Sim et al., 2015) used rating curve functions for transforming measured values of water quality parameters to dimensionless values (Sutadian et al., 2017). The Oregon WQI model applied logarithmic transformations and a nonlinear regression technique to obtain its sub-index values (Dunnette 1979; Cude 2001).

Several WQI models, such as the Almeida index (2012), the House index (1989), and the Hanh surface WQI model (Pham et al., 2011), applied a rating curve technique to obtain the sub-index value. The rating curve system was developed based on water quality parameter standard guidelines that were formulated by legislative bodies or concerned authorities (House, 1989; Pham et al., 2011; Sutadian et al., 2016, 2017). The rating curve relates the measured parameter value to a sub-index scale, which must be first specified (House, 1989). An example is shown in Figure 2.6, where the DO values are related to a sub-index scale ranging from 0 to 100 (Smith, 1990).

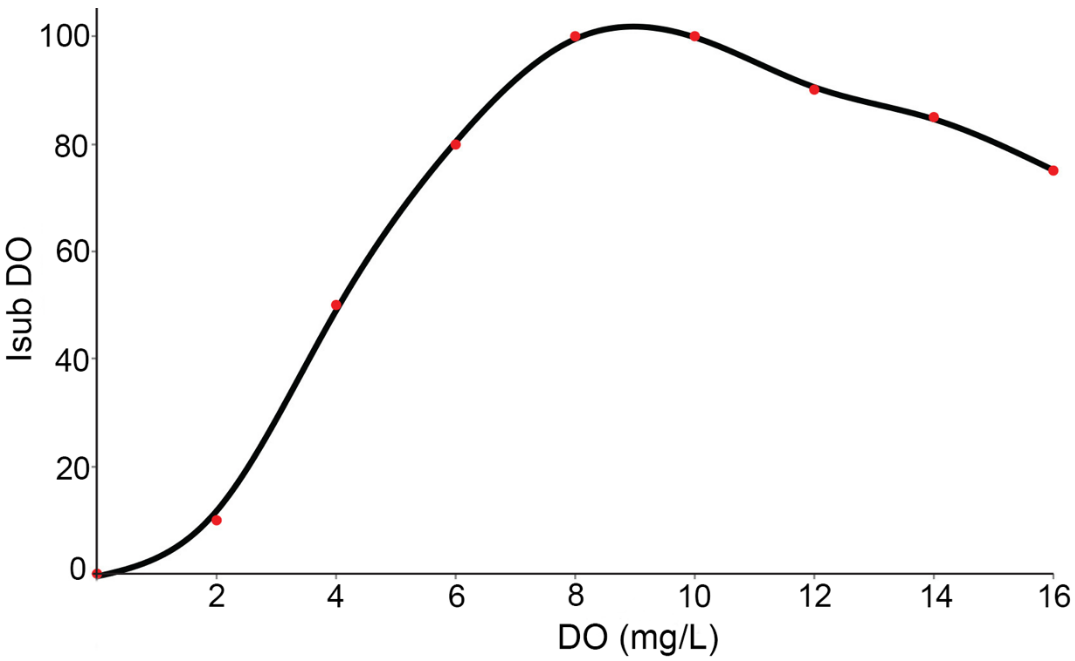


Figure 2.6. Example of sub-index rating curve for dissolved oxygen (Source: Smith, 1990, pp. 1240).

In instances where it has been applied, the rating curve is usually developed by a panel of experts (Smith, 1990; Sutadian et al., 2016) and taking into account the water body type (e.g. groundwater, surface water, marine water, wastewater, etc.) and the use/application (e.g. drinking, agriculture, ecological perspective, recreational, watershed management, wastewater treatment, etc.) (O'Flaherty and Allen, 2001).

2.5.3 Parameter weighting

In general, the parameter weight value is estimated based on the relative importance of the water quality parameter and/or the appropriate guidelines of water quality (Sarkar and Abbasi, 2006). The majority of WQI models applied unequal weighting techniques where the sum of all of the parameter weight values was equal to 1 (Table 2.2 and Table 2.4). The Horton, Bascaron and Ameida index models also used unequal weighting but the weightings were integers and their totals were greater than 1. Some models, such as the Oregon model, used an equal weighting approach where all parameters were assigned an equal weighting. On the other hand, the CCME (2001), the Smith index (1990), and the Dojildo index (1994) models do not require weight values for estimating the final score.

Through the aggregation function (Step 4), the parameter weight values can strongly influence the final index value. WQI model robustness is therefore best developed by using the unequal parameter weighting system and assigning the most appropriate weighting values. This technique reduces the uncertainty in the WQI model and helps improve model integrity. Conversely, if inappropriate weightings are used, i.e. a parameter is given greater importance than it merits, then it can adversely affect the model assessment. Tables 2.4 presents the parameter weighting values recommended for use in the most common WQI models. It can be seen that there is significant variation in the values for a given parameter. Depending on the WQI application, weighting values different to the recommended values may be specified to improve the model outputs. Tables 2.5 and 2.6 compare parameter weight values used for different applications of the same model in the assessment of river and marine waterbodies, respectively.

Two approaches have been commonly used for obtaining appropriate parameter weight values. Many WQI models used expert opinion to inform the parameter weighting process (Sarkar and Abbasi, 2006). The House index adopted the key personnel interview technique to establish the appropriate parameter weight values

(House, 1990), where participants completed questionnaires. The Horton, NSF, SRDD, Ross, EQ, House, Dalmatian and Almeida indices all used the Delphi technique to develop their parameter weightings. Expert panels typically comprise key stakeholders such as water quality experts, policymakers or practitioners, government representatives and non-governmental organizations or authorities responsible for managing water resources quality.

The analytic hierarchy process (AHP) method was developed by Thomas Saaty in the 1970s. It is a technique for decision making in complex environments in which many variables or criteria are considered in the prioritization and selection of alternatives. In the context of WQI parameter weightings, it allows one to determine the most appropriate weightings for given parameters that are reflective of their influence on overall water quality. The parameter pairwise comparisons criteria are employed for generating weight values. This helps to check the reliability of the decision maker's assessments, and it also reduces preconceptions in the decision-making process. The West-Java WQI model applied the AHP technique for formulating parameter weight values (Sutadian et al., 2017). Ocampo-Duque et al. (2006) and Gazzaz et al. (2012) successfully applied the AHP technique for establishing weight values which highlighted the relative significance of the parameters (Sutadian et al., 2017). Several scientists have noted that AHP is an effective method that can minimize model uncertainty and increase the accuracy of the weighting procedure (Sarkar and Abbasi, 2006).

2.5.4 Aggregating functions

The aggregation process is the final step of the WQI model. It is applied to aggregate the parameter sub-indices into a single water quality index score (Sutadian et al., 2016). Most models have used either additive functions or multiplicative functions or a combination of the two (see Table 2.2). The different aggregation functions are discussed briefly here.

Table 2.4: A comparison study of the common water quality parameters weight values applying different WQI model.

WQI	Weight value of the water quality parameters																		
	Tem.	Color	Turb.	SS	TS	pH	DO	BOD	COD	SC	Alk.	Cl-	NH_3-N	FC	TC	TP	NO_3^-	TON	Hard.
Horton						4	4			1	1	1		1					
NSF	0.10		0.08		0.07	0.11	0.17	0.11						0.16		0.10	0.10		
SRDD	0.05			0.07		0.09	0.18	0.15		0.06			0.12	0.12		0.08		0.08	
House	0.02			0.11		0.09	0.2	0.18				0.04	0.16		0.11		0.09		
Bascaron	1	2	4			1	4	3		4		1	3		3		2		
Dalmatian	0.07						0.16	0.1							0.16	0.12		0.16	
WJWQI	0.034			0.044			0.10		0.10			0.077		0.179		0.058	0.065		
Dinius						0.077	0.109	0.097			0.063	0.074		0.090				0.090	0.065
EQI	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1		0.15	0.15	0.15	0.1
Said			0.15				1.5			0.5				15		3.8			
Oregon						0.167	0.167	0.167				0.167		0.167			0.167		
MWQI				0.16		0.12	0.22	0.19	0.16				0.15						
Almeida			3			1			3					1	2	3	3		
Ave.	0.196	1.050	1.466	0.097	0.085	0.675	0.909	0.455	0.840	1.132	0.388	0.351	0.706	1.980	1.318	1.044	0.796	0.120	0.083
SD	0.329	0.950	1.691	0.039	0.015	1.163	1.431	0.900	1.247	1.474	0.433	0.412	1.147	4.617	1.234	1.506	1.111	0.035	0.018
Min	0.020	0.100	0.080	0.044	0.070	0.077	0.100	0.097	0.100	0.060	0.063	0.040	0.100	0.090	0.110	0.058	0.065	0.080	0.065
Max	1	2	4	0.16	0.1	4	4	3	3	4	1	1	3	15	3	3.8	3	0.16	0.1

Table 2.5: Variation of parameter weight values for different applications of the NSF and SRDD models for assessing surface water (river) quality.

WQI	WQ parameters	Model recommended weight values	Researchers defined parameters weight values for the rive water					
			Effendi et al., 2015	*Babaei Semiromi et al., 2011*	*Shah, 2014*	*Hoseinzadeh et al., 2015*	*Ewaid, 2016*	*Tomas et al., 2017*
NSF	DO	0.17	0.2	0.129	0.17	0.17	0.17	0.2857
	pH	0.11	0.11	0.133	0.11	0.12	0.11	0.0714
	BOD	0.11	0.13	-	0.11	0.1	0.11	0.2142
	tem	0.1	0.12	-	0.1	0.1	0.1	-
	TP	0.1	0.12	-	0.1	0.1	0.1	0.1429
	Nitrate	0.1	0.12	0.128	0.1	0.1	0.1	0.1429
	Turbidity	0.08	0.1	0.155	0.08	0.08	0.08	-
	TS	0.07	0.08	0.1	0.07	0.08	0.07	-
	FC	0.16	-	0.182	0.16	0.15	0.16	-
	*TON	-	-	-	-	-	-	0.1429
	*SS	-	-	0.173	-	-	-	-
	Total	**1**	**0.98**	**1**	**1**	**1**	**1**	**1**
			Bordalo et al., 2006	*Oana, 2010*	*Carvalho et al., 2011*			
SRDD	Tem.	0.05	0.05	0.1	0.05			
	SS	0.07	0.07	0.07	0.07			
	pH	0.09	0.09	0.11	0.09			
	DO	0.18	0.18	0.17	0.19			
	BOD	0.15	0.15	0.11	0.15			
	SC	0.06	0.06	-	0.06			
	NH_3-N	0.12	0.12	-	0.12			
	FC	0.12	0.12	-	0.12			
	TP	0.08	0.08	0.1	-			
	TON	0.08	0.08	-	-			
	*NO_3^-	-	-	0.1	-			
	*COD				0.15			
	Total	**1**	**1**	**0.76**	**0.85**			

**researchers modified WQ parameter*

Table 2.6. Parameters weight values used in model applications for assessment of marine ecological status.

WQI	WQ parameters	Model recommended weights values	Researchers defined parameters weight values for marine and coastal water	Application Domains
			Jha et al., 2015	
Horton WQI	[a]DO	4	0.01556	*Andaman Sea, India*
	[a]pH	4	0.00972	
	[b]BOD	-	0.02593	
	[a]S. Con.	1	-	
	[b]Ammonia	-	0.77797	
	[b]Nitrate	-	0.07780	
	[a]Cl-	1	-	
	[b]TP	1	0.07780	
	[a]FC	1	0.00016	
	[b]Chl-a	-	0.01074	
	[a]Alkalinity	1	-	
	[a]Sewage treatment	1	-	
	[a]Carbon chloroforms extract	1	-	
	[b]TSS	-	0.00432	
	Total	**15**	**1**	
			Aminah et al., 2017	
Malaysian Index	[b]TSS	-	0.14	*Port Dickson coast belt*
	[a]SS	0.16	-	
	[a]pH	0.12	-	
	[a]DO	0.22	0.2	
	[a]BOD	0.19	-	
	[a]COD	0.16	-	
	[a]NH_3-N	0.15	0.16	
	[b]FC	-	0.14	
	[b]TP	-	0.11	
	bNO3-	-	0.12	
	[b]O & G	-	0.13	
	Total	**1**	**1**	
			Nives, 1999	
Dalmatian Index	[a]Temperature	0.07	0.07	*Dalmatian Coast, Split, Croatia*
	[a]Mineralization	0.07	0.07	
	[a]Corrosion coefficient	0.06	0.06	
	[a]DO	0.16	0.16	
	[a]BOD	0.1	0.1	
	[a]Total Nitrogen	0.16	0.16	
	[a]Protein nitrogen	0.1	0.1	

	[a]Total phosphorus	0.12	0.12	
	[a]Total coliform	0.16	0.16	
	Total	**1**	**1**	
Said Index			*Said et al., 2004*	*Streams waterbodies, Florida, USA*
	[a]DO	1.5	1.5	
	[a]TP	3.8	3.8	
	[a]Turbidity	0.15	0.15	
	[a]FC	15	15	
	[a]SC	0.5	0.5	
	Total	**20.95**	**20.95**	
WJWQI			*Sutadian et al., 2018*	*Water bodies, coastal area of the west Java sea, Indonesia*
	Temperature	0.034	0.034	
	SS	0.044	0.044	
	COD	0.1	0.1	
	DO	0.1	0.1	
	Nitrite	0.065	0.065	
	Total phosphorus	0.058	0.058	
	Detergent	0.079	0.079	
	Phenol	0.085	0.085	
	Chloride	0.077	0.077	
	Zinc	0.038	0.038	
	Lead	0.061	0.061	
	Mercury	0.079	0.079	
	Faecal coliforms	0.179	0.179	
	Total	**0.99**	**0.99**	

[a]model recommended paramters; [b]researcher's modified WQ parameters

(a) Additive functions

Several WQI models (e.g. Horton model, SRDD model, House index, Malaysian and Dalmatian index models) employed a simple additive aggregation function expressed as:

$$WQI = \sum_{i=1}^{n} s_i w_i \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2.4)$$

where s_i is the sub-index value for parameter i, w_i (which ranges from 0 to 1) is the corresponding parameter weight value and n is the total number of parameters.

(b) Multiplicative functions

Some models (e.g. the NSF, Lious Index model) have used a multiplicative aggregation function expressed as:

$$WQI = \prod_{i=1}^{n} s_i^{w_i} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots .. (2.5)$$

(c) Combined aggregating functions

Several researchers tried to apply combined aggregation (a mix of additive and multiplicative functions) for obtaining the final WQI score (Abbasi and Abassi, 2012; Swamee and Tyagi, 2000). Liou et al., (2004), Ewaid and Abed, (2017) and Alobaidy et al., (2010) successfully applied a combined aggregation function when evaluating water quality in Taiwan. The NSF model uses both additive and multiplicative functions.

(d) Square root of the harmonic mean function

Cude (2001) and Dojlido index (1995) recommended the square root of the harmonic mean function (Eq. 2.6) for the aggregation process. Dojildo et al. (1995) proposed it as a modified aggregation function for the Oregon WQI model (Cude, 2001). Hanh et al. (2011) also applied the harmonic mean function in the Hanh model. The square root of the harmonic mean function is expressed as:

$$WQI = \sqrt{\frac{n}{\sum_{i=1}^{n} \frac{1}{s_i^{2}}}} . \ldots \ldots \ldots . (2.6)$$

(e) Minimum operator function

Smith (1990) applied the minimum operator function (Eq.2.7), in which the minimum sub-index values for parameters are taken as the total water quality index values. Smith developed this index to assess the water quality of the rivers and streams in New Zealand. In mathematical terms this is expressed as:

$$WQI = Min\left(s_i, s_{i+1}, s_{i+2} \ldots \ldots .. I_{sub_n}\right) \ldots \ldots \ldots \ldots (2.7)$$

Shah and Joshi (2015) also applied the Smith index for evaluating surface water quality in India - the first application of the Smith index in the South Asia region although it was recommended only for application in New Zealand (Smith, 1990).

(f) Unique linear/non-linear aggregation functions

A few WQI models applied unique linear or non-linear aggregation functions for aggregation. For instance, the Said index (Eq. 2.8), which uses the parameter concentrations as the sub-index values, aggregates the final WQI using the following unique logarithmic function (Said et al., 2004):

$$WQI = log\left[\frac{(DO)^{1.5}}{(3.8)^{TP}(Turbi)^{0.15}(15)^{fecal/10000} + 0.14(SC)^{0.5}}\right] \ldots \ldots (2.8)$$

where DO, Turbi, TP, fecal and SC are the parameter sub-index values for dissolved oxygen (% oxygen saturation), turbidity (nephelometric turbidity units [NTU]), total phosphates (mg/L), fecal coliforms (counts/100 mL) and specific conductivity (MS/cm at 25°C), respectively**.**

2.6 Major WQI models

The review identified twenty different WQI models; their primary characteristics of all of these models are summarized in Table 2.3. From Table 2.1 it is seen that seven models have been used in four or more applications and together they account for 85% of the 107 WQI applications reviewed. These eight models were therefore selected for a more detailed analysis of their structures i.e. the parameter selection procedures, the sub-index techniques, the parameter weighting systems and the aggregation functions. The West Java Index model, although used in only one study to date, was also selected for a more detailed analysis as it is one of the most recent models published and it purports to have addressed some of the known issues of earlier WQI models. The key features of these eight WQI models are described in the following sections.

2.6.1 The Horton model

The Horton model has been used by many researchers (Appendix 2) in many different countries (Figure 2.3) for the assessment of fresh surface waters. It contains the four standard WQI components, i.e. parameter selection, sub-index calculation, parameter weighting and sub-index aggregation (Alobaidy et al., 2010; Ewaid and Abed, 2017).

(1) Parameter selection

The original Horton model employed eight physicochemical parameters of water quality including DO, pH, coliforms, specific conductivity (specifically measured exact total dissolved solids), carbon chloroforms extract, alkalinity, and chlorides (Shah and Joshi, 2017; Abbasi and Abbasi, 2012). The model also included sewage treatment as an assessment parameter based on entry of the percentage of population upstream served by treatment. The model parameters were determined based on important environmental considerations such as parameter significance, relative influence of other parameters, and authentication and reliability of data (Abbasi and Abbasi, 2012).

(2) Sub-index Generation

To convert parameter values to the sub-index, Horton applied a linear scaling function where sub-index values were assigned based on concentration level or condition of pollution. Sub-index values ranged from 0 to 100; 0 is assigned for conditions of the worst quality and 100 is recommended for excellence. For the sewage treatment sub-index, a value of 100 is assigned when treatment plants are in operation serving pretty much the entire upstream population (95 to 100%) with a direct, measurable influence at the point being considered. If less than 50 per cent of the population is being served a zero value is applied. Rating values between those limits are then graded according to the amount of population served (Horton, 1965).

(3) Parameter weighting

The parameter weight values were established by using the Delphi technique. Environment significance and relative impacts were considered for giving weight values. The expert panel assigned weight values between 1 and 4 to the various water quality parameters. Horton proposed 1 for four parameters (special conductivity, chlorides, alkalinity and carbon chloroform extract), 2 for one parameter (faecal coliforms) and 4 for three parameters (DO, sewage treatment and pH).

(4) Aggregation

An additive function is used to aggregate the final WQI value as follows:

$$WQI = \left[\frac{w_1 s_1 + w_2 s_2 + w_3 s_3 + \cdots . + w_n s_n}{w + w_2 + w_3 \ldots \ldots + w_n}\right] m_1 m_2 \ldots \ldots \ldots \ldots \ldots \ldots . . (2.9)$$

where m1 and m_2 are the coefficients of temperature and obvious pollution, respectively. If the temperature is lower than 34^0C then m_1= 0.5 is used and when the temperature is greater than 34^0C then m_1=1.0 is used. The obvious pollution applies to factors that make sight and smell offensive. Such conditions include, but are not limited to, the creation of sludge deposits, the presence of oil, debris, foam, scum or other liquid materials, and waste discharge causing a disturbance of colour or odour. When the apparent signs of emissions are present, then m_2 is taken as 0.5 otherwise 1.0.

In 1970, Brown completed a critical study on the Horton index. This study concluded that since the two additional parameters temperature and obvious pollution used in the aggregation function were not rated, the index only shows gradations in water quality. Brown also reviewed the model parameters taking into account the expert opinions and their recommended weight values and proposed a weighted average index formula for stream water as follows:

$$Brown\,WQI = \sum_{i=1}^{n} w_i s_i \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots.(2.10)$$

where the weight values summed to 1. Brown concluded that this index function worked well if all water quality parameters were considered independent of each other.

(5) WQI evaluation

The Horton model recommends the following five water quality classes for the value of the final water quality index:

1) Very good (WQI = 91 - 100)
2) Good (WQI = 71 – 90)
3) Poor (WQI = 51 – 70)
4) Bad (WQI = 31 – 50)
5) Very bad (WQI = 0 – 30)

2.6.2 National Sanitation Foundation WQI (NSF-WQI)

The NSF WQI was developed by Brown in 1965 (Abrahão et al., 2007) as a modified version of the Horton model (Lumb et al., 2011). It has been used to evaluate surface water quality in various domains (see Appendix 2 and Figure 2.3 for details). Like the Horton model, it contains the four basic WQI components.

(1) Parameter selection

The Delphi technique was used to select the water quality parameters (Ewaid, 2016; Lobato et al., 2015; Rocha et al., 2015; Tomas et al., 2017). The NSF index proposed eleven water quality parameters divided into five groups: (1) the physical parameters (temperature, turbidity and total solids), (2) the chemical parameters (pH and dissolved oxygen), (3) the microbiological parameters (faecal coliforms and BOD), (4) the nutrient parameters (total phosphate and nitrates) and (5) the toxic parameters (pesticides and toxic compounds) (Abbasi and Abbasi, 2012; Lumb et al., 2011; Sutadian et al., 2016). Brown et al., (1970) recommended that the toxic parameters group be added where most other WQI models omitted toxic elements.

(2) Sub-index generation

The parameter sub-indexing was developed based on expert panel judgement. Sub-index values ranged from 0 to 1 where the sub-index value was considered 1 when the measured value was found to be within the recommended guideline values and 0 otherwise (Lumb et al., 2011; Sutadian et al., 2016).

(3) Parameter weighting

The model uses unequal parameter weight values which sum to 1. The original weight values were obtained by employing an expert panel but subsequent applications of the model have used modified weight values for evaluating surface water quality (Lobato et al., 2015; Noori et al., 2019; Tomas et al., 2017). The original NSF model prescribed weight values for DO (0.17), FC (0.16), pH (0.11), BOD (0.11), temperature (0.10), total phosphate (0.10), nitrates (0.10), turbidity (0.08) and total solids (0.07). Similarly, this model also considered the environmental significance of water quality parameters to allocate the parameter weight value (Harkins, 1974).

(4) Aggregation

The original NSF model used a simple additive aggregation function like equation (2.4). In 1973, Brown proposed an alternative aggregation function (Brown et al., 1973) – the multiplicative function shown in equation (2.5).

(5) WQI evaluation

The model outputs a WQI that ranges from 0 to 100. 0 indicates the worst water quality and 100 indicates excellent water quality. The model proposed five water quality classes:

(1) excellent (WQI = 90 -100)

(2) good (WQI = 70 -89)

(3) medium (WQI = 50 - 69)

(4) bad (WQI = 25 - 49)

(5) very bad quality (WQI = 0 - 24)

2.6.3 Scottish Research Development Department (SRDD) index

The SRDD model has been continually developed by the Scottish Research Development Department since 1970 to evaluate surface water quality (Bordalo, 2001; Dadolahi-Sohrab et al., 2012; Sutadian et al., 2016). Most temperate and tropical-sub-tropical countries apply the SRDD model due to its flexibility and regional convenience. For example, it has been used to assess surface water quality in Iran (Dadolahi-Sohrab et al., 2012), Romania (Ionus, 2010), and Portugal (Carvalho et al., 2011). A modified SRDD model has also been used for evaluating river water quality in Eastern Thailand (Bordalo, 2001 Bordalo et al., 2006).

(1) Parameter selection

The SRDD model also applied the Delphi technique for selecting water quality parameters. It recommended eleven water quality parameters (SRDD, 1973).The model parameters categorized into four water quality groups (Bordalo et al., 2006).There were: (1) the physical group (temperature, conductivity and suspended solids), (2) the chemical group (DO, pH and free and saline ammonia), (3) the organics group (total oxide, nitrogen, phosphate), and (4) the microbiological group (BOD) and *Escherichia coli* (E. coli).

(2) Sub-index generation

The model parameter sub-index values were obtained using the Delphi technique (Bordalo, 2001). Sub-index values range from 0 to 100. The rating curve technique was applied to calculate sub-indices; the curves were developed based on expert opinions (SRDD, 1973). The model also employed the EU water quality standard guidelines to generate the sub-index values (Carvalho et al., 2011).

(3) Parameter weighting

The Delphi process was used to obtain the parameter weight values taking consideration of regional guidelines and characteristics of water quality (Bordalo et al., 2006). The model uses fixed, unequal weightings that must sum to 1. The SRDD recommended weight values were for DO (0.18), BOD (0.15), free and saline ammonia (0.12), pH (0.09), total oxidized nitrogen (0.08), phosphate (0.08), suspended solids (0.07), temperature (0.05), conductivity (0.06) and *E. Coli.* (0.12). The highest weight values were assigned for DO, BOD and *E. coli.* to reflect their importance and influence (Carvalho et al., 2011; Dadolahi-Sohrab et al., 2012).

(4) Model aggregation function

The SRDD model uses the following modified additive function for aggregation:

$$SRDD - WQI = \frac{1}{100}\left(\sum_{i=1}^{n} S_i W_i\right)^2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(2.11)$$

The model also recommended a multiplicative aggregation method (Eq. 2.5) to aggregate the parameters sub-index and weight values. The modified aggregation function of SRDD was developed based on the NSF WQI (Lumb et al., 2011).

(5) WQI Evaluation

The computed WQI can range from 0-100 and the model proposed a seven-category rating scale for evaluating water quality:

(1) clean (WQI = 90 – 100)

(2) good (WQI = 80 – 89)

(3) good without treatment (WQI = 70 – 79)

(4) tolerable (WQI = 40 – 69)

(5) polluted (WQI = 30 – 39)

(6) severe polluted (WQI = 20 – 29)

(7) piggery waste (WQI = 0 – 19)

2.6.4 Canadian Council of Ministers of the Environment (CCME) WQI

The CCME model was developed from the British Colombia WQI Model (BCWQI) in 2001 (Said et al. 2004; Lumb et al., 2011). Worldwide, the CCME WQI model has been applied to a wide range of surface water bodies (Abbasi and Abbasi, 2012;Uddin et al., 2017). Relatively, it is widely used due to its ease of application and because it provides flexibility in choosing the water quality parameters to be included in the model. The review found a range of CCME model applications for the assessment of surface (river or marine) water quality in various regions of the world (see Appendix 2 and Figure 2.3).

(1) Parameter selection

The CCME WQI model requires the use of a minimum of four water quality parameters but does not specify which ones – this is left to the user to decide (Saffran et al., 2001). To order to pick model parameters, the developers suggest using the expert panel evaluation processes.

(2) Sub-index calculation

The CCME model does not include a sub-index calculation component. Comparatively, this is a major deficiency of this model.

(3) Parameter weightings

Parameter weight values are not required to obtain the final WQI.

(4) Aggregation

The aggregation function used by the CCME is quite different to other models. It is expressed as:

$$WQI = 100 - \left[\frac{\sqrt{{F_1}^2 + {F_2}^2 + {F_3}^2}}{1.732}\right] \ldots\ldots\ldots\ldots\ldots..(2.12)$$

The three factors, F_1, F_2 and F_3 are defined as:

(a) F_1: termed the ‘scope’, this is the percentage of the total parameters that do not meet with the specified objectives. It is expressed as:

$$F_1 = \left[\frac{number\ of\ failed\ parameters}{total\ number\ of\ parameters}\right] \times 100 \ldots\ldots\ldots\ldots..(2.13)$$

(b) F_2: termed the 'frequency', this is the percentage of individual tests values that do not meet with the objectives values (failed tests). It is expressed as:

$$F_2 = \left[\frac{number\ of\ failed\ tests}{total\ number\ of\ tests}\right] \times 100 \ldots\ldots\ldots\ldots\ldots (2.14)$$

(c) F_3: termed the 'amplitude', this is a measure of the amount by which test values fail to meet their objectives. The amplitude is calculated by an asymptotic function that scales the normalized sum of the excursions (*nse*) of the test values from the objectives to yield a value between 0 and 100 using:

$$F_3 = \left[\frac{nse}{0.01\ (nse) + 0.01}\right] \ldots\ldots\ldots\ldots\ldots.. (2.15)$$

If a test value falls below the objective value, the excursion for that test value is calculated as:

$$excursion_i = \left[\frac{failed\ test\ value_i}{Objective_j}\right] - 1.. \ldots (2.16)$$

Conversely, if the test value exceeds the objective value, the excursion value is calculated as:

$$excursion_i = \left[\frac{Objective_j}{failed\ test\ value_i}\right] - 1 \ldots\ldots.\ldots. (2.17)$$

The *nse* then is the collective amount by which individual test values are out of compliance and is calculated by summing the excursions of individual tests from their objectives and dividing by the total number of tests (both those meeting objectives and those not meeting objectives). This is expressed mathematically as:

$$nse = \left[\frac{\sum_{i=1}^{n} excursion_j}{total\ number\ of\ test}\right] - 1 \ldots\ldots\ldots\ldots. (2.18)$$

The divisor of 1.732 in equation (2.12) is used as a normalizing factor to ensure the resultant WQI is in the range of 0 to 100 where 0 denotes the "worst" water quality and 100 the "best" (CCME 2001). The factor of 1.732 arises because each of the three individual index factors (F_1, F_2 and F_3) can have a maximum value of 100 giving a maximum value for the numerator of 173.2 (Neary et al., 2001).

(5) WQI evaluation

The CCME model proposed four water quality classes as follows:

(1) excellent (WQI = 95 – 100) - natural water quality

(2) Good (WQI = 80 – 94) - water quality is departed from natural or desirable levels.

(3) fair (WQI = 65 – 79) - water quality condition sometimes departs from natural or desirable levels

(4) marginal (WQI = 45 – 64) - water quality is frequently threatened or impaired; conditions often depart from natural or desirable level

(5) poor (WQI = 0 – 44) - water quality is not suitable for using purposes at any level.

2.6.5 Bascaron index (BWQI)

This model was developed by Bascaron in 1979 to assess water quality based on Spanish water quality guidelines (Abrahão et al., 2007; Sun et al., 2016). The Bascaron model considered the highest water quality parameter to assess surface water quality (Abrahão et al., 2007; Kannel et al., 2007a; Nong et al., 2020). As shown in Figure 2.3, many South American countries adopted the Bascaron model to evaluate surface water quality such as Brazil (Abrahão et al., 2007), Argentina (Pesce and Wunderlin, 2000) and Chile (Debels et al., 2005b). There have been a few applications in the southern Asian region such as Nepal (Kannel et al., 2007) and India (Banerjee and Srivastava, 2009). Several countries have also tried to develop a modified WQI model based on the Bascaron index model, for example, Debels et al., 2005 (Central Chili), and Sun et al., 2016 (China).

(1) Parameter selection

The model proposed 26 water quality parameter representing different groups of water quality characteristics (Abrahão et al., 2007; Pesce and Wunderlin, 2000; Sun et al., 2016). Model parameters were pH, BOD_5, DO, temperature, total coliform (TC), colour, turbidity, permanganate reduction, detergents, hardness, DO, pesticides, oil and grease, sulphates (SO_4^-), nitrate (NO_3^-), cyanides, sodium, free CO_2, ammonia nitrogen (ammonia-N), chloride (Cl), conductivity, magnesium (Mg), phosphorus (P), nitrite (NO_2^-), calcium (Ca) and the visual appearance of water.

(2) Sub-index Generation

The linear transformation function is applied to convert measured parameter values into sub-index values (Kannel et al., 2007; Abbasi and Abbasi, 2012) which range from 0 to 100 (Pesce and Wunderlin, 2000; Sun et al., 2016). The sub-index values are determined based on local water quality guideline values (Abrahão et al., 2007).

(3) Parameter weightings

The model uses an unequal and fixed weighting system where weight values range from 1 - 4. The sum of the weight values of all 26 parameters is 54.

(4) Aggregation

Bascaron proposed two modified additive functions to aggregate sub-indices. The objective aggregation function is defined as:

$$Bascaron - WQI_{obj} = \frac{\sum w_i s_i}{\sum w_i} \dots\dots\dots\dots\dots\dots(2.19)$$

The subjective aggregation function incorporates a subjective assessment of the visual appearance of the water and is expressed as:

$$WQI_{sub} = k\frac{\sum_{i=1}^{n} s_i w_i}{\sum_{i=1}^{n} w_i} \dots\dots\dots\dots(2.20)$$

where k is a constant which is obtained by visual assessment of the water (Pesce and Wunderlin, 2000)). For river water, it takes one of the following values depending on the condition:

(a) 1.00 = clear water without apparent contamination of natural solids suspended.
(b) 0.75 = lightly contaminated water, indicated by light non-natural colour, foam, light turbidity for no natural reason.
(c) 0.50= contaminated water, indicated by non-natural colour, light to moderate odour, high turbidity (non-natural), suspended organic solids, etc.
(d) 0.25= highly contaminated water, indicated by blackish colour, hard odour, visible fermentation, etc.

(5) WQI evaluation

This index adopted five quality classes for assessing the quality of river water.

(1) Excellent (WQI = 90 -100)

(2) Good (WQI = 70 - 90)

(3) Medium (WQI = 50 - 70)

(4) Bad (WQI = 25 – 50)

(5) Very bad (WQI = 0 – 25)

2.6.6 Fuzzy Interface System (FIS)

Fuzzy logic emerged in the 1960s and many researchers and scientists have applied FIS in the environmental risk assessment field (Peche and Rodríguez, 2012). In recent decades, several researchers have adopted FIS-based WQI models to assess river water quality (see Figure 2.5). Examples include Canada (Lu et al., 2014), Brazil (Lermontov et al., 2009), China (Li et al., 2016; Xia and Chen, 2014; Yan et al., 2010), Spain (Ocampo-Duque et al., 2006; Peche and Rodríguez, 2012), Mexico (Carbajal-Hernández et al., 2012), Iran (Nikoo et al., 2011; Sami et al., 2014), India (Mahapatra et al., 2011), Malaysia (Bai Varadharajan et al., 2009; Che Osmi et al., 2016), Sri Lanka (Ocampo-Duque et al., 2013) and Morocco (Mourhir et al., 2014). FIS based WQI models contain four steps which are analagous to the typical WQI components: (1) fuzzy sets and membership function; (2) fuzzy set operations; (3) fuzzy logic; and (4) inference rules (Lermontov et al., 2009).

(1) Fuzzy sets (i.e. parameter selection)

Set functions theory and logical rules are applied to select model parameters but the FIS approach does not recommend any specific water quality parameters for evaluation of the water quality. The FIS model employs correlation studies of the parameters for setting the model parameters. Theoretical and statistical approaches are followed to build a correlation between parameters. A few studies used expert panel opinions for setting water quality parameters (Nikoo et al., 2011).

(2) Fuzzy set operation process (i.e. sub-index generation)

Water quality parameters are normalized by adopting FIS, which allows a numerical value as input, that is then converted to a qualitative value stated by a few FIS functions (member functions, rules, sets and operators) (Lermontov et al., 2009b).

(3) Fuzzy logic function (i.e. parameter weightings)

The weight values of the parameters are generated using FIS logic function.

(4) Interface rules (i.e. aggregation)

A range of fuzzy logic interface rules are applied to aggregate the WQ parameters. The final water quality score is obtained by the defuzzification processes of FIS (Ocampo-Duque et al., 2013, 2006).

2.6.7 Malaysian Water Quality Index (MWQI)

In 1974, the MWQI was developed by the Department of Environment, Malaysia to evaluate the surface water quality and its classification locally. It is also known as the Department of Environment WQI (DOE-WQI) framework. Malaysian national water quality criteria were applied to define the local water quality and their characteristics (Gazzaz et al., 2012). This model comprises the four common components of WQI models.

(1) Parameter selection

Six typical physicochemical water quality parameters - pH, Dissolved Oxygen (DO), Biological Oxygen Demand (BOD), Chemical Oxygen Demand (COD), Ammonical Nitrogen (NH_3-N), Suspended Solid (SS) - were used by the Malaysian WQI model to estimate the surface water quality and its classification. The model parameters were selected based on expert panel opinion (Gazzaz et al., 2012; Khuan et al., 2002)

(2) Sub-index generation

For each selected parameter, a unique quality function (curve) was developed which transforms the measured value to a non-dimensional sub-index value. (Gazzaz et al., 2012). Parameter thresholds and their best fitted sub index equations (i.e. the quality curves) are given in table 2.7.

(3) Parameters weightings

An unequal weighting technique was used to determine parameter weight values by taking into consideration the expert panel opinions (Khuan et al., 2002). The sum of the weight values of the parameters is equal to 1. The highest weight value was assigned for the DO (0.22) and BOD (0.19) separately. The same weight value (0.16) was used for COD and SS, respectively. A weighting of 0.15 was determined for ammonical nitrogen while the lowest weight value was given for pH (0.12) (Gazzaz et al., 2012; Amneera et al., 2013)

Table 2.7. Parameter thresholds range and their sub-index functions for calculation the sub-index value (Department of Environment (Malaysia), 2005).

WQ parameter	Thresholds value	Best fitted Sub- index Equations
DO	for $x \leq 8$	$SI_{DO} = 0$
	for $x \leq 92$	$SI_{DO} = 100$
	for $8 < x < 92$	$SI_{DO} = -0.395 + 0.030x^2 - 0.00020x^3$
BOD	for $x \leq 5$	$SI_{BOD} = 100.4 - 4.23x$
	for $x > 5$	$SI_{BOD} = 108* exp(-0.055x) - 0.1 x$
COD	for $x \leq 20$	$SI_{COD} = -1.33x + 99.1$
	for $x > 20$	$SI_{COD} = 103*exp(-0.01 57x) - 0.04x$
NH_3-N	for $x \leq 0.3$	$SI_{AN} = 100.5 - 105x$
	for $0.3 < x < 4$	$SI_{AN} = 94*exp(-0.573x) - 5* I x - 2 I$
	for $x \geq 4$	$SI_{AN} = 0$
SS	for $x \leq 1 00$	$SI_{SS} = 97.5* exp(-0.00676x) + 0.05x$
	for $100 < x < 1000$	$SI_{SS} = 71 * exp(-0.0061 x) + 0.01 5x$
	for $x \leq 100$	$SI_{SS} = 0$
pH	for $x < 5.5$	$SI_{pH} = 17.02 - 17.2x + 5.02x^2$
	for $5.5 \leq x < 7$ for	$SI_{pH} = -242 + 95.5x - 6.67x^2$
	For $7 \leq x < 8.75$	$SI_{pH} = -1 81 + 82.4x - 6.05x^2$
	for $x \geq 8.75$	$SI_{pH} = 536 - 77.0x + 2.76x^2$

(4) Aggregation

The WQI score was determined using a simple additive aggregation formula where the products of the parameter sub-index values (SI) and their weightings are summed as follows:

$$WQI = 0.22 \times SI_{Do} + 0.19 \times SI_{BOD} + 0.16 \times SI_{COD} + 0.15 \times SI_{AN} + 0.16 \times SI_{ss} + 0.12 \times SI_{pH} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (2.21)$$

(5) WQI evaluation

The DOE, Malaysian (2005) Index proposed three water quality classes to evaluate the surface water quality. There are

(1) Clean (81 – 100)

(2) Slightly polluted (60 – 80)

(3) Polluted (0 – 59)

2.6.8 West Java WQI (WJ-WQI)

Sutadian et al. (2018) developed the West-Java WQI model in 2017. It is the most recently developed WQI model in the literature. This model tried to reduce the uncertainty present in other WQI models by following specific and systematic processes in each step.

(1) Parameters selection

The West-java WQI model prescribes thirteen crucial water quality parameters including six water quality groups (Table 2.2). These are (1) temperature and suspended solids (physical parameters), (2) Chemical Oxygen Demand (COD) and DO (Oxygen depletion parameters), (3) NO_2^- and total phosphate (nutrients), (4) detergent and phenols (organics parameters), chloride (Minerals), (5) Zn, Pb and Hg (heavy metals) and (6) faecal coliforms (microbiological parameters). Model parameters should be selected by first using two screening steps using statistical assessment to determine parameter redundancy, and then using a final step to identify common parameters across all sampling stations (Sutadian et al., 2018).

(2) Sub-index calculation

The linear scaling method is applied for producing the sub-index of temperature while the linear mathematical function of equation (2.1) – (2.2) is used to obtain the sub-index for other water quality parameters.

(3) Parameter weighting

Model parameter weight value were allocated based on expert opinions. The expert panel's opinions were evaluated using the Analytic Hierarchy Process (AHP). Parameters weight values are presented in Table 2.4, which are fixed and unequal values where the sum of the total weight value is equal to 1.

(4) Aggregation

The model uses the same multiplicative aggregation function (see equation (2.5)) as the NSF WQI model.

(5) WQI evaluation

The West-Java WQI model recommended five water quality classes based on the final model output:

(1) Excellent (WQI = 90 -100)

(2) Good (WQI =   75 - 90)

(3) Fair (WQI = 50 - 75)

(4) Marginal (WQI = 25 – 50)

(5) Poor (WQI = 5 – 25)

2.7. Discussion

2.7.1 Model eclipsing problems

One of the main problems with WQI models is that they are not able to deal with the eclipsing problem. The eclipsing term was first used by Ott (1978) and is used to describe how the final model output hides the true nature of the water quality. The eclipsing problem can be caused by inappropriate sub-indexing rules, parameter weightings that do not reflect the true relative influences of parameters, or inappropriate aggregation functions. For instance, consider a WQI model with two parameters whose sub-index values are I_1 =50 and I_2 = 110, and weight values W_1, W_2 are both equal to 0.5. Using a simple additive aggregation function, the final WQI would be 80. This index value (I=80) might indicate acceptable water quality, even though one or other of the parameters may not meet with its guideline value. In this situation, the parameter failure is hidden or “eclipsed” by the aggregation process.

Many scientists have acknowledged that crucial water quality information might be destroyed during the aggregation process (Abbasi and Abassi, 2012). Otte (1978) and Smith (1990) explain eclipsing problems in detail. Several researchers have identified eclipsing issues in WQI models (Steinhart et al. 1982; Smith 1990; Sutadian et al. 2016). They note that it is produced due to the use of extensive mathematical functions in the aggregation stage (Smith, 1990).

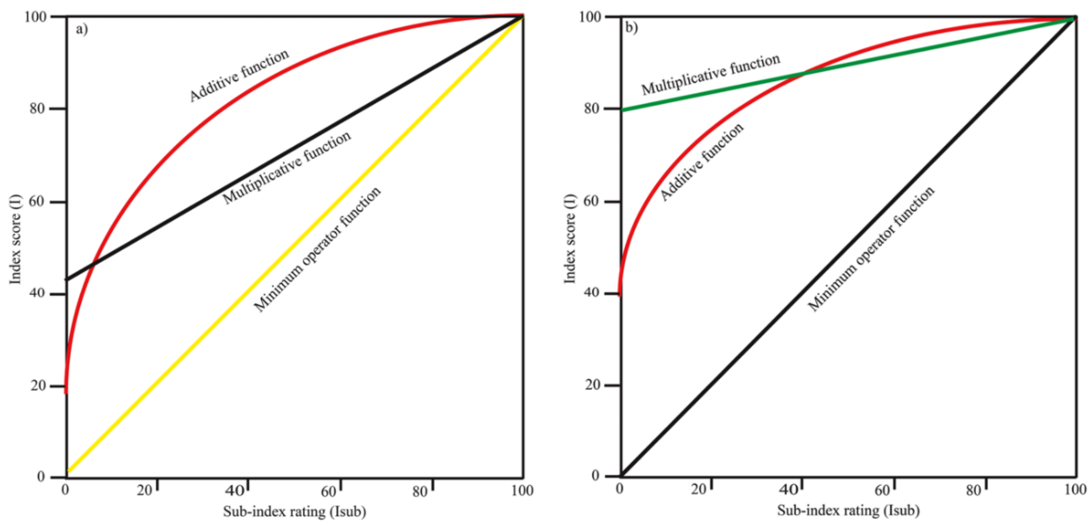


Figure 2.7. Transition of the final WQI score when applying three different aggregation functions and changing just one sub-index rating (I_{sub}) (all others being fixed at their maximum value) for (a) dissolved oxygen concentration changing and (b) faecal coliform concentration changing.

Many researchers have tried to avoid eclipsing issues; for example, the Smith index recommended using the minimum operator index aggregation function to minimize eclipsing problems (Abbasi and Abassi, 2012). If a single determinant's multiple sub-index values are used to implement the different aggregation functions, then the final WQI score is adjusted (Smith, 1990). Smith (1990) argued that the maximum and lowest weight values of 0.30 and 0.12 are the dissolved oxygen and faecal coliform determinants provided for the test. Using different aggregation function, when applying these weighting values, they produce the different WQI scores for the same determinant to calculate the final WQI score (Figure 2.7). That variation is known as the eclipsing problem. Throughout this circumstance, Smith (1990) prescribed that the final WQI score be accomplished without eclipsing the minimal operator function (Eq. 2.7). The minimum operator function not only solves the eclipsing fundamental issue but still produces that much uncertainty during the aggregation process.

2.7.2 Model uncertainty issues

An analysis of index uncertainty focuses on how the variation of the parameter threshold could affect the respective sub-index and end index values. Uncertainty is the fundamental feature of any model and may be correlated with specific parameters of the model. Studies have found that uncertainty in the final indices of WQI models are linked to various sources of the WQI model (Juwana et al., 2016; Seifi et al., 2020). The model uncertainty was contributed by the selection of parameters, the sub-indexing technique and the weighting of parameters (Juwana et al., 2016; Sutadian et al., 2017). The key sources of WQI system eclipses and uncertainty are shown in Table 2.8. The aggregation function has been shown to be a major source of uncertainty (Smith, 1990). Functional uncertainty of the WQI model aggregation was illustrated by Smith (Figure 2.7). Juwana et al., (2016) analyzed the uncertainty and sensitivity of different aggregation functions that applied different weight schemes and found that the final index values were most sensitive to the aggregation function (arithmetic and geometric) used. Several studies have been carried out to identify the sources of uncertainty and to quantify uncertainty. Such studies have used a range of statistical approaches to eliminate ambiguity in parameter selection processes such as correlation analysis, main component analysis, cluster analysis, and discriminant analysis. Some WQI models used expert opinion to mitigate uncertainty in the selection and weighting process of the parameters. Juwana et al. (2016) used the Monte Carlo Simulation method for the coefficient of variation and correlation to estimate the uncertainty and sensitivity of the various aggregation functions. Designing a WQI model should involve defining and quantifying uncertainty so that the final WQI scores can be treated with confidence and used to take proper initiative in water resource management and maintain its good health.

Table 2.8. Comparative analysis of WQI model sources of eclipsing and uncertainty.

WQI Model	Factors contributing to eclipsing	Sources of uncertainty
Oregon Index	(a) Complex parameter selection process that was contributed to eclipsing in WQI	- Aggregation function contributes to uncertainty (Swamee and Tyagi, 2000).
Horton Index	(a) No nutrient elements for the parameter group were included in the model	- The key source of uncertainty is the aggregation function, since the coefficient factors are not well defined. (Brown et al. 1970).
House Index	(a) The eclipsing problem arises through the procedure for parameter selection of the model	- Aggregation function is the main sources of Instability (Sutadian et al. 2016).
NSF Index	(a) Parameter selection phase contributes to the eclipsing of the model	- Brown et al . (1973) introduced a new multiplicative aggregation function due to the lack of original function sensitivity (Ashok Lumb et al. 2011).
CCME Index	(a) Model does not specified the WQ parameters (b) Weighting value does not required, both are responsible for eclipsing problems	- The CCME model uses a number of complex aggregation functions, which could lead to the ambiguity of the end index ranking.

Smith Index	(a) Number of required WQ parameters does not specified (b) Complicated subindex equations used for the subindex resulting from the eclipsing problems (c) Parameters weight values does not required	- Not referenced
Malaysian Index	(a) Model only used very common WQ parameters (b) Not included any oxic and biological indicators	- Not referenced
Said Index	(a) Literature based parameter selection process (b) parameter standardization not required	- Not referenced
Hanh Index	(a) complex parameter selection procedures (mixed) (b) equal weight assigned for all selected parameters	- Hybrid aggregation methods produce the uncertainty in the final score (Sutadian et al. 2016).
Dojildo Index	(a) Number of required WQ parameters does not specified (b) Parameter selection processes were based on the intent of the end user	- Aggregated index does not reflect the overall quality of water (Smith, 1990).
Almeida Index	(a) There is no scope for incorporating other essential WQ parameters for the potential implication of closed parameter selection processes. (b) Actual WQ concentration values used explicitly as a sub-index	- The key source of uncertainty is the aggregation process (Swamee and Tyagi, 2000).
Liou Index	(a) The eclipsing problem is a form of fixed-parameter selection that arises due to the lack of other critical parameters.	- The aggregation function leads to uncertainty since the final value is not correlated with the lowest sub-index ranking (Smith, 1990; Sutadian et al. 2016; Swamee and Tyagi, 2000).
West Java WQI	(a) Model parameter selection process is mainly source of eclipsing due to the model parameters were selected based on availability of monitoring data	- Not referenced
FIS	(a) The technique of parameter selection can help to enhance the eclipsing of data into the model.	- Fuzzy logic rules are the main origin of uncertainty at final index

2.7.3 Parameter selection

The number of parameters used by WQIs to assess water quality varies significantly between models. A few models, such as the CCME WQI (2001) and Said index (2004) employed only four parameters to assess water quality. It would seem that this is too few to be able to express the complete picture of the water quality since water quality depends on many different natural and anthropogenic factors. On the other extreme, the WJI requires 26 parameters and it is unlikely that measured data for all 26 would be easily available. Most WQI model parameter lists are selected based on the judgements of expert panels while one must also consider the availability and quality of the monitoring data.

Some models offer user-flexibility in parameter selection while others do not. In open systems, e.g. the CCME model, users can easily select WQ parameters using their own justification. In fixed systems such as the NSF, SRDD, Ross and Bascaron models users can only considering the model-recommended parameters. Mixed systems such as the Dojildo index (1994) allow some flexibility. Expert knowledge and experience should be used for selecting parameters. Some researchers applied statistical tools to analyse the opinions of expert panels. The Delphi technique is a popular tool to obtain the best parameter selection from an expert panel, but a few studies found this technique produced data uncertainty and reduced model accuracy. Local water quality guideline should also be used when selecting parameters and the purpose of the assessment (e.g. to assess for drinking water quality, bathing water quality, shellfish cultivation, etc.) should be taken into account. Recently, the use of statistical approaches to aid parameter selection has become popular. Ma et al. (2020), for example, used Spearman's rank correlation coefficient to measure the interaction between parameters and excluded those parameters that showed no significant correlation with the others.

Data availability is a major concern in the parameter selection process. Some WQI models need comprehensive water quality data on physical, Chemical, biological, toxic and pesticide parameters (Ongley and Booty, 1999). This is particularly difficult for developing countries because of the cost and labour intensity of water quality monitoring programs. Recent studies have recognized the monitoring program as a main source of errors and uncertainty through improper site selection and planning, inaccurate measurement due to poorly calibrated equipment or sample contamination, poor sampling techniques, inconsistent recording and data transcription, management and storage capability (Department of Water, 2009). Many developing countries are also unable to construct modern advanced laboratory facilities due to their lack of adequate capital, such as economic support, skilled human resources and effective water management boards (Debels et al. 2012).

Models should be updated when new data or new evidence of parameter importance becomes available. The Oregon WQI model has been updated repeatedly and temperature and total phosphorus were incorporated to improve the model (Cude, 2001). Many researchers have used principal component analysis (PAC) to determine parameter importance (Abrahão et al., 2007; Debels et al. , 2005; Gazzaz et al. , 2005; Gazzaz et al. , 2011; Sun et al. , 2016; Wu et al. , 2018) while others have used cluster analysis (CA) (Wu and Kuo, 2012; Sim et al., 2015). Traditionally, faecal coliforms have been used as an indicator organism for faecal contamination and microbiological water quality; this is reflected in the inclusion of faecal coliforms in many of the reviewed WQI models (Odonkor and Ampofo, 2013). Nowadays, it is commonly accepted that *E-coli* are a better indicator of faecal contamination and microbiological water pollution than faecal coliforms and international bodies such as the World Health Organization (Ashbolt et al. 2001) and the EU, via the Water Framework Directive (WFD, 2000), recommend the use of *E. coli* over faecal coliforms. Newly developed WQI models should therefore include E. coli as well as, or instead of, faecal coliforms, particularly if their purpose is for assessment of drinking or bathing waters.

2.7.4 Parameter sub-index calculation

Although sub-index calculation would appear to be a crucial component of the WQI model system given its influence on the final WQI, it is omitted by a small number of WQI models, such as CCME (2001), while some WQI models such as the Oregon, British Colombia, House, SRDD, Stoner's and Smith Index used the measured parameter values directly as sub-index values. Of those who do calculate sub-indexes, many have used experts' opinions to develop the sub-index rule for parameters and some of the sub-index generating procedures are quite complex. When developing the techniques to obtain the sub-index values, care must be taken so that the generated values do not conceal the parameter's importance / influence. According to Swamee and Tyagi (2000), a major limitation of sub-indexing strategies is that they bury the original knowledge of water quality. The local guideline values for water quality can, and should, be used to develop appropriate sub-indexing rules; these should be aligned where possible with international guideline values (e.g. WHO and EU Water Framework Directive) to provide more uniformity across WQI models.

2.7.5 Parameter weighting

The parameter weighting attributes the relative influence of a water quality parameter on the final WQI and is therefore another crucial component in the WQI model. However, some models, e.g. the CCME, Smith and Dojildo models, do not apply weightings at all. Unequal weightings are most popular as they can distinguish between the influence of different parameters. Many models obtained parameter weight values based on expert panel opinion (e.g. the NSF, House and SRDD models). The expert panels have generally based their weightings on the environmental significance of the parameter, recommended guideline values and the applications/uses of the water body. The weightings used for the same parameters vary significantly between models – thus demonstrating the difficulty in assigning appropriate weight values and the variation in the influence of a parameter depending on the purpose of the assessment. An example is dissolved oxygen which has been attributed the following range of weight values by different models: 4, 0.17, 0.18, 0.2, 4, 0.16, 0.10, 8, 0.167 and 0.22. The AHP technique has been used to determine parameters significance and therefore reduces uncertainty resulting from inappropriate weighting of parameters.

2.7.6 Aggregation function

A large range of aggregation techniques have been applied by researchers. Simple additive or multiplicative functions have been most popular. However, they have been identified as a major source of uncertainty in WQI models and as contributing to the eclipsing problem. As discussed earlier, Smith proposed the minimum operator function to minimize eclipsing problems while Stambuk Giljanovic recommended an automated aggregation function for treating this problem (Eq. 2.8). Many researchers have proposed modified aggregation techniques to aggregate parameter sub-index with less uncertainty and have had some success (Debels et al., 2005; Hallock, 2002; Hurley et al., 2012; Khan et al., 2004; Şener et al., 2017; Sun et al., 2016; Wu et al., 2018). Computer-based aggregation techniques using fuzzy interface systems and artificial neural networks have also has some success here (Kloss and Gassner, 2006; Lermontov et al., 2009; Li et al., 2016; Mahapatra et al., 2011; Nikoo et al., 2011; Ocampo-Duque et al., 2013, 2006; Peche and Rodríguez, 2012; Ross, 1995; Sami et al., 2014; Xia and Chen, 2014 and Gazzaz et al., 2012).

Furthermore, for identical water quality data different aggregation functions formulate different index ratings. A range of variations in the water quality classes were observed as a result. The water quality classes does not match the output score for the WQI model. Thus, it is difficult to identify what the accurate water quality scenarios are. The weakness of the aggregation process in the WQI model reflects these types of uncertainty. Specific guidelines for the development of an ideal WQI model for assessing real surface water quality scenarios are therefore crucial. After that, an effective WQI model could be obtained to evaluate the quality of the surface water without any uncertainty.

2.8. Conclusions

Given the relative simplicity and easily relatable output, the WQI models have been widely used for water quality assessment but many different versions have been developed to date. This review was conducted to investigate the structures and mathematical techniques used in WQI models. The study found that while most models had broadly similar structures, the finer details of the four main components varied greatly. The study also highlighted the issues of eclipsing and uncertainty due to the process of model development. The following are the main conclusions from the review:

- Most WQI models involve four stages: (1) selection of water quality parameters, (2) determination of parameter sub-indices, (3) determination of parameter weightings and (4) aggregation of the sub-indices to compute the overall water quality index. Although most models have been developed in a generic manner such that they are easily transferrable to other sites, model applications are quite region/site-specific. Selection of parameters, sub-indexing rules and weightings are all very dependent on the waterbody type (river / lake / estuary / groundwater), its current / intended uses (e.g. drinking water, industrial use, bathing, fisheries, etc.), local water quality guidelines / assessment protocols and data availability.
- There is significant variability in the number and type of water quality parameters that have been included in WQI models, the weightings attributed to particular parameters and the criteria (e.g. guideline values) used to develop sub-index values. As such, there is very little uniformity between models making it difficult to compare applications to different study areas. Some streamlining of the structure and processes of WQI models, such as incorporation of international guideline values (e.g. WHO, EU WFD or similar) may make them more attractive tools for water quality assessment. Updating of models considering new parameters of interest is also crucial for increased use; for example, the inclusion of E. Coli as the preferred indicator (by WHO and EU WFD) of faecal contamination and a measure of microbiological water quality, nutrients (e.g. nitrogen and phosphorous) that are important for eutrophication and toxins. For new studies,

care must be taken to determine which model suits best, whether a new/modified model is needed and to ensure that the model is applied in the most appropriate manner.

- Eclipsing and uncertainty are two of the key issues with regard to trust in the accuracy of model outputs. All four stages of WQI models can contribute here. Model development to date has relied heavily on expert panel opinions with regard to parameter selection, development of sub-indexing rules and determination of appropriate weightings. While this is preferable to reliance on a single person's opinions, it can still introduce uncertainty into the models. More recently mathematical techniques like principal component analysis and cluster analysis have been used to better inform the selection of parameters and their weightings and computer-based techniques like fuzzy interface systems and artificial neural networks have been used to reduce uncertainty resulting from the final aggregation process. The use of these techniques should be pursued in order to provide more certainty around the accuracy of the final computed indices. At the very least, model uncertainty should be assessed and quantified for any WQI application.

2.9 Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

2.10 Acknowledgements

The authors would like to acknowledge the Hardiman Research Scholarship of the University of Galway, Ireland which funded the first author as part of his PhD program. The reserach was also supported by MaREI, the SFI Research Centre for Energy, Climate, and Marine [Grant No: 12/RC/2302_P2].

2.11 References

Abrahão, R., Carvalho, M., Da Silva, W.R., Machado, T.T.V., Gadelha, C.L.M., Hernandez, M.I.M., 2007. Use of index analysis to evaluate the water quality of a stream receiving industrial effluents. Water SA.

Almeida, C., González, S.O., Mallea, M., González, P., 2012. A recreational water quality index using chemical, physical and microbiological parameters. Environ. Sci. Pollut. Res. 19, 3400–3411. https://doi.org/10.1007/s11356-012-0865-5

Alobaidy, A.H.M.J., Abid, H.S., Maulood, B.K., 2010. Application of Water Quality Index for Assessment of Dokan Lake Ecosystem, Kurdistan Region, Iraq. J. Water Resour. Prot. https://doi.org/10.4236/jwarp.2010.29093

Amneera, W. a., Najib, N.W. a. Z., Mohd Yusof, S.R., Ragunathan, S., 2013. Water quality index of Perlis River, Malaysia. Int. J. Civ. Environ. Eng. 13, 1–6. https://doi.org/10.1017/S0022112095002084

Ashbolt, Nicholas J., Willie O.K. Grabow and Mario Snozzi, 2001. Indicators of microbial water quality. World Health Organization (WHO). Water Quality: Guidelines, Standards and Health. Ed. by Lorna Fewtrell and Jamie Bartram. Pub. by IWA Publishing, London, UK. ISBN: 1 900222 28 0.

Babaei Semiromi, F., Hassani, A.H., Torabian, A., Karbassi, A.R., Hosseinzadeh Lotfi, F., 2011. Evolution of a new surface water quality index for Karoon catchment in Iran. Water Sci. Technol. https://doi.org/10.2166/wst.2011.780

Bai Varadharajan, raman, Bai, raman V, Bouwmeester, reinier, 2009. Fuzzy logic Water Quality index and importance of Water Quality Parameters. Air, Soil Water Res. 2, 51–59. https://doi.org/10.4137/ASWR.S2156

Bakan, G., Özkoç, H.B., Tülek, S., Cüce, H., 2010. Integrated Environmental Quality Assessment of the Ki{dotless}zi{dotless}li{dotless}rmak River and its Coastal Environment. Turkish J. Fish. Aquat. Sci. 10, 453–462. https://doi.org/10.4194/trjfas.2010.0403

Banerjee, T., Srivastava, R.K., 2009. Application of water quality index for assessment of surface water quality surrounding integrated industrial estate-Pantnagar. Water Sci. Technol. https://doi.org/10.2166/wst.2009.537

Bonanno, G., Giudice, R. Lo, 2010. Application of two quality indices as monitoring and management tools of rivers. Case study: The Imera Meridionale River, Italy. Environ. Manage. 45, 856–867. https://doi.org/10.1007/s00267-010-9450-1

Bordalo, A., 2001. Water quality and uses of the Bangpakong River (Eastern Thailand). Water Res. 35, 3635–3642. https://doi.org/10.1016/S0043-1354(01)00079-3

Bordalo, A.A., Teixeira, R., Wiebe, W.J., 2006. A water quality index applied to an international shared river basin: The case of the Douro River. Environ. Manage. 38, 910–920. https://doi.org/10.1007/s00267-004-0037-6

Brown, R.M., McClelland, N.I., Deininger, R.A. and Tozer, R.G., 1970. A water quality index-do we dare. Water and sewage works, 117(10).Carbajal-Hernández, J.J., Sánchez-Fernández, L.P., Carrasco-Ochoa, J.A., Martínez-Trinidad, J.F., 2012. Immediate water quality assessment in shrimp culture using fuzzy inference systems. Expert Syst. Appl. 39, 10571–10582. https://doi.org/10.1016/j.eswa.2012.02.141

Carvalho, L., Cortes, R., Bordalo, A.A., 2011. Evaluation of the ecological status of an impaired watershed by using a multi-index approach. Environ. Monit. Assess. 174, 493–508. https://doi.org/10.1007/s10661-010-1473-9

Che Osmi, S.F., Malek, M.A., Yusoff, M., Azman, N.H., Faizal, W.M., 2016. Development of river water quality management using fuzzy techniques: a review. Int. J. River Basin Manag. 14, 243–254. https://doi.org/10.1080/15715124.2015.1105232

Cude, C.G., 2001. Oregon water quality index: A tool for evaluating water quality management effectiveness. J. Am. Water Resour. Assoc. https://doi.org/10.1111/j.1752-1688.2001.tb05480.x

Dadolahi-Sohrab, A., Arjomand, F., Fadaei-Nasab, M., 2012. Water quality index as a simple indicator of watersheds pollution in southwestern part of Iran. Water Environ. J. 26, 445–454. https://doi.org/10.1111/j.1747-6593.2011.00303.x

Debels, P., Figueroa, R., Urrutia, R., Barra, R., Niell, X., 2005. Evaluation of water quality in the Chill??n River (Central Chile) using physicochemical parameters and a modified Water Quality Index. Environ. Monit. Assess. 110, 301–322. https://doi.org/10.1007/s10661-005-8064-1

Debels, P., Figueroa, R., Urrutia, R., Barra, R., Niell, X., 2005c. Evaluation of water quality in the Chillán River (Central Chile) using physicochemical parameters and a modified Water Quality Index. Environ. Monit. Assess. https://doi.org/10.1007/s10661-005-8064-1

Department of Water, 2009. Water quality monitoring program design - A guideline for field sampling for surface water quality.

Dinius, S.H., 1987. Design of an Index of Water Quality. JAWRA J. Am. Water Resour. Assoc. 23, 833–843. https://doi.org/10.1111/j.1752-1688.1987.tb02959.x

Dunnette, D.A., 1979. A Geographically Variable Water Quality Index Used in Oregon. Source J. (Water Pollut. Control Fed. https://doi.org/https://www.jstor.org/stable/pdf/25040240.pdf

Ewaid, S.H., 2016. Water quality evaluation of Al-Gharraf river by two water quality indices. Appl. Water Sci. https://doi.org/10.1007/s13201-016-0523-z

Ewaid, S.H., Abed, S.A., 2017. Water quality index for Al-Gharraf River, southern Iraq. Egypt. J. Aquat. Res. https://doi.org/10.1016/j.ejar.2017.03.001

Fulazzaky, M.A., Seong, T.W., Masirin, M.I.M., 2010. Assessment of water quality status for the

selangor river in Malaysia. Water. Air. Soil Pollut. 205, 63–77. https://doi.org/10.1007/s11270-009-0056-2
Gazzaz, N.M.N.M., Yusoff, M.K.M.K., Aris, A.Z.A.Z., Juahir, H., Ramli, M.F.M.F., 2012. Artificial neural network modeling of the water quality index for Kinta River (Malaysia) using water quality variables as predictors. Mar. Pollut. Bull. 64, 2409–2420. https://doi.org/10.1016/j.marpolbul.2012.08.005
Gupta, N., Pandey, P., Hussain, J., 2017. Effect of physicochemical and biological parameters on the quality of river water of Narmada, Madhya Pradesh, India. Water Sci. 31, 11–23. https://doi.org/10.1016/j.wsj.2017.03.002
Gupta, S., Nayek, S., Chakraborty, D., 2016. Hydrochemical evaluation of Rangit river, Sikkim, India: using Water Quality Index and multivariate statistics. Environ. Earth Sci. https://doi.org/10.1007/s12665-015-5223-8
Hallock, D., 2002. A Water Quality Index for Ecology's Stream Monitoring Program. Environ. Assess. Progr. https://doi.org/10.1021/jp905202x
Hasan, H.H., Jamil, N.R., Aini, N., 2015. Water Quality Index and Sediment Loading Analysis in Pelus River, Perak, Malaysia. Procedia Environ. Sci. 30, 133–138. https://doi.org/10.1016/j.proenv.2015.10.024
Horton, R.K., 1965. An index-number system for rating water quality. J. Water Pollut. Control Fed. 37, 300–306. https://doi.org/10.2307/25035251
House, M.A., 1980. A water quality index for rivers. Water Int. 5, 16–21. https://doi.org/10.1080/02508068008685872
Hurley, T., Sadiq, R., Mazumder, A., 2012. Adaptation and evaluation of the Canadian Council of Ministers of the Environment Water Quality Index (CCME WQI) for use as an effective tool to characterize drinking source water quality. Water Res. 46, 3544–3552. https://doi.org/10.1016/j.watres.2012.03.061
Ichwana, I., Syahrul, S., Nelly, W., 2016. Water Quality Index by Using National Sanitation Foundation-Water Quality Index (NSF-WQI) Method at Krueng Tamiang Aceh. Proceeding First Int. Conf. Technol. Innov. Soc. 110–117. https://doi.org/10.21063/ICTIS.2016.1019
Ionuş, O., 2010. Water Quality Index -Assessment Method of the Motru River Water Quality (Oltenia, Romania). Geogr. Univ. DIN CRAIOVA Ser. Geogr. 13, 74–83.
Islam, S., Rasul, T., Alam, J. Bin, Haque, M.A., 2010. Evaluation of Water Quality of the Titas River Using NSF Water Quality Index. J. Sci. Res. 3. https://doi.org/10.3329/jsr.v3i1.6170
Kannel, P.R., Lee, S., Lee, Y.-S., Kanel, S.R., Khan, S.P., 2007. Application of Water Quality Indices and Dissolved Oxygen as Indicators for River Water Classification and Urban Impact Assessment. Environ. Monit. Assess. 132, 93–110. https://doi.org/10.1007/s10661-006-9505-1
Khan, A.A., Paterson, R., Khan, H., 2004. Modification and application of the Canadian Council of Ministers of the Environment Water Quality Index (CCME WQI) for the communication of drinking water quality data in Newfoundland and Labrador. Water Qual. Res. J. Canada. https://doi.org/10.1007/s10661-005-9092-6
Khuan, L.Y., Hamzah, N., Jailani, R., 2002. Prediction of water quality index (WQI) based on artificial neural network (ANN), in: 2002 STUDENT CONFERENCE ON RESEARCH AND DEVELOPMENT, PROCEEDINGS: GLOBALIZING RESEARCH AND DEVELOPMENT IN ELECTRICAL AND ELECTRONICS ENGINEERING. https://doi.org/10.1109/SCORED.2002.1033081
Kloss, F.R., Gassner, R., 2006. Bone and aging: Effects on the maxillofacial skeleton. Exp. Gerontol. 41, 123–129. https://doi.org/10.1016/j.eswa.2012.02.141
Koçer, M.A.T., Sevgili, H., 2014. Parameters selection for water quality index in the assessment of the environmental impacts of land-based trout farms. Ecol. Indic. https://doi.org/10.1016/j.ecolind.2013.09.034
Lermontov, A., Yokoyama, L., Lermontov, M., Machado, M.A.S., 2009. River quality analysis using fuzzy water quality index: Ribeira do Iguape river watershed, Brazil. Ecol. Indic. 9, 1188–1197. https://doi.org/10.1016/j.ecolind.2009.02.006
Li, R., Zou, Z., An, Y., 2016. Water quality assessment in Qu River based on fuzzy water pollution index method. J. Environ. Sci. (China) 50, 87–92. https://doi.org/10.1016/j.jes.2016.03.030
Liou, S.-M., Lo, S.-L., Wang, S.-H., 2004. A Generalized Water Quality Index for Taiwan. Environ. Monit. Assess. 96, 35–52. https://doi.org/10.1023/B:EMAS.0000031715.83752.a1
Lobato, T.C., Hauser-Davis, R.A., Oliveira, T.F., Silveira, A.M., Silva, H.A.N., Tavares, M.R.M., Saraiva, A.C.F., 2015. Construction of a novel water quality index and quality indicator for reservoir water quality evaluation: A case study in the Amazon region. J. Hydrol. 522, 674–683. https://doi.org/10.1016/j.jhydrol.2015.01.021

Lu, F., Chen, Z., Liu, W., 2014. A Gis-based system for assessing marine water quality around offshore platforms. Ocean Coast. Manag. 102, 294–306. https://doi.org/10.1016/j.ocecoaman.2014.10.003

Lumb, A., Sharma, T.C., Bibeault, J.-F., 2011. A Review of Genesis and Evolution of Water Quality Index (WQI) and Some Future Directions. Water Qual. Expo. Heal. https://doi.org/10.1007/s12403-011-0040-0

Ma, Z., Li, H., Ye, Z., Wen, J., Hu, Y., Liu, Y., 2020. Application of modified water quality index (WQI) in the assessment of coastal water quality in main aquaculture areas of Dalian, China. Mar. Pollut. Bull. 157. https://doi.org/10.1016/j.marpolbul.2020.111285

Mahapatra, S.S., Nanda, S.K., Panigrahy, B.K., 2011. A Cascaded Fuzzy Inference System for Indian river water quality prediction. Adv. Eng. Softw. https://doi.org/10.1016/j.advengsoft.2011.05.018

Medeiros, A.C., Faial, K.R.F., do Carmo Freitas Faial, K., da Silva Lopes, I.D., de Oliveira Lima, M., Guimarães, R.M., Mendonça, N.M., 2017. Quality index of the surface water of Amazonian rivers in industrial areas in Pará Brazil. Mar. Pollut. Bull. 123, 156–164. https://doi.org/10.1016/j.marpolbul.2017.09.002

Misaghi, F., Delgosha, F., Razzaghmanesh, M., Myers, B., 2017. Introducing a water quality index for assessing water for irrigation purposes: A case study of the Ghezel Ozan River. Sci. Total Environ. 589, 107–116. https://doi.org/10.1016/j.scitotenv.2017.02.226

Mladenović-Ranisavljević, I.I., Žerajić, S.A., 2018. Comparison of different models of water quality index in the assessment of surface water quality. Int. J. Environ. Sci. Technol. 15, 665–674. https://doi.org/10.1007/s13762-017-1426-8

Mojahedi, S.A., Attari, J., 2009. A Comparative Study of Water Quality Indices for Karun River. World Environ. Water Resour. Congr. 2009 1–9. https://doi.org/10.1061/41036(342)246

Mourhir, A., Rachidi, T., Karim, M., 2014. River water quality index for Morocco using a fuzzy inference system. Environ. Syst. Res. 3, 1–12. https://doi.org/10.1186/s40068-014-0021-y

Naubi, I., Zardari, N.H., Shirazi, S.M., Ibrahim, N.F.B., Baloo, L., 2016. Effectiveness of water quality index for monitoring Malaysian river water quality. Polish J. Environ. Stud. 25, 231–239. https://doi.org/10.15244/pjoes/60109

Neary, B., Cash, K., Hebert, S., Khan, H., Saffran, K., Swain, L., Williamson, D., 2001. Canadian Water Quality Guidelines for the Protection of Aquatic Life CCME Water Quality Index 1.0 Technical Report. Can. Counc. Minist. Environ.

Nikoo, M.R., Kerachian, R., Malakpour-Estalaki, S., Bashi-Azghadi, S.N., Azimi-Ghadikolaee, M.M., 2011. A probabilistic water quality index for river water quality assessment: A case study. Environ. Monit. Assess. https://doi.org/10.1007/s10661-010-1842-4

Nives, Š.-G., 1999. Water quality evaluation by index in Dalmatia. Water Res. 33, 3423–3440. https://doi.org/10.1016/s0043-1354(99)00063-9

Nong, X., Shao, D., Zhong, H., Liang, J., 2020. Evaluation of water quality in the South-to-North Water Diversion Project of China using the water quality index (WQI) method. Water Res. 178. https://doi.org/10.1016/j.watres.2020.115781

Noori, R., Berndtsson, R., Hosseinzadeh, M., Adamowski, J.F., Abyaneh, M.R., 2018. A critical review on the application of the National Sanitation Foundation Water Quality Index. Environ. Pollut. 244, 575–587. https://doi.org/10.1016/j.envpol.2018.10.076

Ocampo-Duque, W., Ferré-Huguet, N., Domingo, J.L., Schuhmacher, M., 2006. Assessing water quality in rivers with fuzzy inference systems: A case study. Environ. Int. https://doi.org/10.1016/j.envint.2006.03.009

Ocampo-Duque, W., Osorio, C., Piamba, C., Schuhmacher, M., Domingo, J.L., 2013. Water quality analysis in rivers with non-parametric probability distributions and fuzzy inference systems: Application to the Cauca River, Colombia. Environ. Int. https://doi.org/10.1016/j.envint.2012.11.007

Odonkor, S.T., Ampofo, J.K., 2013. Escherichia coli as an indicator of bacteriological quality of water: an overview. Microbiol. Res. (Pavia). https://doi.org/10.4081/mr.2013.e2

Oni, O., Fasakin, O., 2016. Open Access The Use of Water Quality Index Method to Determine the Potability of Surface Water and Groundwater in the Vicinity of a Municipal Solid Waste Dumpsite in Nigeria . American Journal of Engineering Research (AJER). Am. J. Eng. Res. 96–101.

Ortega, D.J.P., Pérez, D.A., Américo, J.H.P., De Carvalho, S.L., Segovia, J.A., 2016. Development of index of resilience for surface water in watersheds. J. Urban Environ. Eng. 10, 72–82. https://doi.org/10.4090/juee.2016.v10n1.007282

Othman, F., Alaa Eldin, M.E., 2012. Assessment of the Klang River Quality Using the Water Quality Indices. Adv. Mater. Res. 599, 237–240. https://doi.org/10.4028/www.scientific.net/AMR.599.237

Panda, P.K., Panda, R.B., Dash, P.K., 2016. Assessment of Water Quality Index of River Salandi at

Hadagada Dam and Its Down Stream upto. Am. J. Water Resour. 4, 44–53. https://doi.org/10.12691/ajwr-4-2-3
Peche, R., Rodríguez, E., 2012. Development of environmental quality indexes based on fuzzy logic. A case study. Ecol. Indic. 23, 555–565. https://doi.org/10.1016/j.ecolind.2012.04.029
Pesce, S.F., Wunderlin, D.A., 2000. Use of water quality indices to verify the impact of Cordoba City (Argentina) on Suquia River. Water Res. https://doi.org/10.1016/S0043-1354(00)00036-1
Pham, T.M.H., Sthiannopkao, S., Ba, D.T., Kim, K.W., 2011. Development of Water Quality Indexes to Identify Pollutants in Vietnam's Surface Water. J. Environ. Eng. 137, 273–283. https://doi.org/10.1061/(ASCE)EE.1943-7870.0000314.
Rocha, F.C., Andrade, E.M., Lopes, F.B., 2015. Water quality index calculated from biological, physical and chemical attributes. Environ. Monit. Assess. 187. https://doi.org/10.1007/s10661-014-4163-1
Ross, T.J., 1995. FUZZY LOGIC WITH ENGINEERING APPLICATIONS Fourth Edition Title: Fuzzy logic with engineering applications.
Saffran, K., Environment, A., Cash, K., Canada, E., 2001. Canadian Water Quality Guidelines for the Protection of Aquatic Life CCME WATER QUALITY INDEX 1 . 0 User ' s Manual. Quality 1–5.
Said, A., Stevens, D.K., Sehlke, G., 2004. An innovative index for evaluating water quality in streams. Environ. Manage. https://doi.org/10.1007/s00267-004-0210-y
Sami, M., Shiekhdavoodi, M.J., Pazhohanniya, M., Pazhohanniya, F., 2014. Environmental comprehensive assessment of agricultural systems at the farm level using fuzzy logic: A case study in cane farms in Iran. Environ. Model. Softw. https://doi.org/10.1016/j.envsoft.2014.02.014
Sánchez, E., Colmenarejo, M.F., Vicente, J., Rubio, A., García, M.G., Travieso, L., Borja, R., 2007. Use of the water quality index and dissolved oxygen deficit as simple indicators of watersheds pollution. Ecol. Indic. 7, 315–328. https://doi.org/10.1016/j.ecolind.2006.02.005
Seifi, A., Dehghani, M., Singh, V.P., 2020. Uncertainty analysis of water quality index (WQI) for groundwater quality evaluation: Application of Monte-Carlo method for weight allocation. Ecol. Indic. 117. https://doi.org/10.1016/j.ecolind.2020.106653
Şener, Ş., Şener, E., Davraz, A., 2017. Evaluation of water quality using water quality index (WQI) method and GIS in Aksu River (SW-Turkey). Sci. Total Environ. 584–585, 131–144. https://doi.org/10.1016/j.scitotenv.2017.01.102
Shah, K.A., Joshi, G.S., 2017. Evaluation of water quality index for River Sabarmati, Gujarat, India. Appl. Water Sci. 7, 1349–1358. https://doi.org/10.1007/s13201-015-0318-7
Singh, P.K., Panigrahy, B.P., Verma, P., 2018. Evaluation of the Surface Water Quality Index of Jharia Coal Mining Region and Its Management of Surface Water Resources, in: Environmental Pollution. Springer Nature Singapore Pte Ltd.2018, pp. 429–437. https://doi.org/10.1007/978-981-10-5792-2_34
Smith, D.G., 1990. A better water quality indexing system for rivers and streams. Water Res. https://doi.org/10.1016/0043-1354(90)90047-A
Štambuk-Giljanović, 2003. Comparison of Dalmatian Water Evaluation Indices. Water Environ. Res. 75, 388–405. https://doi.org/10.2175/106143003X141196
Sun, W., Xia, C., Xu, M., Guo, J., Sun, G., 2016. Application of modified water quality indices as indicators to assess the spatial and temporal trends of water quality in the Dongjiang River. Ecol. Indic. 66. https://doi.org/10.1016/j.ecolind.2016.01.054
Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2018. Development of a water quality index for rivers in West Java Province, Indonesia. Ecol. Indic. 85, 966–982. https://doi.org/10.1016/j.ecolind.2017.11.049
Tomas, D., Čurlin, M., Marić, A.S., 2017. Assessing the surface water status in Pannonian ecoregion by the water quality index model. Ecol. Indic. 79, 182–190. https://doi.org/10.1016/j.ecolind.2017.04.033
Uddin, M.G., Moniruzzaman, M., Khan, M., 2017. Evaluation of Groundwater Quality Using CCME Water Quality Index in the Rooppur Nuclear Power Plant Area, Ishwardi, Pabna, Bangladesh. Am. J. Environ. Prot. 5, 33–43. https://doi.org/10.12691/env-5-2-2
Uddin, M.G., Moniruzzaman, M., Quader, M.A., Hasan, M.A., 2018. Spatial variability in the distribution of trace metals in groundwater around the Rooppur nuclear power plant in Ishwardi, Bangladesh. Groundw. Sustain. Dev. https://doi.org/10.1016/j.gsd.2018.06.002
Wu, Z., Wang, X., Chen, Y., Cai, Y., Deng, J., 2017. Assessing river water quality using water quality index in Lake Taihu Basin, China. Sci. Total Environ. 612, 914–922. https://doi.org/10.1016/j.scitotenv.2017.08.293
Xia, R., Chen, Z., 2014. Integrated Water-Quality Assessment of the Huai River Basin in China. J.

Hydrol. Eng. 20, 1–8. https://doi.org/10.1061/(ASCE)HE.1943-5584.0001030
WFD, 2000.Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy. Available at: http://data.europa.eu/eli/dir/2000/60/2014-11-20
Yan, H., Zou, Z., Wang, H., 2010. Adaptive neuro fuzzy inference system for classification of water quality status. J. Environ. Sci. https://doi.org/10.1016/S1001-0742(09)60335-1
Yidana, S.M., Yidana, A., 2009. Assessing water quality using water quality index and multivariate analysis. Environ. Earth Sci. 59, 1461–1473. https://doi.org/10.1007/s12665-009-0132-3
Zandbergen, P.A., Hall, K.J., 1998. Analysis of the British Columbia Water Quality Index for watershed managers: A case study of two small watersheds. Water Qual. Res. J. Canada.
Zeinalzadeh, K., Rezaei, E., 2017. Determining spatial and temporal changes of surface water quality using principal component analysis. J. Hydrol. Reg. Stud. 13, 1–10. https://doi.org/10.1016/j.ejrh.2017.07.002

3. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment

This chapter was published in the Journal of **“Water Research”** on May 1, 2022.
Details can be found at the following web resource:
https://doi.org/10.1016/j.watres.2022.118532

3.1 Chapter highlights

- A comprehensive method was developed for the improvement of water quality index (WQI) models in order to assess coastal water quality assessment using Cork Harbour, Ireland, as the case study.
- That was the first initiative to develop the WQI model using systematic mathematical approaches.
- Four identical components were proposed for improved WQI model, including (i) the selection of water quality indicators, (ii) sub-indexing functions, (iii) weighting technique, and (iii) an aggregation function.
- Advanced machine learning techniques were utilized in order to reduce model uncertainty.
- The XGBoost algorithm was optimized and recommended and can be used to rank and select water quality indicators for inclusion based on their relative importance to overall water quality status.
- Sensitivity analysis of the XGBoost algorithm using spatio-temporal water quality data.
- Transparency, dissolved inorganic nitrogen, ammoniacal nitrogen, BOD5, chlorophyll, temperature, and orthophosphate were found to be important for summer, and total organic nitrogen, dissolved inorganic nitrogen, pH, transparency, and dissolved oxygen were suggested for winter, respectively.
- Three brand new linear rescaling interpolation sub-index functions were developed, incorporating the WFD guidelines for coastal waters, and tested in terms of avoiding the eclipsing problem.

- A comprehensive technique incorporating the XGBoost algorithm and a statistically based rank order centroid method was developed for estimating indicators' weight values most accurately compared to the typical approach of expert opinion.
- Eight aggregation functions are included, including five widely used in the existing WQI system and three newly appointed for computing the WQI score and sensitivity testing across various functions in terms of protecting the model ambiguity problem.
- A brand new classification scheme was developed for rating coastal water quality using WFD guidelines.
- A practical methodology was provided for determining the nature and causes of model eclipsing and ambiguity problems.
- The assessment of aggregation functions found that a weighted quadratic mean (WQM) aggregation function and an unweighted arithmetic mean function (AM) resulted in the lowest instances of eclipsing and ambiguity and are therefore recommended for WQI approaches.

3.2 Abstract

Here, we present an improved water quality index (WQI) model for assessment of coastal water quality using Cork Harbour, Ireland, as the case study. The model involves the usual four WQI components – selection of water quality indicators for inclusion, sub-indexing of indicator values, sub-index weighting and sub-index aggregation – with improvements to make the approach more objective and data-driven and less susceptible to eclipsing and ambiguity errors. The model uses the machine learning algorithm, XGBoost, to rank and select water quality indicators for inclusion based on relative importance to overall water quality status. Of the ten indicators for which data were available, transparency, dissolved inorganic nitrogen, ammoniacal nitrogen, BOD_5, chlorophyll, temperature and orthophosphate were selected for summer, while total organic nitrogen, dissolved inorganic nitrogen, pH, transparency and dissolved oxygen were selected for winter. Linear interpolation functions developed using national recommended guideline values for coastal water quality are used for sub-indexing of water quality indicators and the XGBoost rankings are used in combination with the rank order centroid weighting method to determine sub-index weight values. Eight sub-index aggregation functions were tested - five from existing WQI models and three proposed by the authors. The computed indices were compared with those obtained using a multiple linear regression (MLR) approach and R^2 and RMSE used as indicators of aggregation function performance. The weighted quadratic mean function ($R^2 = 0.91$, RMSE = 4.4 for summer; $R^2 = 0.97$, RMSE = 3.1 for winter) and the unweighted arithmetic mean function ($R^2 = 0.92$, RMSE = 3.2 for summer; $R^2 = 0.97$, RMSE = 3.2 for winter) proposed by the authors were identified as the best functions and showed reduced eclipsing and ambiguity problems compared to the others.

Keyword: water quality; water quality index model; coastal waters; machine learning algorithm; rank order centroid method; aggregation function

3.3 Introduction

Surface water quality poses significant environmental, sociological, and economic risks in many parts of the world. As such, sustainable management of water resource has become a challenge of critical importance. Due to population growth, industrialisation and urbanisation observed over many decades, freshwater usage and wastewater production have significantly increased (Javed et al., 2017; Uddin et al., 2018). Both human activities and natural processes have caused a continuous degradation of surface water quality in recent decades. Many countries have adopted a range of policies and guidelines to manage surface water quality and provide more effective water resource management in order to reverse this negative trend. Member states of the European Union (EU), for example, adopted the Water Framework Directive (WFD) in 2000 and it has been an effective instrument for the management of the quality of water and its ecosystem (Carsten Von Der Ohe et al., 2007; Zotou et al., 2018). The WFD envisaged the achievement of at least a "good environmental status" of all waterbodies such as coastal and transitional water, rivers and lakes by 2015 (Brack et al., 2017; Carsten Von Der Ohe et al., 2007; EPA, 2001; European Union, 2009; Hering et al., 2018; Santos et al., 2021).

The WFD and other similar frameworks rely on assessment of water quality. In recent years a range of tools and techniques has been developed to assess the quality of surface waters and diagnose the health of aquatic ecosystems. Water quality index

(WQI) models are an example. WQI models use mathematical algorithms to convert available water quality indicator monitoring data into a single number which can be used as a measure of water quality. The method is relatively easy to apply and its results are easy to interpret by both professionals and non-experts (Abbasi and Abbasi, 2012; Nives, 1999; Sutadian et al., 2018; Uddin et al., 2021). WQI models typically consist of four components: water quality indicator selection, sub-indexing, indicator weighting and index aggregation. Over the years, some components of WQI models have been modified and/or newly developed. An extensive review of existing WQI models and their evolution is presented in Uddin et al., (2021) along with a critical discussion of model structures, applications, sources of model uncertainty and eclipsing problems.

Indicator selection and sub-index weighting are two of the prime sources of uncertainty in the implementation of a WQI model (Sutadian et al., 2016; Uddin et al., 2021). Traditionally, both have been conducted based either on a literature review of the importance and contribution of a given indicator to the overall water quality (Ashok Lumb et al., 2011) or on the opinions and judgements of experts (Sutadian et al., 2016; Uddin et al., 2021). However, these approaches have received much criticism as they are overly complex and rather subjective (Abbasi and Abbasi, 2012). They can lead to inclusion of irrelevant indicators or omission of important ones and to the attribution of weightings that are not truly reflective of real-world indicator importance. Determination of weightings is particularly open to error; while a decisionmaker may be quite comfortable ranking indicators based on their relative importance; they will likely struggle with the precision imposed by the eliciting of exact weights. This is true even for a group of experts who may struggle to agree on a ranking of indicators never mind precise weightings.

Recently, some studies have used more objective mathematical approaches for indicator selection such as logistic regression models (Ewaid et al., 2018; Feng et al., 2018; Huan et al., 2020; Li et al., 2020; Wang et al., 2017) and machine learning algorithms (Azhar and Thomas, 2019; Das et al., 2017; Jović et al., 2015; Momenzadeh et al., 2019). Here, we utilize the extreme gradient boosting (XGBoost) machine learning algorithm to rank indicators based on their measured values and their influence on water quality status. This ranking is essential in determining indicator selection and weightings for further analysis. The rank order centroid method is employed to attribute weights based on the ranking results. Another important component of a WQI model is the sub-index function, which allows conversion of indicator concentrations into dimensionless values. Sub-index generation has been reported in several studies to be one of the main sources of uncertainty (Abbasi and Abbasi, 2012) as the process can conceal the integral information of water quality (Ashok Lumb et al., 2011; Sutadian et al., 2016; Uddin et al., 2021). To address these issues, sub-index functions were developed in this study using surface water quality guidelines adopted by the Environmental Protection Agency (EPA), Ireland.

The final and most crucial component of a WQI model is the aggregation function which determines the overall index. Various WQI aggregation functions have been intercompared in the literature (Mladenović-Ranisavljević and Žerajić, 2018; Zotou et al., 2019) and significant variations in formulations has been found (Gupta et al., 2003; A. Lumb et al., 2011; Zotou et al., 2018). Several studies report that the aggregation function is another source of model uncertainty (Abbasi and Abbasi, 2012; Sutadian et al., 2016). In this study, eight aggregation functions (weighted and unweighted) are tested and their effects on WQI scores examined were - five of the functions are commonly used in existing WQI models and three are proposed new by the authors.

The aim of this research was to develop an improved, objective WQI methodology for assessing coastal water quality. To date, most WQI models have been developed for river and lakes and, to the best of our knowledge, no WQI models that have been specifically developed for coastal water quality assessment. The novel aspects of the research are the:

(1) utilization of the XGBoost machine learning algorithm for selection of key water quality indicators for inclusion in the WQI
(2) development of new sub-indexing functions specifically for coastal waters which convert water quality indicator data into dimensionless values without losing any information;
(3) calculation of indicator weight values using mathematical formulae to reduce reliance on expert opinion;
(4) determination of the most accurate aggregation function by comparing different weighted and unweighted functions; and finally,

(5) development of a WQI method for assessing coastal water quality that is systematic, objective, and aided by machine learning.

The paper is structured as follows: Section 3.4 describes the study domain, Section 3.5 provides a concise description of materials and methods, Section 3.6 presents results and discusses the methodology, and Section 3.8 summarizes the main conclusions.

3.4 Model study area – Cork Harbour

Cork Harbour, located on the southwest coast of Ireland, was selected as the case study site. It is the largest natural Harbour in Ireland and is a macro-tidal estuary with a typical spring tide range of 4.2 m at the entrance to the Harbour (Hartnett and Nash, 2015). Water depths are generally relatively shallow with much of the estuary having a depth of less than 5 m on spring tides. During periods of low water, a significant portion of the Harbour area becomes exposed, revealing extensive mudflats and sandflats (Figure 3.1). The Harbour deepens towards the mouth in the main Channel to depths of about 30 m. A number of rivers flow into the estuary, the largest being the River Lee which flows through Cork City and accounts for approximately 75% of the freshwater delivered to the estuary (Uddin et al., 2020).

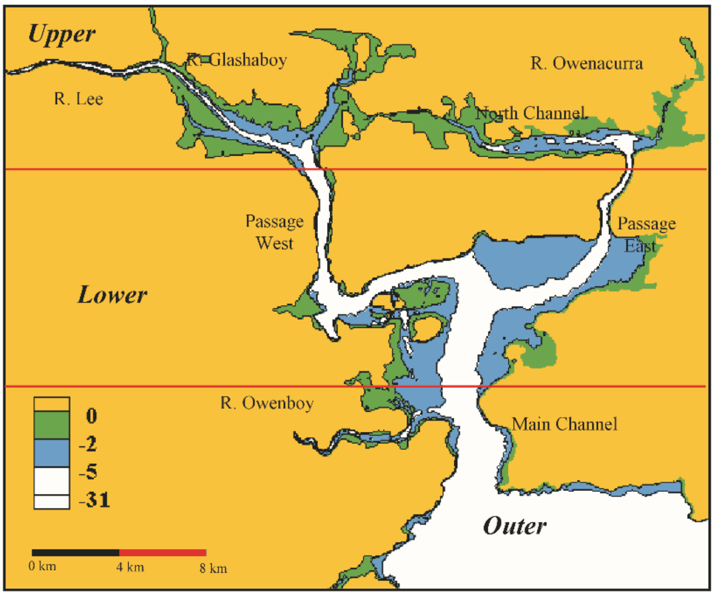


Figure 3.1. Map of Cork Harbour showing mean water depths (green areas are inter-tidal).

Cork Harbour is heavily populated and industrialized. Cork City, located at the mouth of the River Lee, is home to a population of approximately 125,000. When its immediate suburbs are included, the population rises to approximately 200,000 (Hartnett and Nash, 2015). The city is the industrial hub of the Irish southwest region and the surrounding hinterlands are subject to relatively intense agricultural activities which impact water quality in the region. Like much of Ireland, agriculture is widespread in the River Lee catchment, which covers an area of approximately 1,200 km^2. Additionally, effluent discharges (Figure 3.2) from seven wastewater treatment plants (WWTPs) which further impact water quality in the Harbour (EPA, 2016). For the purpose of regional evaluation, the Cork Harbour domain was divided into three regions delineated with the red lines in Figure 3.1: (1) Upper Harbour (including River Lee, River Glashaboy, North Channel and River Owenacurra), (2) Lower Harbour (including Passage West and Passage East) and (3) Outer Harbour (including River Owenboy and the main channel of the harbour).

3. 5 Materials and methods

3.5.1 Data collation

Water quality in Cork Harbour is monitored by the Irish EPA at 36 stations as part of the national monitoring programme. The EPA have a comprehensive quality control/quality assurance system in place to ensure that data generated by the national monitoring programme are reliable and of sufficient accuracy and precision (see EPA (2021) for more detail). Water samples are typically gathered at approximately high and low tides on two dates during winter (October – March) and two dates during summer (April – September).

This study used data from 29 of the 36 monitoring stations (Figure 3.2) for the calendar year October 2019 – September 2020; the stations were selected based on availability of a full suite of water quality indicator data and coverage of the full extents of the Harbour. For consistency, only samples taken from 1 m below the water surface were used. Data for eleven water quality indicators were available: salinity (SAL), water temperature (TEMP), pH, transparency (TRAN), dissolved oxygen (DOX), biological oxygen demand (BOD_5), total organic nitrogen (TON), ammoniacal nitrogen (AMN), dissolved inorganic nitrogen (DIN), molybdate reactive phosphorus (MRP), and chlorophyll-a (CHL) (as a measure of algae). Data were depth-averaged and seasonal average concentrations of the water quality indicators were obtained by calculating the mean of the measurements in a particular season (summer or winter). This produced singular summer and winter values for each indicator at each station (see Appendix 3a and 3b for values).

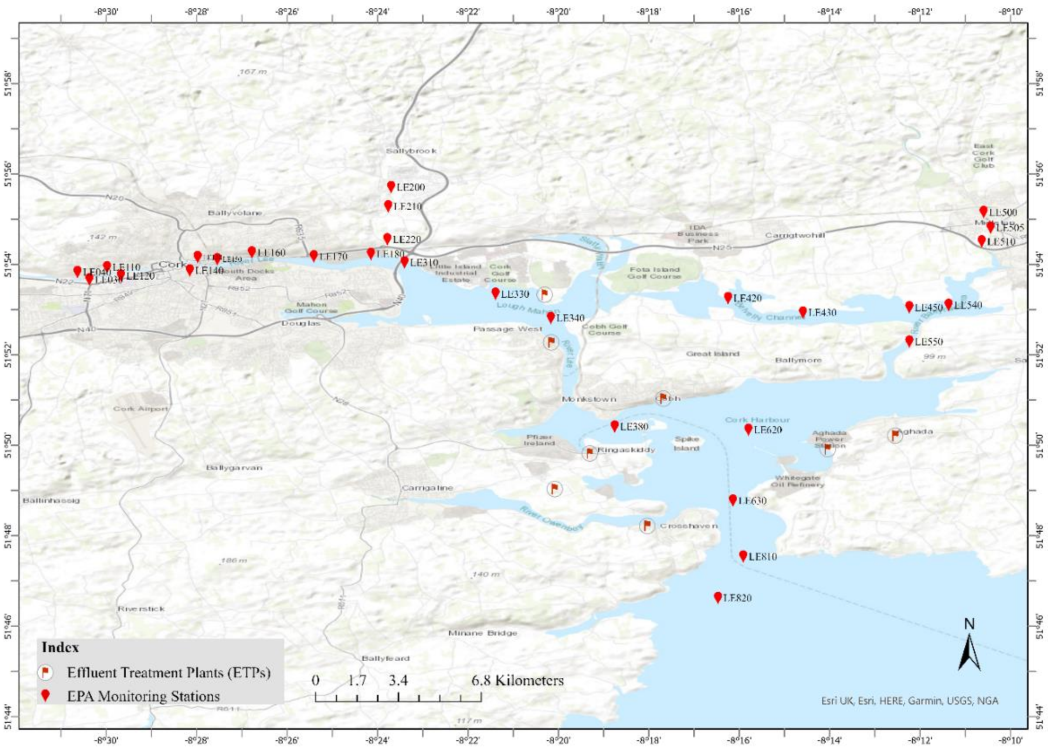


Figure 3.2. Monitoring and discharge locations in Cork Harbour.

3.5.2 Methodology for WQI model development

The WQI model consists of four components: (a) indicator selection process, (b) sub-index function, (c) indicator weighting process and (d) aggregation function. These are now described for the developed methodology.

3.5.2.1 Indicator selection process

Machine learning techniques use programmed algorithms that analyse input data (or features) to predict output values within an acceptable range of accuracy. In doing so, they attribute relative importance to input variables based on their influence on model output and can therefore potentially be used for identifying significant water quality indicators from datasets (Chen et al., 2020; Muttil and Chau, 2007). In this study, an initial assessment of four machine-learning algorithms including (1) decision tree, (2) random forest, (3) Boruta, and (4) XGBoost was performed using the Cork summer data as the test dataset. As explained in the next section, the water quality indicator data were used as the model input and a computed water quality status based on the indicator data was the desired model output. XGBoost achieved the highest prediction accuracy for water quality status - 97% compared to 92% for random forest, 79% for Boruta and 72% for decision tree – and was therefore chosen for the WQI indicator selection process.

XGBoost is a widely used ensemble machine learning technique that uses a gradient boosting framework (Naghibi et al., 2020; Tanha et al., 2020). It is one of the most commonly used machine learning algorithms due to lower prediction errors compared to other algorithms (Islam Khan et al., 2021). Unlike regular machine learning techniques, which train a single model, or an ensemble of models in isolation of each other, boosting techniques train models in succession with each new model being trained to correct the errors of the previous ones and then added to the ensemble model. Gradient boosting techniques specifically train new models to predict the residuals (errors) of previous models. A number of studies have utilized XGBoost to extract the key variables of water quality for developing models (Huan et al., 2020; Naghibi et al., 2020). Here, we implemented the XGBoost algorithm for selection of important indicators using the approach of Huan et al., (2020); this involved the following four steps.

(i) Input Data

Ten water quality indicators were used as inputs to the XGBoost model. Salinity, although not used as a direct model input, was used for obtaining the standard threshold values of coastal water quality. The summer and winter data for the ten water quality indicators at the 29 monitoring stations were used to determine a water quality status at each station which was used as the desired XGBoost output. Water quality status was determined by comparing measured data values with the recommended water quality standards given in Table 3.1. Where coastal water quality standards were available, site specific values were determined using median salinity values and the Irish EPA’s Assessment of Trophic Status of Estuaries and Bays in Ireland (ATSEBI) system (see Toner et al., (2005) for details). Where coastal water quality standards were not available, the most appropriate bathing or surface water quality standards were used instead. In Appendix 3c, the detailed applicable values of each of the criteria for the entire range of salinities are tabulated. By comparing measured values with the standard values, an initial water quality status was determined using a simple binary function. If all water quality indicator values met the guideline values, the water quality status was assigned a binary value of 0 indicating 'unpolluted'; if any water quality indicator failed to meet the guideline values, then a binary value of 1 was assigned indicating 'polluted' status. The water quality data and associated water quality status for each monitoring station are presented in Appendix 3a and 3b.

Table 3.1. Guideline values of water quality indicators for coastal water quality.

Indicator	unit	Standard threshold (summer)		Standard threshold (winter)	
		Lower	Upper	Lower	Upper
CHL[(i)]	μg/l	0.0	14.2	0.0	14.7
DOX[(i)]	% sat	72	128	71	129
MRP[(i)]	mg/l P	0.0	0.057	0.0	0.059
DIN[(i)]	mg/l N	0.0	1.208	0.0	1.336
AMN[(ii)]	mg/l	0	1.5	0	1.5
BOD_5[(ii)]	mg/l	0	7	0	7
pH[(iii)]	-	5	9	5	9
TEMP[(ii)]	^0C	-	25	-	25
TON[(iv)]	mg/l N	0.0	2	0.0	2
TRAN[(v)]	m/depth	>1	-	>1	-

(i) ATSEBI standards, determine the standard values based on median value of Salinity (see details Toner et al., (2005)*, pp. 72 – 76).*
(ii) EPA, Ireland (2001), recommended values for the surface water/freshwater/river water/aquatic life.
(iii) Estuary Monitoring Manual for pH and Alkalinity, EPA,USA
(iv) The European Communities (Quality of surface water intended for the abstraction of drinking water) regulations, 1989 (S.I. No. 294/1989).
(v) Bathing Water Quality Regulations 2008, (S.I. No. 79/2008).

(ii) Model validation:

Evaluating the performance of a machine learning algorithm requires the use of different train and test datasets. The input data were therefore randomly split into two groups: a training group containing data from 23 (80%) stations and a testing group containing data from the remaining 6 (20%) stations. The simplest method of evaluation of model performance uses one training dataset and one test dataset, but this can result in high variance and over-fitting. Over-fitting is a major concern for machine learning algorithms. It occurs when the model fits overly closely to its training data (including noise or random fluctuations) and cannot then perform well when applied to other unseen data, thus yielding poor model accuracy. k-fold cross-validation can be used to protect against over-fitting (Ghatak, 2017; Natekin and Knoll, 2013). This involves dividing the input data set randomly into k number of segments, or folds. One segment of data is reserved for testing the performance of the model while all other segments are used for training. A model is then fit to the training data and subsequently used to predict the test data. This is repeated k number of times using a different segment as the training data each time until each segment has served as both a training and test dataset. The overall model performance is taken as the average of each fold's results. A 5-fold cross-validation technique was employed here to reduce variance and the risk of over-fitting.

(iii) XGBoost hyperparameter tuning:

In machine learning, hyperparameters are parameters whose values control the learning process and must be tuned for each application. The grid search optimization method was used to adjust XGBoost's hyperparameters to increase model prediction accuracy (Huan et al., 2020; Touzani et al., 2018). A grid of different combinations of hyperparameter values was constructed. Models were developed for each point of the optimisation grid and the RMSE of model predictions calculated using equation (3.1).

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \quad \ldots\ldots.\ldots\ldots\ldots\ldots.(3.1)$$

where n is the number of pairs of observed/predicted water quality status (i.e. the number of monitoring stations), y_i is the observed status (determined in step (i)) and $\hat{y}_i$ is the XGBoost model-predicted value. For each optimisation grid point, the average RMSE was calculated across the 5-folds of the k-fold cross-validation and the optimal grid point (and thus best combination of hyperindicator values) was identified as that with the smallest RMSE. The optimized indicators determined for this study are listed in Table 3.6 while Table 3.7 shows the average RMSEs for each of the five folds of the final optimised model.

(iv) Indicator importance:

XGBoost can rank features based on their relative importance. It determines the importance of a feature using the model’s structural gain at each segment of a decision tree (Malohlava et al., 2017; Touzani et al., 2018). The more a feature is used to make key decisions within a decision trees, the higher its relative importance. For a single decision tree, T, Breiman et al. (1984) proposed the following equation to estimate the importance of a feature X_l (see Hastie, 2009):

$$I_l^2(T) = \sum_{t=1}^{j-1} \hat{\imath}_t^2 \, I(v(t) = l), \ldots \ldots \ldots \ldots \ldots . \ldots \ldots . (3.2)$$

where $\hat{\imath}_t^2$ is the maximal improvement in squared error risk for each node splitting, j is the number of leaf nodes in the XGBoost decision tree, $v(t)$ is the variable used to partition the region associate with each node t, and $I_l^2(T)$ for a particular feature is the sum of the improvement in squared error risk over all internal nodes for which that feature was chosen as the splitting variable. The global importance of a feature can then be easily estimated by averaging the feature importance across all decision trees as:

$$\hat{I}_l^2 = \frac{1}{M} \sum_{m=1}^{M} I_l^2 \, (T_m), \ldots \ldots \ldots \ldots \ldots \ldots \ldots (3.3)$$

where $\hat{I}_l^2$ is the averaged value of the feature importance measure (I_l^2) across all M decision trees in the model.

3.5.2.2 Establishing sub-index rules

Sub-index (SI) rules are used to transform the measured values of water quality indicators into dimensionless values, generally using a scale of 0-100 with 0 and 100 indicating poor and excellent status of the indicator, respectively. Many researchers have found that SI functions have significantly contributed to WQI model uncertainty (Abbasi and Abbasi, 2012 ; Sutadian et al., 2016), thus, sub-indexing is a crucial step in WQIs. A range of techniques have been used to generate SI values for water quality indicators (see Uddin et al. (2021) and Sutadian et al. (2016) for examples). A number of WQI models use interpolation techniques to establish SI values using limits set by recommended guideline values from legislative standards (Uddin et al., 2021), while others directly use the actual indicator concentration as the SI value ei.g Dinius, (1987) and Said et al., (2004).

For all water quality indicators, excluding TEMP, we developed linear interpolation rescaling functions (equations 3.4-3.6) to compute SI values using the threshold guideline values presented in Table 3.1. For TEMP, we applied a binary rule. Table 3.2 shows how SI values are determined in combination with equations (3.4 – 3.6).

Table 3.2. Sub-indexing functions for various water quality indicators.

Indicators	Conditions	Sub-index functions
BOD_5, CHL, MRP, DIN, AMN, TON	-	Eq. (3.4)
DOX	(i) if DOX > 100 (ii) if, DOX < 100 (iii) if, DOX = 100	Eq. (3.5) Eq. (3.6) SI = 100
pH	(i) If, pH ≥ 5.0 and pH < 7.5 (ii) If, pH > 8.5 and pH ≤ 9.0 (iii) If, pH ≥ 7.5 and pH ≤ 8.5	Eq. (3.5) Eq. (3.6) 100
TEMP	(i) If, TEMP ≤ 25 (ii) If, TEMP > 25	100 0.0
TRAN	(i) If. TRAN < 1.0 (ii) If. TRAN ≥ 1.0	Eq. (3.6) 100

$$SI = (SI_u - SI_l) - \frac{(SI_u \times WQ_m)}{(STD_u - STD_l)} \ldots\ldots\ldots..(3.4)$$

$$SI = \frac{\left(WQ_{i_m} - STD_l\right)}{(STD_u - STD_l)} \times SI_u \ldots\ldots\ldots..(3.5)$$

$$SI = (SI_u - SI_l) - \frac{\left(WQ_{i_m} - STD_l\right)}{(STD_u - STD_l)} \times SI_u \ldots\ldots\ldots..(3.6)$$

In equations (4-6), SI_l and SI_u are the lower and upper limits of possible SI values (0 and 100, respectively), STD_l and STD_u are the lower and upper threshold values, and WQ_m is the measured water quality indicator concentration.

3.5.2.3 Obtaining indicator weight values

Indicator weight values should reflect the relative importance of the water quality indicators included in the WQI. Here, a novel, objective weighting approach is employed combining two processes: (i) the XGBoost ranking of indicators; and (ii) the Rank Order Centroid (ROC) weights method which is used to attribute weightings based on rank. This combined approach is fundamentally different from the more subjective methods (e.g. expert opinion) used in the literature and designed to reduce the risk of eclipsing caused by inappropriate weightings. The ROC approach is a relatively simple way of assigning weights to a ranked list if items. It takes the ranks as inputs and converts them to weights. The maximum error of the weights is minimised by identifying the centroid of all possible weights whilst maintaining the rank order (Roszkowska, 2013). The method has been used extensively for solving multi-criteria decision-making problems in a range of scientific research. The ROC weights of a set of *N* variables, ranked from *i = 1 to N*, are calculated according to:

$$w_i = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{i} \quad \dots\dots\dots\dots\dots\dots\dots(3.7)$$

3.5.2.4 Aggregation process

Aggregation is the final stage of a WQI model. Its purpose is to convert multi-indicator water quality information into a single value that expresses the overall status of water quality. Three categories of aggregation functions are commonly used in WQI modelling: weighted, unweighted and multiplicative functions (Ashok Lumb et al., 2011; Sutadian et al., 2018). Several studies have addressed WQI model uncertainty issues related to aggregation functions (Smith, 1990). In this research, the performances of eight different aggregation functions were compared. Functions from five existing WQI models were selected: (i) National Sanitation Foundation (NSF) index, (ii) Scottish Research Development Department (SRDD) index, (iii) Canadian Council of Ministers of the Environment (CCME) index, (iv) Hanh index and (v) West Java (WJ) index, and three new functions were proposed: (i) weighted quadratic mean (WQM), (ii) arithmetic mean (AM), and (iii) root mean square (RMS), to compare with the traditional aggregation approaches and help select the best method for calculating WQI values in terms of addressing the existing problems in WQI models. Table 3.3 provides an overview of the aggregation functions and their properties.

Table 3.3. An overview of different WQI model aggregation functions and their components

Types of functions	WQIs Models	Aggregation functions		References
(a) Weighted	NSF index [Weighted Arithmetic Mean (WAM)]	$NSF = \sum_{i=1}^{n} s_i w_i$	(3.8)	(Gupta & Gupta, 2021; Smith, 1990)
	Weighted Quadratic Mean (WQM)	$WQM = \sqrt{\sum_{i=1}^{n} w_i\, s_i^2}$	(3.9)	Proposed by authors.

	SRDD index (modified additive function)	$$SRDD = \frac{1}{100}\left(\sum_{i=1}^{n} S_i W_i\right)^2 \quad (3.10)$$	(Bordalo et al., 2006; Carvalho et al., 2011)
	West Java WQI [Weighted Geometric Mean (WGM)]	$$WJ = \prod_{i=1}^{n} {s_i}^{w_i} \quad (3.11)$$ where s_i is the SI value for indicator *i*; w_i is weight value of respective variables and *n* is the number of indicators.	(Sutadian et al., 2018)
	Root Mean Squared (RMS)	$$RMS = \sqrt{\frac{1}{n}\sum_{i=1}^{n} s_i^2} \quad (3.12)$$	Proposed by authors.
	Arithmetic Mean (AM)	$$AM = \frac{1}{n}\sum_{i=1}^{n} s_i \quad (3.13)$$	Proposed by authors.
(b) Unweighted	CCME Index	$$CCME = 100 - \left[\frac{\sqrt{{F_1}^2 + {F_2}^2 + {F_3}^2}}{1.732}\right] \quad (3.14)$$ Where, F1, F2 and F3 are the factors that are estimated using the separate equation. The CCME details are discussed in Uddin et al., 2020. The divisor 1.732 used as a normalizing factor to ensure the resultant WQI is in the range of 0 to 100.	(Gupta and Gupta, 2021; Hurley et al., 2012; Saffran et al., 2001)
	Hanh index	$$WQI_b = \left[\frac{1}{n}\sum_{i=1}^{n} q_i \times \frac{1}{n} q_j \times q_k\right]^{1/3} \quad (3.15)$$	(Pham et al., 2011)

	Where, WQI_b is the basic water quality index; q_i is the subindex value of the organic; q_j is the inorganic substance; q_k is the subindex value of the biological or bacterial groups components; n is the number of components each group

3.5.2.5 WQI model score interpretation

The final output of the WQI model is a numerical score (the *index*) that typically ranges from 0-100. The score is commonly interpreted with the help of a classification scheme that defines classes of water quality. Classification schemes vary between models with different models sometimes assigning different classes of water quality for the same score. Table 3.4 shows the classification schemes of the five models whose aggregation functions were tested.

Table 3.4. Classification schemes of different WQI models.

WQI model	Classification schemes
NSF index (1965)	(1) excellent (90 - 100) (3) good (70 - 89) (4) medium (50 - 69) (5) bad (25 - 49) (6) very bad (0 - 24)
SRDD Index (1970)	(1) clean (90 - 100) (2) good (80 - 89) (3) good with treatment (70 - 79) (4) tolerable (40 - 69) (5) polluted (30 -39) (6) severely polluted (20 - 29) (7) piggery waste (0 - 19)
CCME (2001)	(1) excellent (95 – 100) (2) good (80 – 94) (3) fair (65 – 79) (4) marginal (45 – 65) (5) poor (0 – 44)
Hanh Index (2010)	(1) excellent (91 - 100) (2) good (76 - 90) (3) fair (51 - 75) (4) marginal (26 - 50) (5) poor (<25)
West Java Index (2017)	(1) excellent (90 - 100) (2) good (75 - 90) (3) fair (50 - 75) (4) marginal (25 - 50) (5) poor (5 – 25)

To enable comparison of the aggregation functions, we proposed a new classification scheme which could be applied to the scores from all of the aggregation functions.

Table 3.5 presents the classification which comprises four classes of water quality ranging from good to poor with higher index scores indicating better water quality. The new classification scheme was developed by analysing the classifications and corresponding index intervals for schemes in Table 3.4 and attempting to generalize these. For example, 'poor' status in the new scheme has a range of 0-29. The upper limit here was guided by the corresponding upper limits of 24 for 'very bad' in NSF, 29 for 'severely polluted' in SRDD, 44 for 'poor' in CCME, 25 for 'poor' in Hanh and 25 for 'poor' in West Java.

Table 3.5. Proposed a new classification scheme for assessing coastal water quality using WQI model.

Classifications scheme	Range of score	Descriptions
(i) Good	80 - 100	Good waterbodies are those that meet the guidelines' values. Water quality is maintained and is suitable for all uses.
(ii) Fair	50 - 79	Waterbodies that a few indicators meet the guidelines values; water quality is usually protected with a minor degree of impairment.
(iii) Marginal	30 – 49	The majority of water quality indicators failed to meet the criteria; water quality is unprotected, which may be posing a risk for aquatic life.
(iv) Poor	0 - 29	Poor waterbodies are those that fail to meet all of the criteria. Water quality is completely unprotected and unsuitable for many specifics uses

3.5.3 Analysis of WQI model sensitivity

The multilinear regression (MLR) technique was used to assess the level of sensitivity in the WQI models. This technique has been employed in several water quality studies to investigate the effect of model predictors on the response. The approach involved the prediction of WQI scores using both MLR and the aggregation functions and comparison of the results using the coefficient of determination or R^2 value. To predict WQI values using MLR, the same indicators and values included in the WQI model were used. i.e. seven indicators for summer and five indicators for winter.

MLR analysis was carried out using regression learner apps in MATLAB 2021b to develop the besting fitting MLR function of the following form:

$$y = b_0 + b_1x_1 + b_2x_2 + \cdots b_nx_n \qquad (3.16)$$

where y is the MLR-predicted WQI score, x_n is the MLR input value for the n^{th} water quality indicator, b_0 is the regression constant, and b_n is the regression coefficient for the n^{th} indicator. To compare with unweighted WQI functions, x_n in equation 3.16 was simply set to the corresponding sub-index value (SI_n) whereas, to compare with weighted functions, sub-index values were multiplied by their corresponding weights, i.e. $x_n = SI_n.w_n$.

Once the MLR-WQI scores were predicted, scatter plots were produced to visualize the relationship between the original and MLR-predicted WQI scores and obtain the R^2 from the linear fit model to analyse the sensitivity of WQI model. Three other common statistical measures of model performance were also used to help assess model sensitivity and uncertainty; these were (i) root mean squared error (RMSE), (ii) mean absolute error (MAE), and (iii) mean squared error (MSE), defined as follows.

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \widehat{y_i}| \qquad (3.17)$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{y_i})^2 \qquad (3.18)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \widehat{y_i})^2}{\sum_{i=1}^{n}(y_i - \hat{y})^2} \qquad (3.19)$$

where $\hat{y}$ is the mean of the predicted values.

3.6 Results and Discussion

The following sections present results from the XGBoost model validation exercise, the various stages of the WQI model process, and comparative analysis of the eight aggregation functions assessed.

3.6.1 XGBoost Validation

Table 3.6 shows the final tuned hyperparameter values for the XGBoost model obtained using the grid-search optimization method. These were the combination of hyperparameters that resulted in the lowest RMSEs between the predicted and observed water quality statuses; the average RMSEs are presented in Table 3.7 for each of the five folds of the final optimised model. A maximum tree depth of 10 was used for the summer analysis, and 6 for winter, to increase the maximum effects of interactions between variables. A learning rate of 0.05 and 0.01 were applied for 3400 and 600 trials for summer and winter, respectively. Whereas model training and testing accuracy was found to be 0.96 and 0.67 for the summer, and 1 for both the winter respectively which are acceptable levels of accuracy.

Table 3.6. Optimized XGBoost hyperparameter values.

Model hyperparameters	Optimum hyperparameter value	
	Summer	Winter
nrounds	3400	600
learning rate	0.05	0.01
max.depth	10	6
gamma	0	0
subsample	0.4	0.95
colsample_bytree	1	1
cv.folds	5	5
training accuracy	0.96	1
testing accuracy	0.67	1

Another measure of model performance is the AUC-ROC (area under the curve - receiver operating characteristics) curve (Feng et al., 2018; Huan et al., 2020). Of particular interest is the AUC value, with a value of 1 indicating an excellent model and 0 indicating a poor model (Walter, 2005). Table 3.7 shows the AUC values for the 5 folds of the optimised model. For both the summer and winter seasons, the AUC was estimated 0.98 and 1, respectively, for all of the training iterations.

The log loss error is a commonly used probability-based metric which can be plotted for each model iteration to produce a model learning curve which shows how model performance varies with each iteration. Figure 3.3 presents the model learning curves for the training and test datasets for both summer and winter for the optimized model. The x-axis shows the number of iterations of trees added to the ensemble and the y-axis shows the log loss of the model. As desired, the log loss error reduces with each iteration showing improved model performance. Both figures show that the model performance is better during training (blue line) than testing (red line), as would be expected. The test model performance is better for the winter season, but the summer performance is also acceptable.

Table 3.7. 5 folds cross-validation results of the XGBoost model.

Temporal variation	Iteration	Training				Validating			
		RMSE		AUC		RMSE		AUC	
		Mean	Std.	Mean	Std.	Mean	Std.	Mean	Std.
summer	1	0.241	0.042	0.98	0.026	0.379	0.040	0.81	0.01
	2	0.163	0.067	0.98	0.026	0.375	0.056	0.81	0.01
	3	0.163	0.067	0.98	0.026	0.375	0.057	0.81	0.01
	4	0.164	0.067	0.98	0.026	0.375	0.057	0.81	0.01
	5	0.164	0.067	0.98	0.026	0.375	0.058	0.81	0.01
winter	1	0.199	0.002	1.0	0	0.239	0.074	0.98	0.05
	2	0.115	0.011	1.0	0	0.172	0.114	0.98	0.05
	3	0.116	0.010	1.0	0	0.175	0.110	0.98	0.05
	4	0.118	0.011	1.0	0	0.177	0.109	0.98	0.05
	5	0.118	0.011	1.0	0	0.177	0.108	0.98	0.05

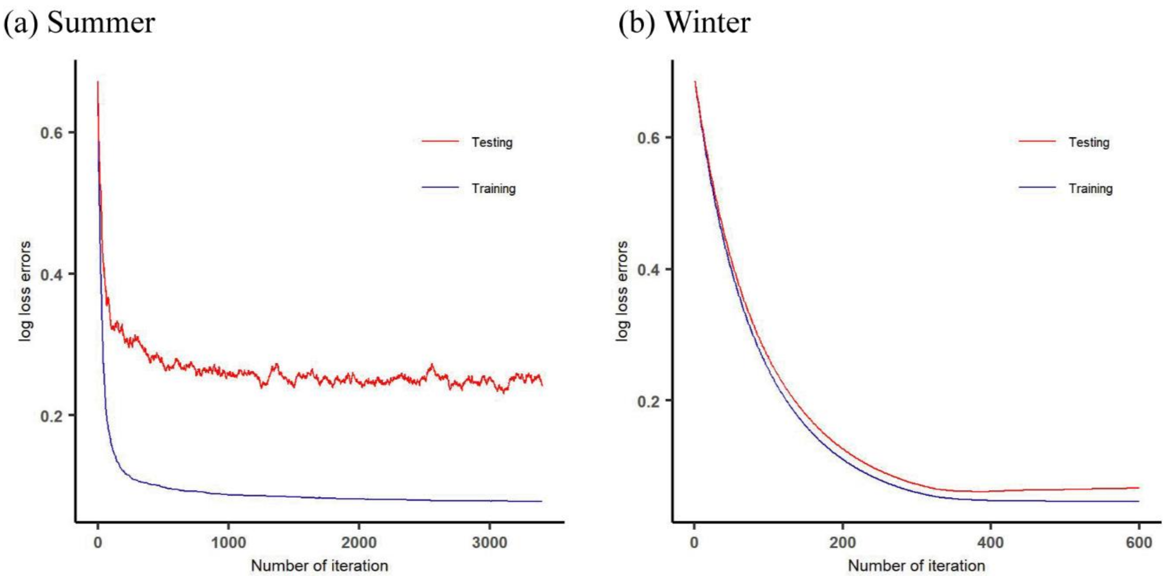


Figure 3.3. Plot of loss function against number of iterations for training and testing.

3.6.2 Analysis of WQI model components

This section of the study presents results from each of the WQI's four model components to demonstrate the application of the proposed methodology to Cork Harbour.

3.6.2.1 Indicator selection

The validated XGBoost model was used to select water quality indicators for inclusion in the WQI of Cork Harbour based on their relative importance in terms of contribution to water quality status. XGBoost outputs an ‘importance’ matrix with a number of different importance metrics. One of these metrics, the importance score, is used here to rank indicators as it implies the relative contribution of the respective indicators to the model calculated by taking each indicator’s contribution for each tree in the model.

Table 3.8. XGBoost ranking of ‘important’ water quality indicators by gain score for summer and winter.

Temporal variability	Indicators	Features selection criteria
		Importance
Summer (2019)	TRAN	0.439
	DIN	0.240
	TEMP	0.085
	CHL	0.083
	AMN	0.079
	MRP	0.029
	BOD_5	0.022
Winter (2019)	TON	0.9253
	DIN	0.0629
	pH	0.0111
	TRAN	0.0003
	DOX	0.0002

Table 3.8 shows the relative importance results obtained from the XGBoost algorithm. Seven of the ten water quality variables were determined as important for summer, and five were deemed important for winter. The highest importance scores obtained for summer were TRAN, DIN, TEMP and CHL whereas the lowest importance scores were calculated for AMN, MRP and BOD_5. For winter, the highest importance values were obtained for TON and DIN and the lowest for TRAN and DOX. While the selection of indicators was broadly in line with those of previous studies (Chen et al., 2020; Nong et al., 2020; Wu et al., 2021), most WQI studies have previously assigned the highest priority to DOX; however, this key difference is likely due to the fact that most previous studies were focussed on fresh waterbodies while this one is focussed on marine waters.

(i) Reliability of XGBoost output using outlier detection analysis

Figure 3.4 provides a statistical overview of the summer and winter indicator values input to the XGBoost model. These variables obviously impact on water quality in Cork Harbour over the study period. Comparatively, a significant statistical difference was found in water quality variables between seasons in Cork Harbour. The maximum standard deviation was found for CHL, DOX, DIN and TON for summer, while it was observed for DOX, DIN and TON for winter. This means these indicators' concentrations are not distributed evenly in Cork Harbour over the monitoring periods.

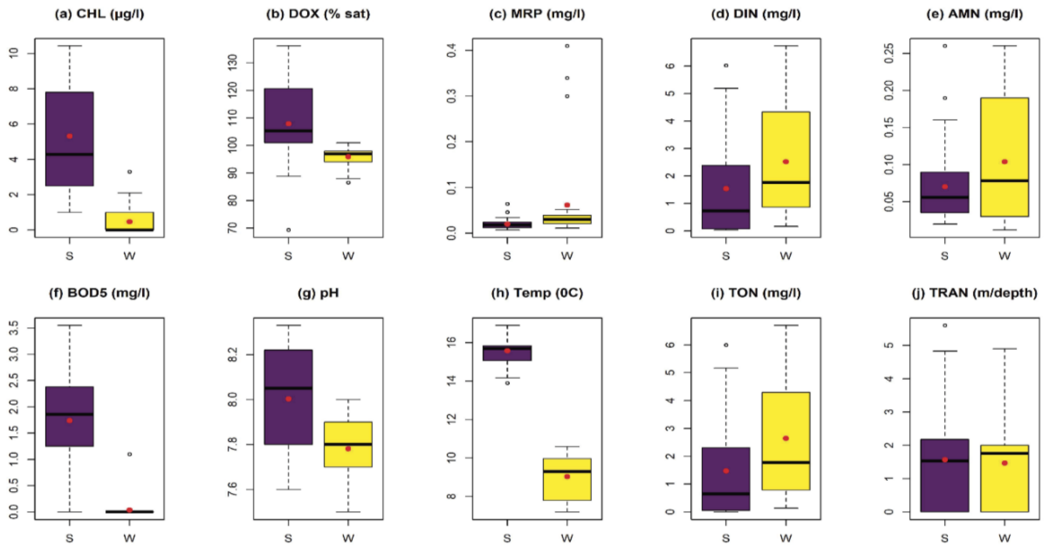


Figure 3.4. Whisker plot analysis of water quality indicators showing outlier attributes. Note: S and W on x-axes indicate summer and winter.

For the determination of water quality indicator impacts on the XGBoost model, outlier detection analysis was carried out on the water quality dataset. Figure 3.4 presents the results of the Whisker box-plots analysis for detecting data outliers of the model input variables. Outlier results were validated using Dixon's Q test (see Rorabacher (1991) for details) because this technique is widely used in statistics for the identification and rejection of outliers. As shown in Figure 3.4, CHL, DOX, BOD_5, pH, and TEMP are normally distributed during summer while DOX, DIN, AMN, pH, TEMP, TON and TRAN are normally distributed during winter. These water quality indicators had a significant positive effect on the XGBoost model and these indicators meet with the coastal water quality standard values. On the other hand, outliers were detected for MRP, DIN, AMN, TON and TRAN during summer and for CHL, MRP and BOD_5 in winter.

The outlier results indicate that these water quality indicators had extremely negative impacts on water quality in Cork Harbour. Consequently, the average WQI value in Cork Harbour decreases due to these variables. But, as can be seen from Table 3.8 (above), XGBoost does not regard TON as a critical variable for the summer season nor CHL, BOD_5, and MRP for the winter season. When the results are compared to the standard values of coastal water quality, it is seen that the XGBoost algorithm does not completely accurately identify the most influential indicators of water quality. Although the XGBoost algorithm is widely used in machine-learning techniques for selecting critical attributes in a dataset, these results show that it should be used with care when identifying critical water quality indicators.

3.6.2.2 SI function

Figure 3.5 shows the summer SI values calculated using equations (3.4-3.7) for all ten water quality indicators at all of the monitoring stations. Each black dot represents the SI value at a particular station for the particular indicator. $SI = 100$ indicates excellent water quality while SI = 0 indicates the poorest water quality. The values are presented in tabular form in Appendix 3f and 3g.

A number of studies have revealed that the sub-indexing method is one of the major contributors to uncertainty in WQI models (Abbasi and Abbasi, 2012; Sutadian et al., 2018; Juwana et al., 2016; Uddin et al., 2021). Commonly, uncertainty is produced by the SI method when it estimates smaller values without any input indicators exceeding the critical indicator thresholds. Another complication arises when the SI function estimates higher values for input indicators that exceed the critical indicator thresholds. These types of problems are well known as ambiguity in WQI models. To avoid model ambiguity from this step, the present research proposed three SI functions that were implemented based on appropriate coastal water quality standards. Comparison of the SI graphs in Figure 3.5 with the SI functions and standards in Table 3.2 show that a larger SI value is only calculated when the actual concentration of the indicator fall below, or within, the permissible thresholds; otherwise, a smaller SI value is calculated.

The SI results obtained from equations (3.4 – 3.6) can be compared using the statistical summary in Figure 3.6. A significant difference was found between the summer and winter SI values. Relatively, higher SI values were obtained during summer than winter. Looking at the individual indicators, the largest ranges were found for TRAN, DIN, and CHL during summer, and for TRAN, DIN, and TON during winter. TRAN had the greatest range of variation, ranging from 0 to 100 with an average and standard deviation of 68 ± 46 and 58.6 ± 49 for the summer and winter seasons, respectively.

DIN values ranged from 0 to 97 in the summer and 0 to 87 in the winter, with an average and standard deviation of 43.4 ± 43 in the summer and 21.4 ± 31 in the winter.

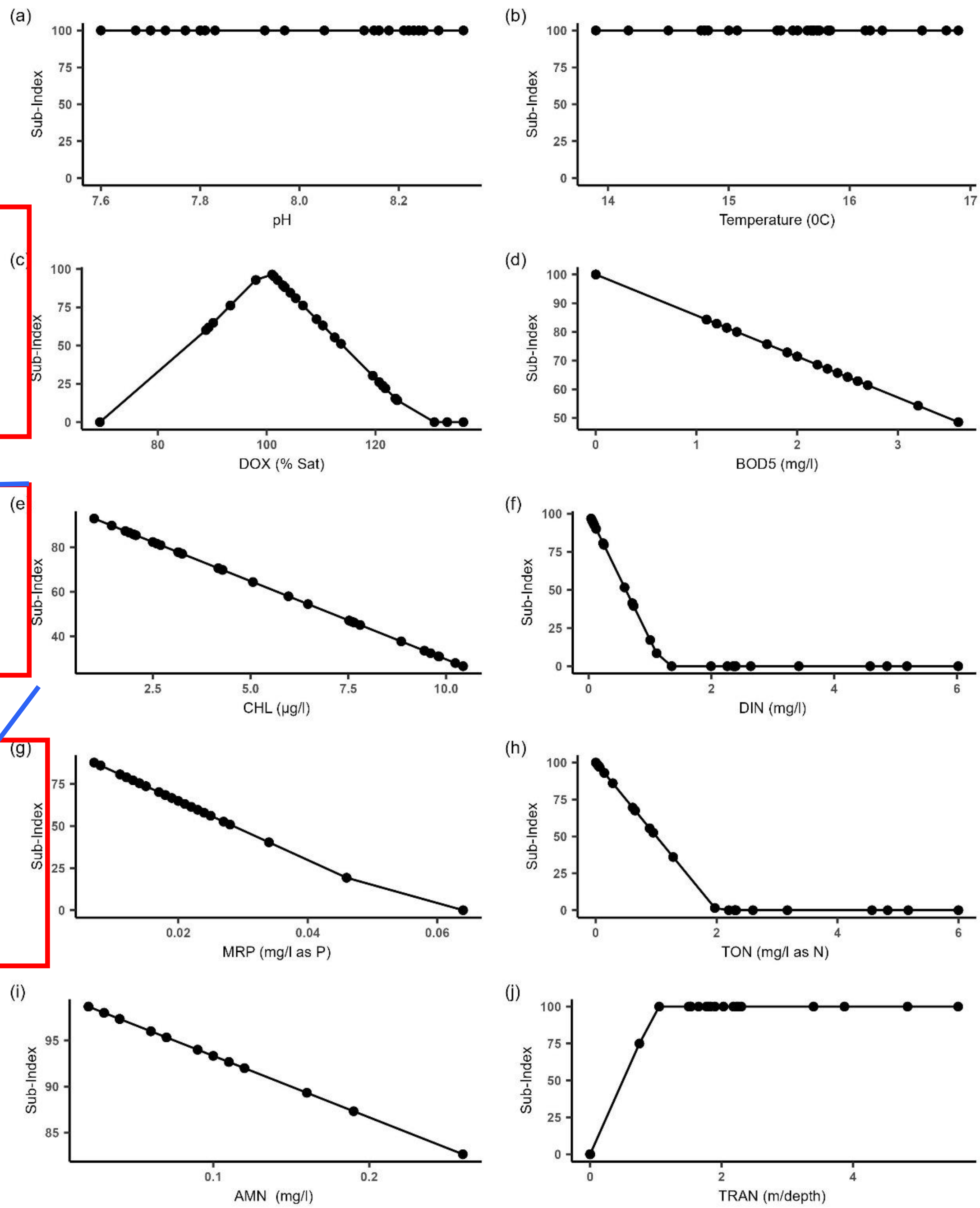


Figure 3.5. Summer SI values versus corresponding indicator value for every station for each water quality indicator. Each black dot represents the SI value calculated for the particular indicator at one of the 29 monitoring stations.

CHL summer values ranged from 27 to 93, with an average and standard deviation of 62.5 ± 22, while TON winter values ranged from 0 to 93 with an average and standard deviation of 30.6 ± 35. Regarding spatial variation of SI in the Harbour, SI values were lower in the upper and lower Harbour and higher in the outer Harbour (Appendix 3f – 3g). This is as expected as Figure 3.2 shows that all of the WWTPs that discharge effluent to the harbour are located in the upper and lower harbour regions. Taken as a whole, the results of SI functions appear to reflect the true state of the water quality indicators in Cork harbour. The SI functions presented here are fundamentally different from existing SI procedures in the literature, because they are developed specifically for coastal water quality.

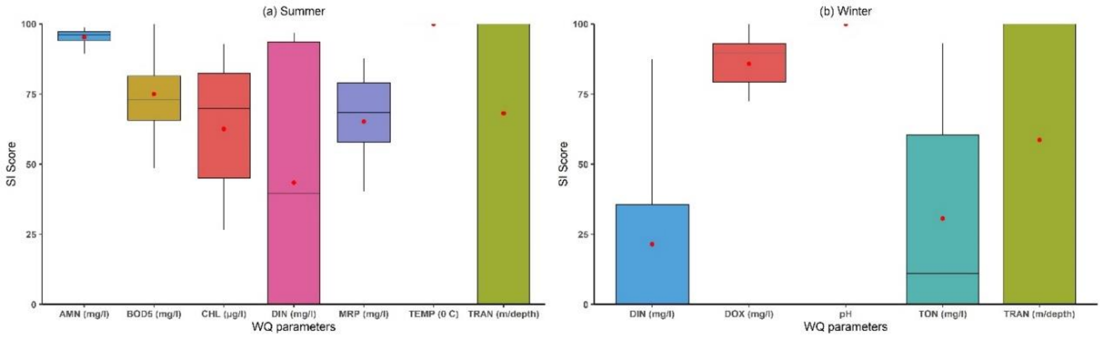


Figure 3.6. Statistical summary of calculated SI values of selected important water quality indicators in Cork Harbour.

3.6.2.3 Weight factor

Table 3.9 presents the weights calculated for the ranked indicators using the ROC method. The weights follow the same order as the rankings of model indicators with TRAN, DIN, TEMP and CHL having the largest weight values for the summer, and TON, DIN and pH having the highest weight values for winter. The weighting method used here should reduce model uncertainty compared to other models which use weightings based on expert opinions.

Table 3.9. Ranks and weight values of water quality indicators.

Summer (2019)			Winter (2019)		
Indicators	Rank	Weight	Indicators	Rank	weight
TRAN	1	0.370	TON	1	0.45
DIN	2	0.228	DIN	2	0.257
TEMP	3	0.156	pH	3	0.157
CHL	4	0.109	TRAN	4	0.090
AMN	5	0.073	DOX	5	0.040
MRP	6	0.044	Sum of weight		1.0

BOD_5	7	0.020
Sum of weight		1.0

3.6.2.4 Aggregation function WQI scores

Eight different aggregation functions were used to calculate WQI values in this study. The aggregation functions were classified into two types for analysis: (i) weighted functions and (ii) unweighted functions. Figure 3.7 shows the range of WQI scores computed by each function throughout Cork Harbour for the summer and winter periods. As might be expected, WQI values were significantly different between functions.

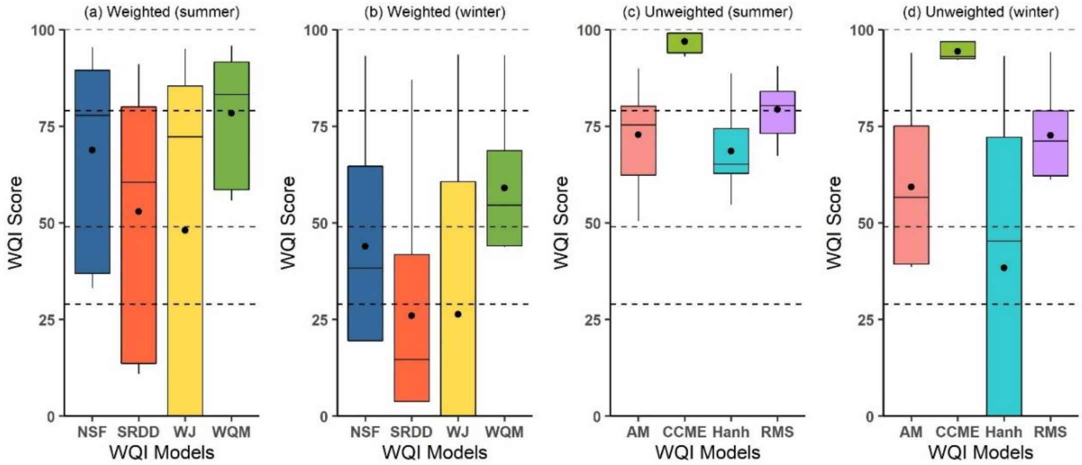


Figure 3.7. Range of WQI scores computed throughout Cork Harbour by eight different aggregation functions for summer and winter. The horizontal dashed lines indicate the scores used to classify water quality (see Table 3.5). The circle indicates the mean score and the solid black line in each box is the median WQI score.

The effect of using a weighting in the aggregation function is very clear. In general, the weighted functions produced a much greater spread of scores and lower mean scores in both summer and winter. The weighted functions appear to be much more sensitive to the input water quality values. Directly comparing the NSF scores which uses a weighted arithmetic mean (WAM) function with those from the unweighted arithmetic mean function (AM), the same observations can be made. With the exception of the Hanh function, weighted function scores showed much greater seasonal variation than the unweighted function scores, again indicating that the weighted functions are more sensitive to the input water quality values. Finally, the CCME model function appears to be highly insensitive to variations in the input water quality data. It produced very similar scores for both summer and winter and very little variation in scores across the harbour. This may be due to eclipsing problems.

Commonly, the eclipsing problem occurs due to overestimation of the WQI index by the aggregation function. Most commonly, eclipsing occurs when some water quality indicator values exceed their critical levels, but the overall index does not reflect this. The extent to which eclipsing affected the aggregation functions was determined by checking compliance of the water quality measurements for the indicators included in the WQI models with their guideline values to determine the numbers of breaches of the guideline values at each monitoring station. These numbers were then compared with the typical number of breaches of recommended guideline values that might be expected for a WQI classification (Table 3.10). For example, one would not expect any breach of guideline values for any indicator where a classification of ‘good’ status was determined by the model. For any station, if the number of breaches was greater than expected for a particular water quality status then the aggregation function was deemed to have overestimated the water quality status, and if the number of breaches was less than expected then the function was deemed to have underestimated the status. Appendix (3d) and (3e) present the occurrences of eclipsing for the different WQI aggregation functions. The results are summarised in Table 3.11 which shows the total numbers of instances of eclipsing for each function.

Table 3.10 Criteria for the determination of eclipsing problem in WQI model.

Quality status	**Expected number of breaches of indicator guideline values**
Good	0
Fair	1-2
Marginal	3
Poor	>3

** The term "criteria" refers to the threshold value of standard guideline. Details are given in Table 1 above.*

Table 3.11 Numbers of stations at which eclipsing occurred for each WQI function. The number in brackets indicates how many of the total were overestimation eclipsing.

	Weighted				**Unweighted**			
	NSF	**WQM**	**SRDD**	**WJ**	**RMS**	**AM**	**Hanh**	**CCME**
Summer	12 (0)	10 (1)	19 (5)	17 (6)	5 (2)	7 (0)	9 (0)	12 (12)
Winter	25 (8)	7 (0)	26 (0)	22 (6)	10 (3)	2 (0)	8 (1)	13 (8)
Total	37 (8)	17 (0)	45 (5)	39 (12)	15 (5)	9 (0)	17 (1)	25 (20)

From Table 3.11, eclipsing is seen to occur for all aggregation functions during both seasons. Instances of eclipsing were more prevalent for the weighted functions – the NSF, SRDD and WJ functions all resulted in much higher eclipsing numbers than the highest of the unweighted functions (25 for CCME). Of the weighted functions, the WQM method was clearly the best performer in terms of eclipsing with just 17 instances compared to the next best of 37 for NSF. Of the unweighted functions, the AM method resulted in the lowest number (9) compared to 15 and 17 for RMS and Hanh, respectively. There was a slight seasonal bias towards eclipsing with 5 of the 8 functions yielding higher instances in winter than summer. There also appeared to be a spatial bias towards eclipsing as during both seasons, across all functions, the majority of cases of eclipsing were found in monitoring sites in the Upper Harbour (see Appendix (3d) and (3e)).

The underestimating eclipsing problem was observed more often across all aggregation functions with the exception of the CCME function which suffered more from overestimation (20 of the 25 CCME instances of eclipsing were overestimation). During summer, the CCME function determined "good" water quality status at many monitoring locations in Cork Harbour even though some of the water quality indicators at those locations exceeded the guideline values. All 12 summer instances of eclipsing were overestimation. For winter, 8 of the 13 eclipsing instances were overestimation. It can be concluded that the CCME displays a consistent bias towards attributing higher water quality status even when that is not the case.

Ambiguity is another important source of the WQI model uncertainty. Ambiguity hides the actual water quality information contained in the model inputs. Consequently, the model produces considerable uncertainty that results in the misclassification of water quality for environmental mangers or assessors. Commonly two types of ambiguity contribute to uncertainty:

Type-I: Underestimation ambiguity - if the aggregation function estimates a smaller index without any of the sub-indices exceeding the critical level (nearly zero or unacceptable value)

Type-II: Overestimation ambiguity - if the aggregation function estimates a larger index with one or more sub-indices exceeding the critical level (nearly zero or unacceptable value)

The results show type-I ambiguity having occurred in the weighted SRDD and WJ models during both seasons. The aggregation functions have calculated lower index values but the SI values do not reflect this (Appendix 3f – 3g). Type-II ambiguity occurred in the unweighted CCME methodology for both seasons with higher index values calculated for all monitoring locations even though the SI values contain some low values. Relatively, the NSF and WQM and unweighted AM and RMS aggregation methods produce indices during both seasons that reflect the true quality of the water.

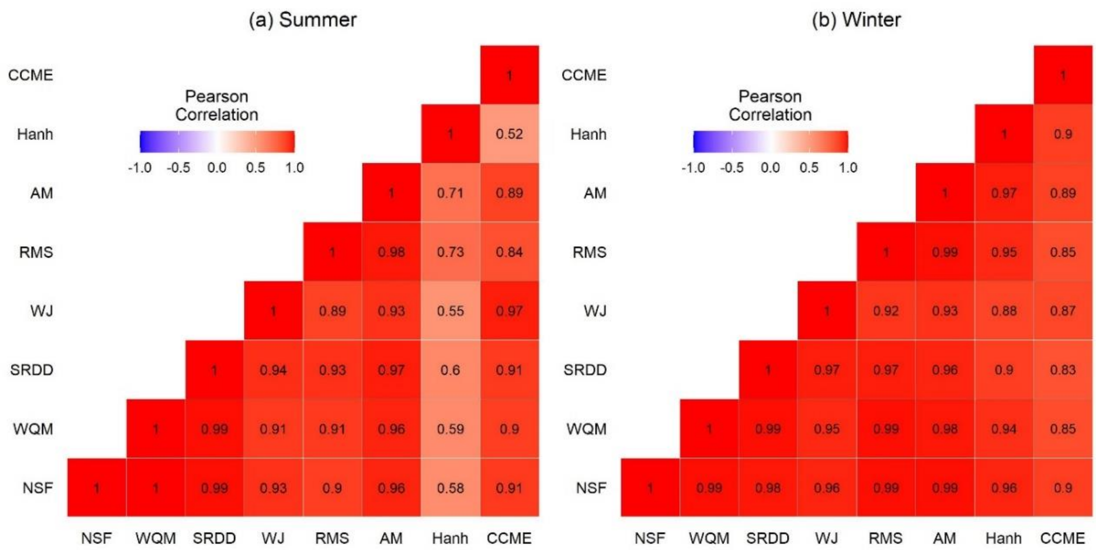


Figure 3.8. Correlation coefficients among WQI methodologies.

Another significant aspect of the aggregation functions is the relationship between them. To assess the similarity of model results, the Pearson correlation coefficient was calculated with R software using the ggcorplot package. The statistical significance level was set at 0.01. As shown in Figure 8, all WQI functions, with the exception of the CCME, were highly positively associated with one another for both seasons.

3.6.3 Spatio-temporal-variability of different WQI methods

Figure 3.9 presents the WQI scores computed at each monitoring location by the different aggregation functions. It can be seen that the WQI scores varied significantly across the monitoring locations in Cork Harbour. During both seasons, higher WQI values were found in the lower and outer Harbour for all functions. Comparatively, lower values were found in the upper monitoring stations of Harbour over the study period. For all of the WQI functions, there was a significant temporal variation between seasons. The results of the WQI models show that the water quality in the Harbour degrades significantly during the winter at all monitoring sites.

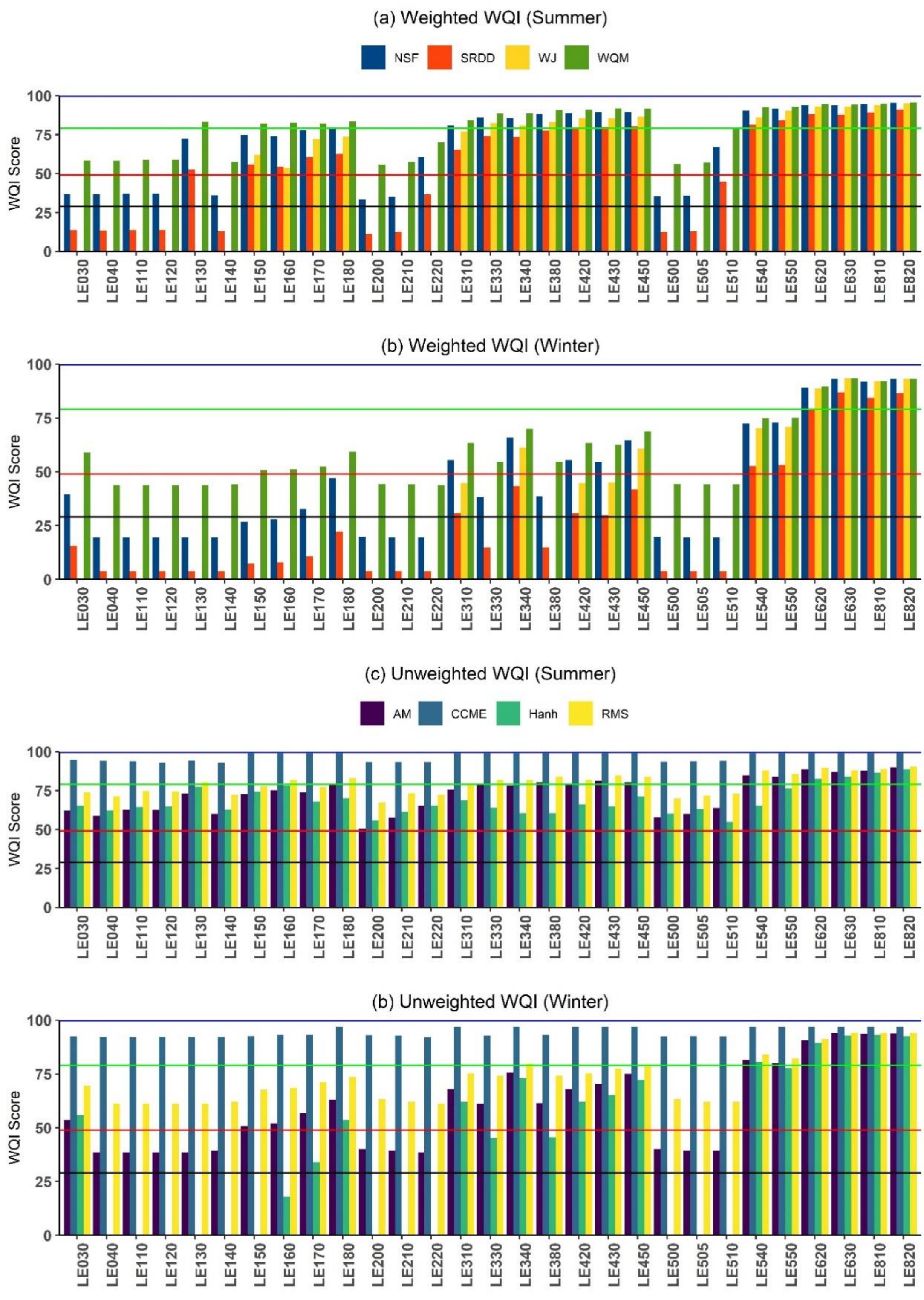


Figure 3.9. Monitoring location based WQI results of different WQI models in Cork Harbour: The black solid line represents the poor class; the red solid line indicates the maximum range of the potentially poor class; the green solid line refers to Fair water. The purple solid line denotes the good status of water quality.

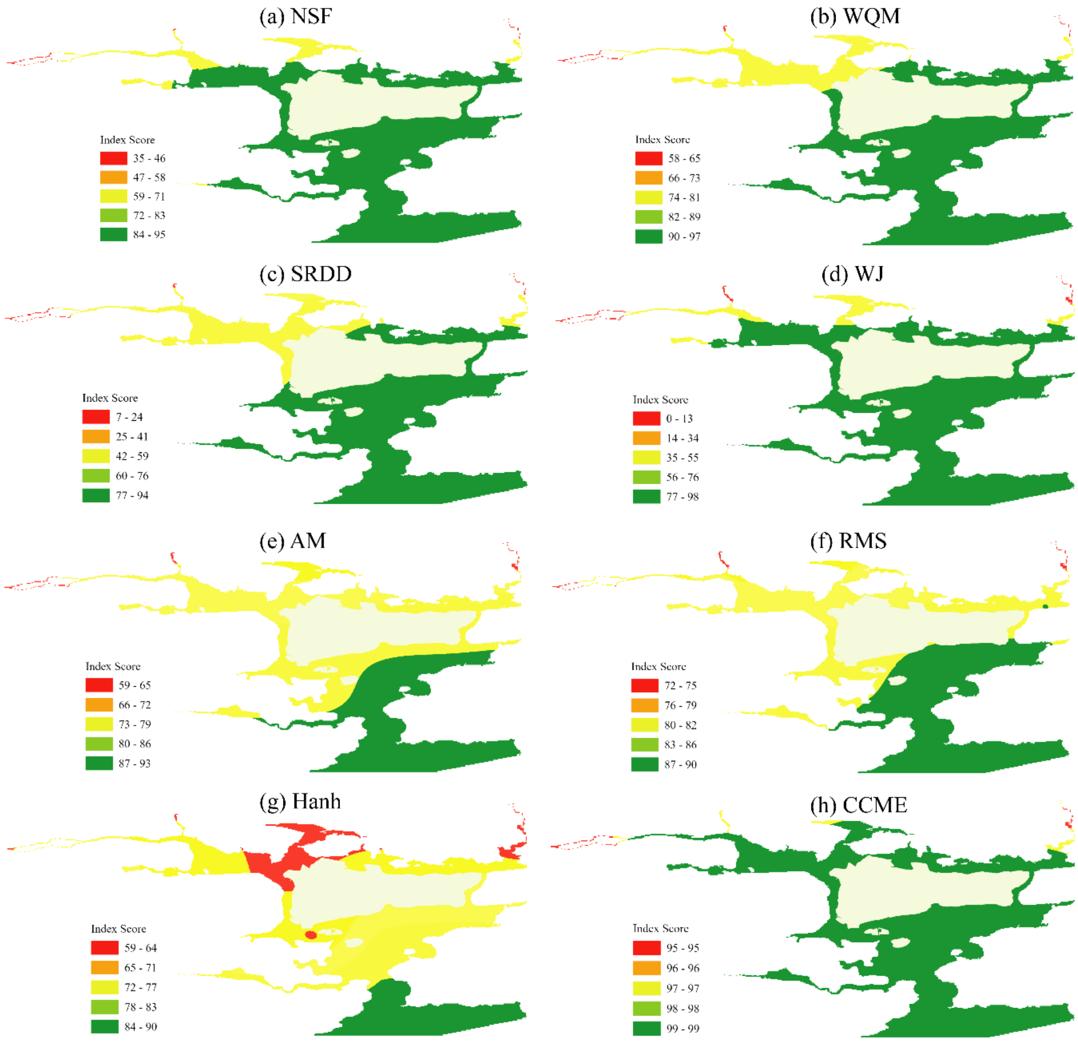


Figure 3.10. Spatial distribution of simulated WQI scores in Cork Harbour for different WQI models during summer.

The advanced geo-statistical Empirical Bayesian Kriging (EBK) technique was utilized to spatially interpolate calculated WQI scores at the monitoring stations onto the whole domain of Cork Harbour (ESRI, 2016). A detailed description of the procedure can be found in Uddin et al., 2020. Figures 3.10 and 3.11 show the spatial and temporal variations of WQI scores in Cork Harbour throughout the summer and winter seasons, respectively. Relatively, all of the functions computed higher WQI scores in the outer Habour, while lower index scores were obtained in the upper Habour. According to recent studies, the upper harbour has received significant pollutant loads from a variety of sources over the years, including farmlands, WWTPs, industries, etc. (EPA, 2018; Hartnett and Nash, 2015).

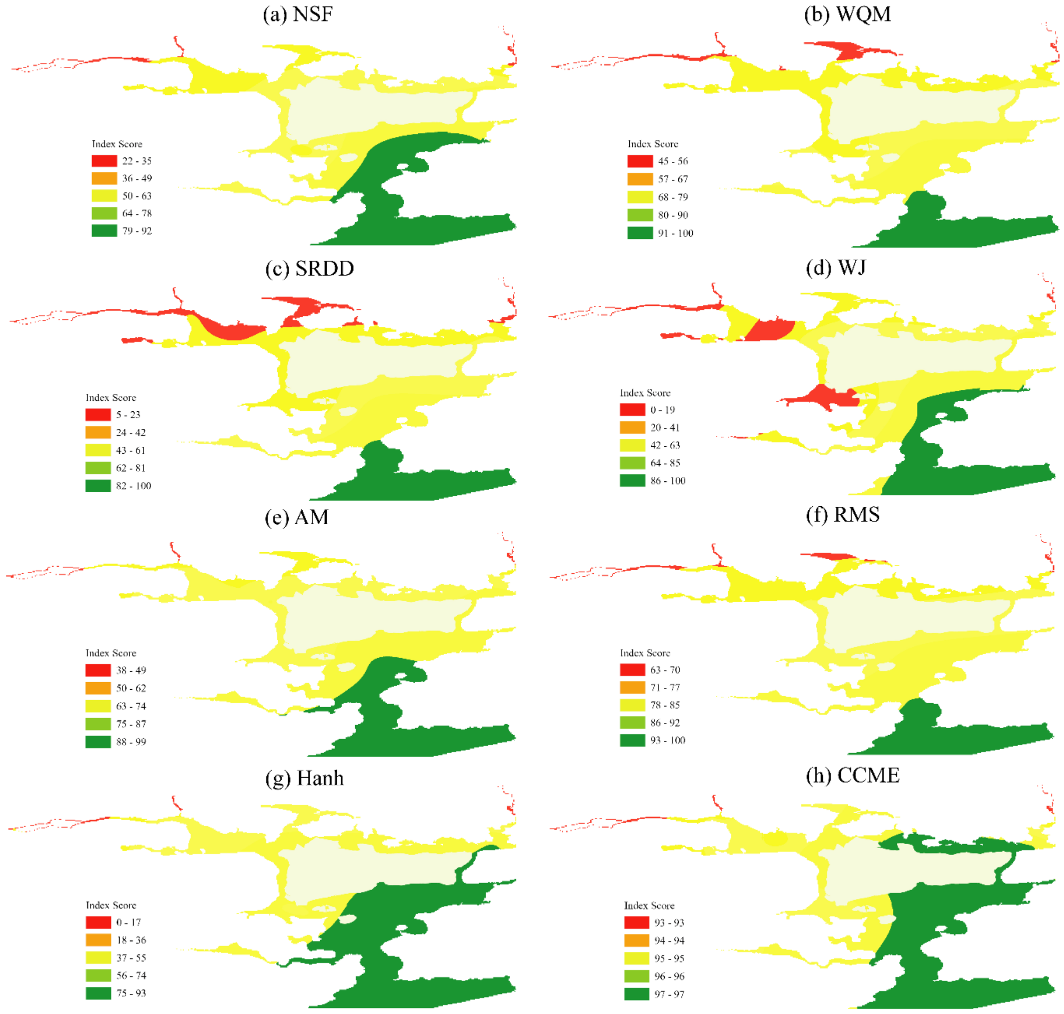


Figure 3.11. Spatial distribution of simulated WQI scores in Cork Harbour for different WQI models during winter.

There was a greater difference in spatial variation between the weighted and unweighted techniques over the study periods. Figure 3.12 shows the spatial variation in the standard deviations of the indices computed by the different WQI models. During both seasons, the WQI scores predicted by the different models at monitoring stations in the upper Harbour varied significantly more than those predicted by the different models in the lower and outer areas of the Harbour.

When comparing the weighted and unweighted models, the unweighted method had the lowest deviation during the summer season, while the weighted methods had the highest during the winter season. The results show that the spatial distribution of water quality factors can have a significant impact on the WQI model because a higher density of diverse water quality was observed in the present study in the upper Harbour.

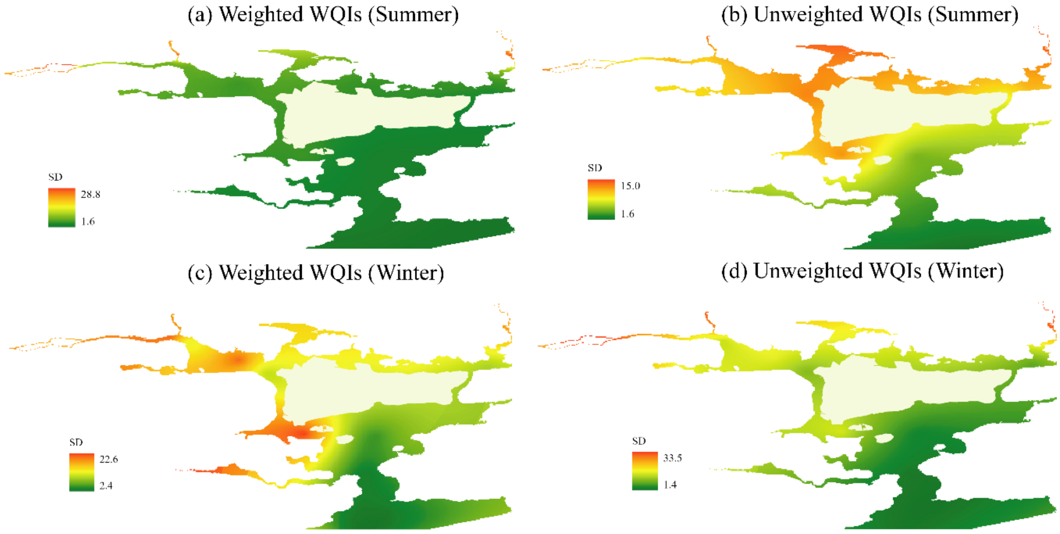


Figure 3.12. Standard deviations (SD) of WQI models in Cork Harbour.

3.6.4 Comparative analysis of WQI model performance

MLR analysis was used to predict WQI scores in order to compare model performance. All statistical analyses were conducted at a significance level of 0.05. R^2, RMSE, MSE, and MAE were used to evaluate the performance of the MLR models versus the WQI functions. The R^2 for the regression analysis of WQI scores are shown in Figures 3.13 – 3.16 for the weighted (summer and winter) and unweighted (summer and winter) aggregation models.

Looking at the weighted models, a significant difference was found between seasons over the models. Similarly high levels of agreement ($R^2 > 0.9$) were observed for all unweighted functions for the summer while poorer agreements were observed in winter for the NSF, WJ and particularly the SRDD models. The WQM model showed highest levels of agreement with 91% and 97% of prediction variance in summer and winter, respectively.

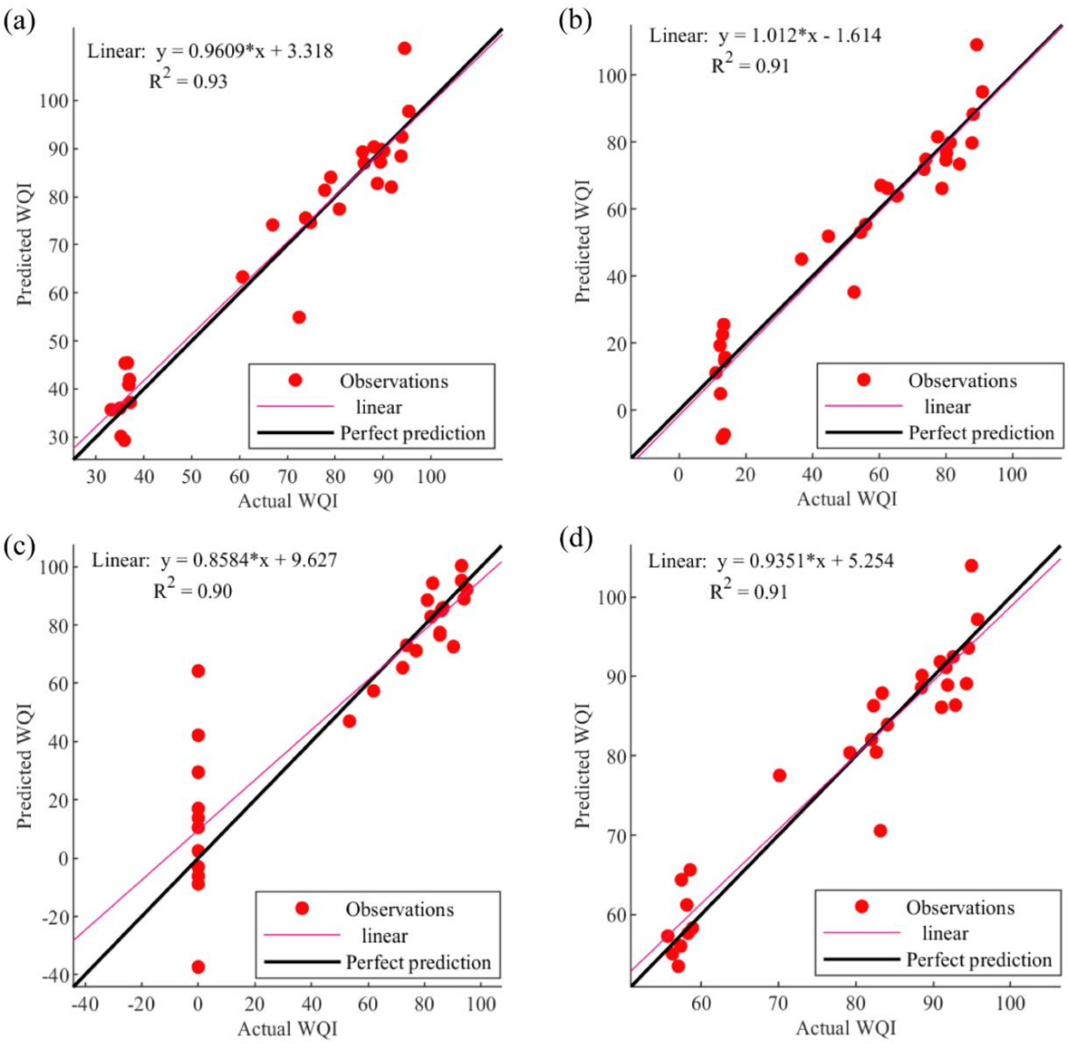


Figure 3.13. Comparison between predicted and actual WQI scores based on the testing dataset of different weighted WQI models in Cork Harbour during summer: (a) NSF, (b) SRDD, (c) West Java, (d) WQM.

In contrast, there is a significant variation in R^2 values for the unweighted prediction models during both seasons. A higher proportion of variance, 92% and 97% respectively for summer and winter, is explained by the AM model than any other unweighted model. There were also high levels of correlation for the RMS model; 89% and 79% of the variance was explained for summer and winter. respectively. Poor correlations were found for the CCME model with just 72% and 70% of variance explained in summer and winter, respectively.

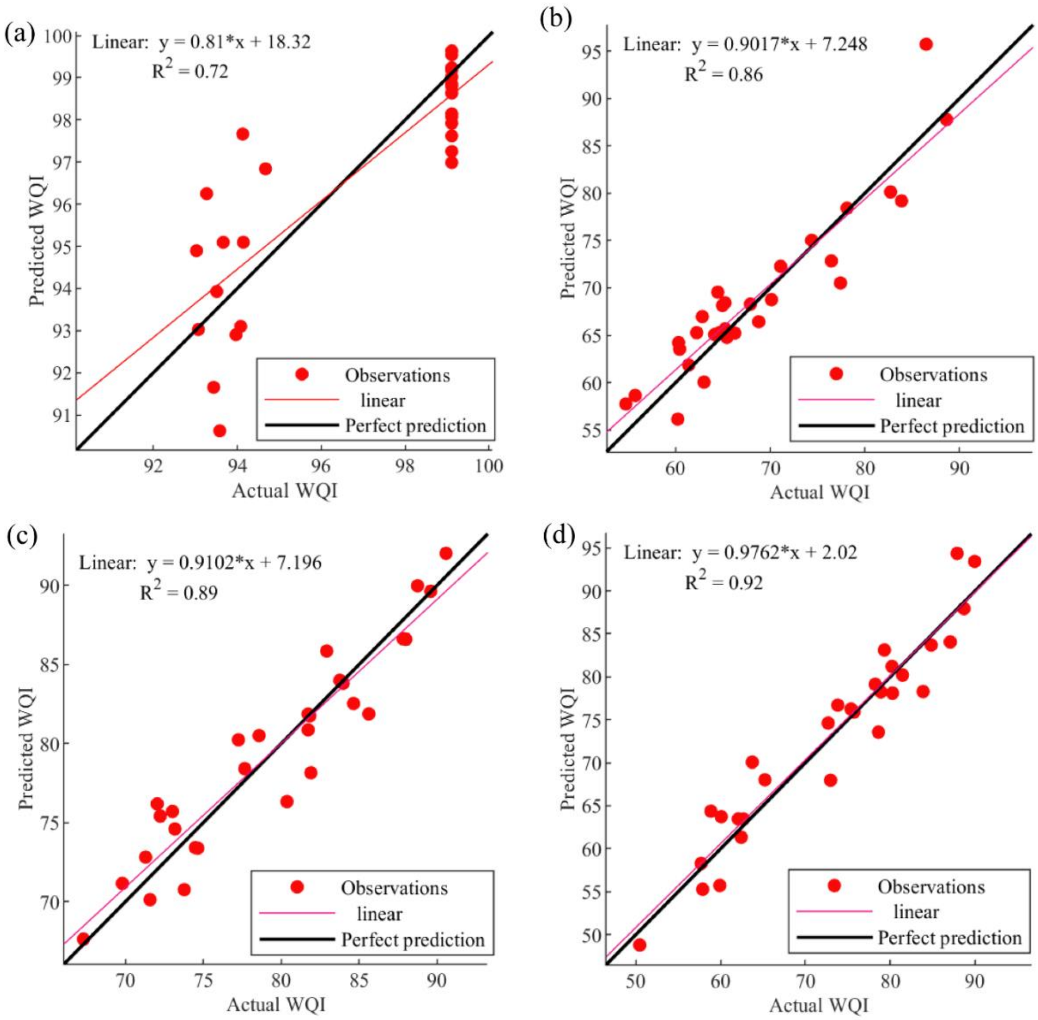


Figure 3.14. Comparison between predicted and actual WQI scores based on the testing dataset of different unweighted WQI models in Cork Harbour during summer: (a) CCME, (b) Hanh, (c) RMS and (d) AM.

RMSE, MAE and MSE statistical metrics for the MLR models are shown in Figure 3.17. Smaller values (close to zero) of the metrics indicate better performance of the MLR model. As shown in Figure 3.17, during both seasons RMSE, MAE, and MSE are lowest for the weighted WQM models while the highest prediction errors was calculated for the SRDD and WJ models respectively. In contrast, the unweighted Hanh model exhibits the highest errors during both seasons. The Hanh model performance varied significantly between seasons; the highest RMSE, MAE and MSE were found during the winter season, whereas the lowest during the summer season. The results of the performance metrics reveal that of the weighted models, the WQM-WQI model exhibits excellent performance and the best fit for the predicted WQI scores. Overall, the AM and CCME models had the lowest model error for both seasons.

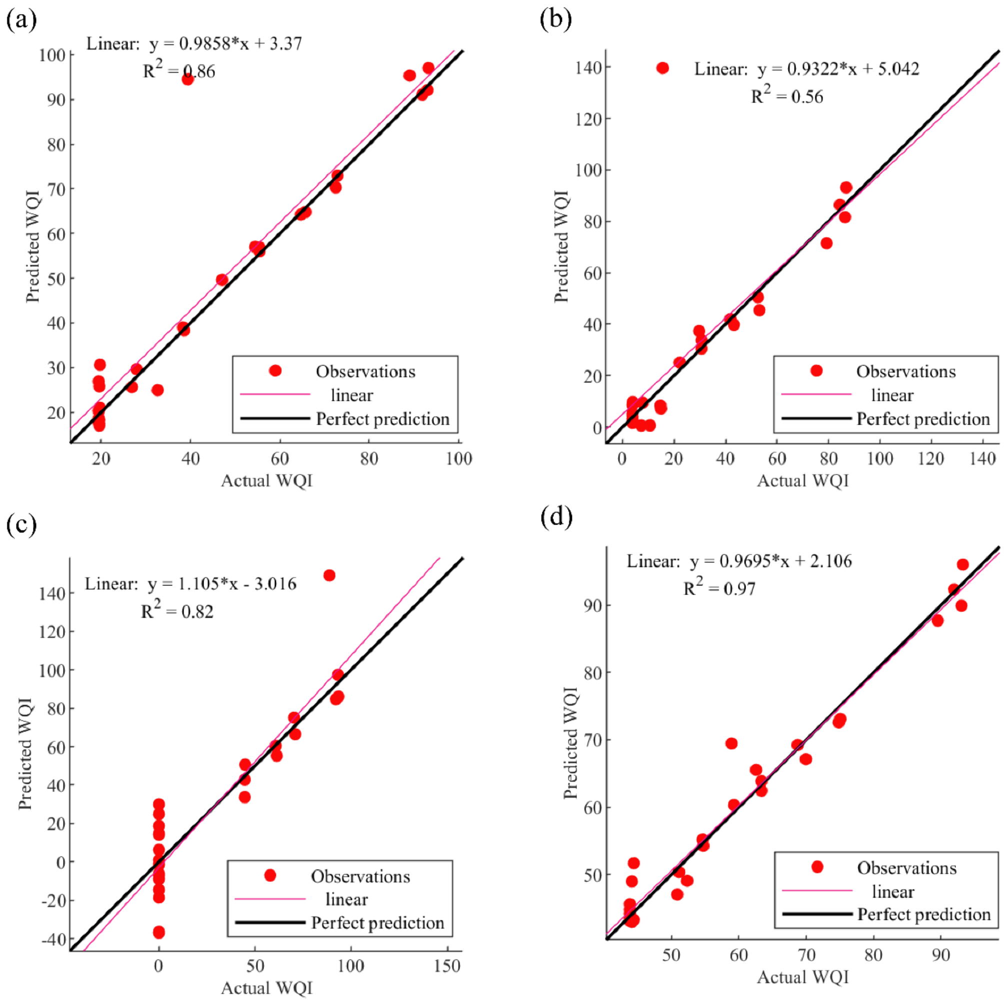


Figure 3.15. Comparison between predicted and actual WQI scores based on the testing dataset of different weighted WQI models in Cork Harbour over the winter: (a) NSF, (b) SRDD, (c) West Java, (d) WQM.

Ranking the models in terms of sensitivity, it was found that the WQM aggregation function was more sensitive than other aggregation functions. This approach also had less error than other weighted methods based on the MLR model performance metrics. The methodology has a distinct advantage, in terms of eclipsing and ambiguity problems over the other methodologies. The NSF function, while being less sensitive than the WQM, showed better sensitivity than the WJ and the SRDD models. Looking at the unweighted functions, the pooret sensitivity was found for the CCME and Hanh functions in the summer and winter seasons, respectively, whereas the AM showed high sensitivity during both seasons.

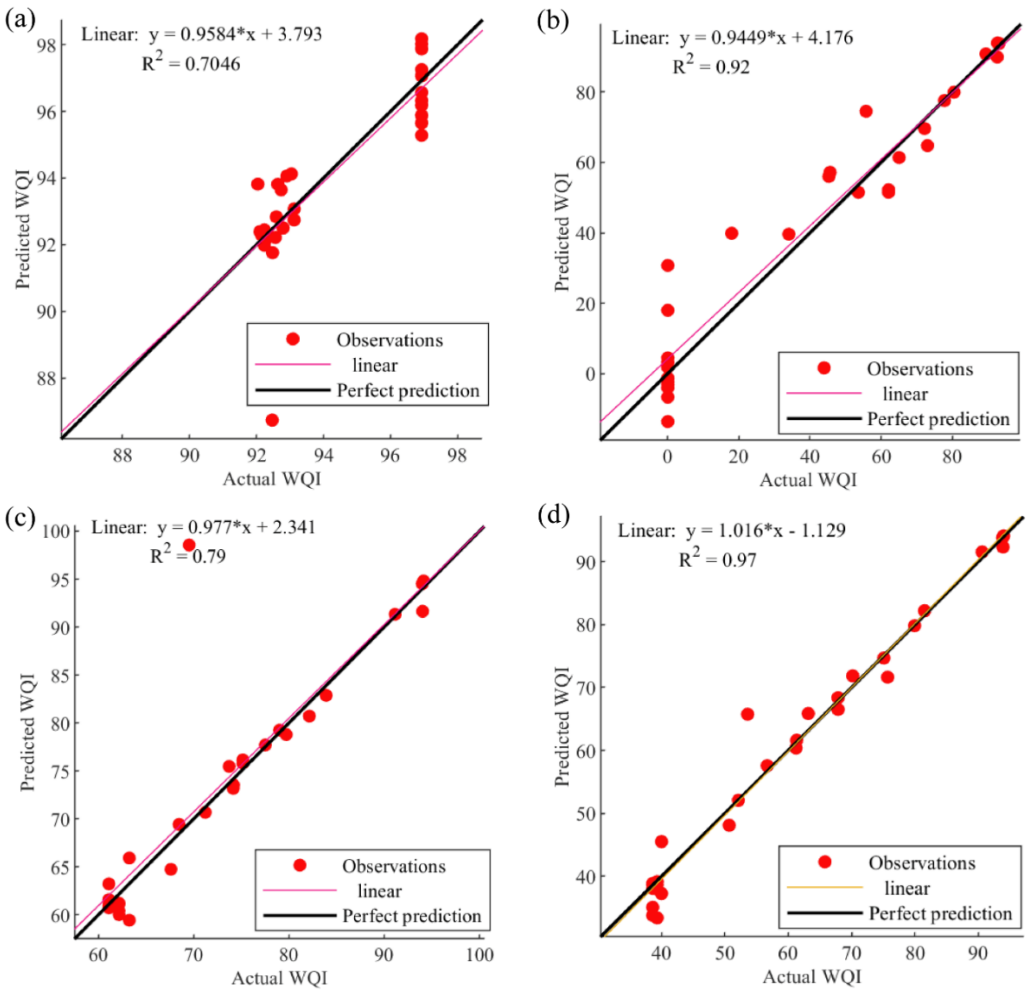


Figure 3.16. Comparison between predicted and actual WQI scores based on the testing dataset of different unweighted WQI models in Cork Harbour over the winter season: (a) CCME, (b) Hanh, (c) RMS and (d) AM.

Model performances were ranked (see Table 3.12) taking on the R^2 values from Figures 3.13-3.16 (above) as a measure of model sensitivity and the RMSE values from Figure 3.17 as a measure of prediction error. Taking the weighted models as an example, models were first scored from 1-4 separately for each metric with 1 indicating best performance and 4 worst. These scores were then added, giving each metric equal weighting, and the models ranked based on the cumulative scores. For the weighted models, Table 3.12 shows that the WQM model was ranked first for both seasons. For the unweighted models, the AM model was ranked first for both seasons.

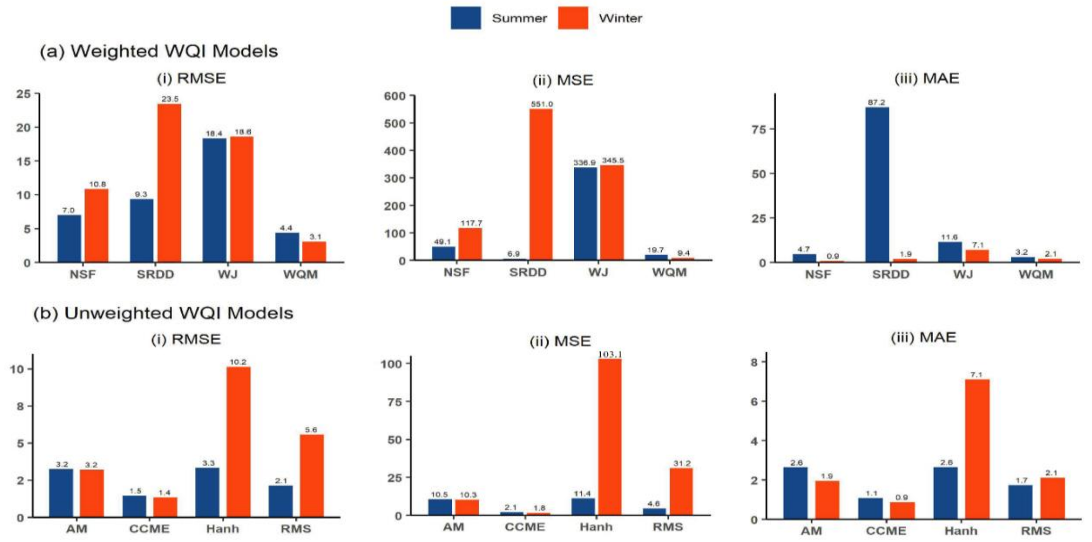


Figure 3.17. Model performance comparison of the eight WQI models using different statistical measures metrics.

Table 3.12. Ranking of WQI model performance based on sensitivity (R^2) and prediction error (RMSE). S = summer, W = winter.

WQI models	R^2 Score		RMSE Score		R^2 Score		RMSE Score		Total Score		Rank	
	S	W	S	W	S	W	S	W	S	W	S	W
Weighted												
WQM	91	97	4.4	3.1	2	1	1	1	3	2	1	1
NSF	93	86	7.0	10.8	1	2	2	2	3	4	1	2
SRDD	91	56	9.3	23.5	2	4	3	4	5	8	3	4
WJ	90	82	18.4	18.6	4	3	4	3	8	6	4	3
Unweighted												
AM	92	97	3.2	3.2	1	1	3	2	4	3	1	1
RMS	89	79	2.1	5.6	2	3	2	3	4	6	1	3
Hanh	86	92	3.3	10.2	3	2	4	4	7	6	4	3
CCME	72	70	1.5	1.4	4	4	1	1	5	5	3	2

3.7 Comparison of water quality statuses

The ultimate goal of the WQI model is to assess water quality and determine its status. For the purpose of coastal water quality assessment, the results presented thus-far suggest that the weighted WQM and unweighted AM approaches are the most appropriate techniques for calculating WQI scores as they suffered least from eclipsing and ambiguity difficulties. Figure 3.18 shows the computed water quality status at 29 monitoring stations in Cork Harbour for the WQM and the AM methods. Table 3.13 provides the percentage of stations attributed particular statuses by the two methods.

Table 3.13 Assessment of monitoring sites water quality in Cork Harbour using WQM and AM methods.

WQI methods	water quality classifications							
	summer				winter			
	Good	Fair	Marginal	Poor	Good	Fair	Marginal	Poor
WQM	28% (8)	72% (21)	0	0	14% (4)	48% (14)	38% (11)	0
AM	31% (9)	69% (20)	0	0	17% (5)	45% (13)	38% (11)	0

Total number of monitoring sites 29 used in this assessment.

In summer, the WQM method classified 72% of stations as ‘fair’ and 28% ‘good’ while the AM method classified 69% as ‘fair’ and 31% ‘good’. From Figure 3.18 (a) and (b), it can be seen that ‘fair’ water quality was found in the upper part of the Harbour (River Lee, Glashaboy River and River Owenacurra) for both methods in the area that is most strongly affected by urban pressures (EPA, 2017).

During the winter period, the WQM method classified 38% of stations as ‘potentially poor’, 48% as ‘fair’ and 14% as ‘good’, whereas the AM method classified 38% of stations as ‘potentially poor’, 45% as ‘fair’ and 17% ‘good’. As seen in Figure 3.18 (c) and (d), the poorest water quality was assessed in the upper Harbour by both methods while the best water quality was found in the lower and outer Harbour. However, the qualitative assessment of WQI models showed a significant spatial variation of water quality classes in Cork Harbour. This could be due to the combined impacts of various edaphic and non-edaphic activities on Harbour water (Xia et al., 2015). A number of factors can contribute to poor water quality, including industrial effluents, home waste, and agricultural activities (farming, fishing, etc.) in the upper Harbour.

In this study, all WQI methods used the same indicators and SI values to calculate WQI. The results of the study show that there are considerable differences in WQI model outcomes for similar water quality inputs. The differences are therefore entirely due to the different aggregation functions and use of weighted versus unweighted aggregation functions.

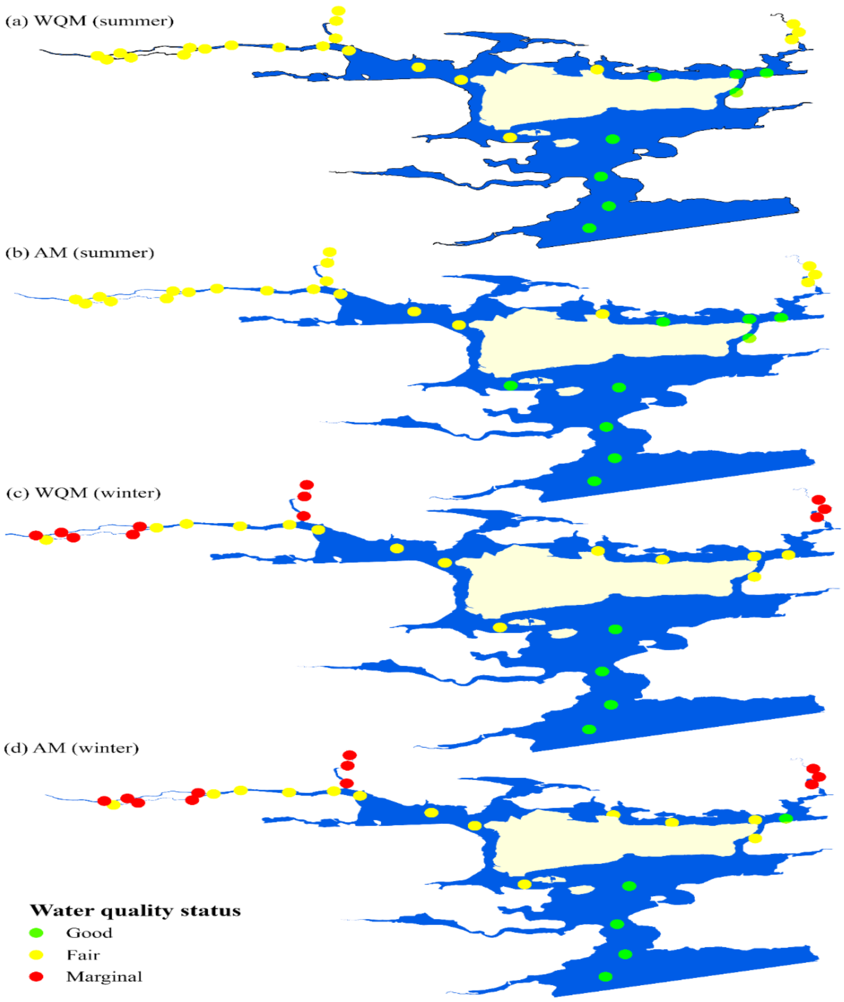


Figure 3.18. States of water quality in Cork Harbour.

3.8 Conclusion

The main aim of this study was to develop an improved WQI methodology for assessment of coastal water quality. This was achieved by using the XGBoost machine learning algorithm to identify water quality indicators for inclusion in a WQI model, using the XGBoost rankings the rank order centroid weighting method to attribute sub-index weightings and testing a large number of aggregation functions to determine their input on model performance. The key conclusions from the research are as follows:

- XGBoost can be used to objectively rank water quality indicators based on their significance in terms of water quality. Although XGBoost was shown to work well here, it requires further investigation using longer term datasets. Its's use requires both input (i.e. indicator data) and some desired output which, here, was an initial water quality status determined using binary analysis of the indicator data. However, the XGBoost ranking is sensitive to the desired output and it should therefore be carefully chosen.

- The rank order centroid weighting method is a useful means of objectively weighting the indicators in a WQI model but it must be used in conjunction with some ranking method such as the XGBoost method. Use of objective, mathematical approaches like these have the potential to reduce model uncertainty that might be introduced by the use of rankings/weightings based on expert opinion which can obviously vary between expert.
- The assessment of aggregation functions found that a weighted quadratic mean aggregation function and an unweighted arithmetic mean function resulted in the lowest instances of eclipsing and ambiguity and are therefore recommended for WQI approaches. However, the present study only used one year of monitoring data and their performance in mutli-year analyses should be further investigated.

In this research, the proposed methodology with two new identical aggregation methods should be recommended for assessing coastal water quality using the WQI model. Because, they not only could reduce the eclipsing and ambiguity problems, but also could provide accurate information on water quality to water managers. Therefore, further studies should be required on the measurement of uncertainty of this approach for the assessment of coastal water quality efficiently. This could help to improve the efficiency of the methodology.

3.9 Declaration of competing interest

The authors state that they have no known competing financial interests or personal relationships that the work reported in this paper could have seemed to influence.

3.10 Acknowledgement

This research was funded by the Hardiman Research Scholarship of the National University of Ireland Galway, which funded the first author as part of his PhD program. The authors would like to thank the Environmental Protection Agency of Ireland for providing water quality data. MaREI, the SFI Research Centre for Energy, Climate, and Marine and Ryan Institute, NUIG, Galway, Ireland, also supported the research. The authors also sincerely acknowledge Charles Sturt University for

providing all necessary supports to this PhD project through the international co-supervision.

3.11 References

Abbasi, T., Abbasi, S., 2012. Water Quality Indices, Water Quality Indices. https://doi.org/10.1016/C2010-0-69472-7

Azhar, M.A., Thomas, P.A., 2019. Comparative Review of Feature Selection and Classification modeling. 2019 6th IEEE Int. Conf. Adv. Comput. Commun. Control. ICAC3 2019. https://doi.org/10.1109/ICAC347590.2019.9036816

Bordalo, A.A., Teixeira, R., Wiebe, W.J., 2006. A water quality index applied to an international shared river basin: The case of the Douro River. Environ. Manage. 38, 910–920. https://doi.org/10.1007/s00267-004-0037-6

Carvalho, L., Cortes, R., Bordalo, A.A., 2011. Evaluation of the ecological status of an impaired watershed by using a multi-index approach. Environ. Monit. Assess. 174, 493–508. https://doi.org/10.1007/s10661-010-1473-9

Chen, K., Chen, H., Zhou, C., Huang, Y., Qi, X., Shen, R., Liu, F., Zuo, M., Zou, X., Wang, J., Zhang, Y., Chen, D., Chen, X., Deng, Y., Ren, H., 2020. Comparative analysis of surface water quality prediction performance and identification of key water parameters using different machine learning models based on big data. Water Res. 171, 115454. https://doi.org/10.1016/j.watres.2019.115454

Das, A.K., Das, S., Ghosh, A., 2017. Ensemble feature selection using bi-objective genetic algorithm. Knowledge-Based Syst. 123, 116–127. https://doi.org/10.1016/j.knosys.2017.02.013

Dinius, S.H., 1987. Design of an Index of Water Quality. JAWRA J. Am. Water Resour. Assoc. 23, 833–843. https://doi.org/10.1111/j.1752-1688.1987.tb02959.x

EPA, 2018. Lee-Cork Harbour Catchment Assessment 2015.

EPA, 2017. Urban Waste Water Treatment, Official Journal of the European Union.

EPA, 2016. Urban Waste Water Treatment in 2015.

EPA, 2021. Ireland’s National Water Framework Directive Monitoring Programme 2019-2021.

Ewaid, S.H., Abed, S.A., Kadhum, S.A., 2018. Predicting the Tigris River water quality within Baghdad, Iraq by using water quality index and regression analysis. Environ. Technol. Innov. 11, 390–398. https://doi.org/10.1016/j.eti.2018.06.013

Feng, T., Wang, C., Hou, J., Wang, P., Liu, Y., Dai, Q., Yang, Y., You, G., 2018. Effect of inter-basin water transfer on water quality in an urban lake: A combined water quality index algorithm and biophysical modelling approach. Ecol. Indic. 92, 61–71. https://doi.org/10.1016/j.ecolind.2017.06.044

Gupta, A.K., Gupta, S.K., Patil, R.S., 2003. A comparison of water quality indices for coastal water. J. Environ. Sci. Heal. - Part A Toxic/Hazardous Subst. Environ. Eng. 38, 2711–2725. https://doi.org/10.1081/ESE-120024458

Gupta, S., Gupta, S.K., 2021. A critical review on water quality index tool: Genesis, evolution and future directions. Ecol. Inform. 63, 101299. https://doi.org/10.1016/j.ecoinf.2021.101299

Hartnett, M., Nash, S., 2015. An integrated measurement and modeling methodology for estuarine water quality management. Water Sci. Eng. 8, 9–19. https://doi.org/10.1016/j.wse.2014.10.001

Hastie, T. et. all., 2009. The Elements of Statistical Learning. Math. Intell. 27, 83–85.

Huan, J., Li, H., Li, M., Chen, B., 2020. Prediction of dissolved oxygen in aquaculture based on gradient boosting decision tree and long short-term memory network: A study of Chang Zhou fishery demonstration base, China. Comput. Electron. Agric. 175, 105530. https://doi.org/10.1016/j.compag.2020.105530

Hurley, T., Sadiq, R., Mazumder, A., 2012. Adaptation and evaluation of the Canadian Council of Ministers of the Environment Water Quality Index (CCME WQI) for use as an effective tool to characterize drinking source water quality. Water Res. 46, 3544–3552. https://doi.org/10.1016/j.watres.2012.03.061

Javed, S., Ali, A., Ullah, S., 2017. Spatial assessment of water quality parameters in Jhelum city (Pakistan). Environ. Monit. Assess. 189. https://doi.org/10.1007/s10661-017-5822-9

Jović, A., Brkić, K., Bogunović, N., 2015. A review of feature selection methods with applications. 2015 38th Int. Conv. Inf. Commun. Technol. Electron. Microelectron. MIPRO 2015 - Proc. 1200–1205. https://doi.org/10.1109/MIPRO.2015.7160458

Juwana, I., Muttil, N., Perera, B.J.C., 2016. Uncertainty and sensitivity analysis of West Java Water Sustainability Index - A case study on Citarum catchment in Indonesia. Ecol. Indic. 61, 170–178. https://doi.org/10.1016/j.ecolind.2015.08.034

Li, X., Ding, J., Ilyas, N., 2020. Machine learning method for quick identification of water quality index (WQI) based on Sentinel-2 MSI data: Ebinur lake case study. Water Supply 1–22. https://doi.org/10.2166/ws.2020.381

Lumb, Ashok, Sharma, T.C., Bibeault, J.-F., 2011. A Review of Genesis and Evolution of Water Quality Index (WQI) and Some Future Directions. Water Qual. Expo. Heal. https://doi.org/10.1007/s12403-011-0040-0

Lumb, A., Sharma, T.C., Bibeault, J.-F., Klawunn, P., 2011. A Comparative Study of USA and Canadian Water Quality Index Models. Water Qual. Expo. Heal. 3, 203–216. https://doi.org/10.1007/s12403-011-0056-5

Malohlava, M., Candel, A., Bartz, A., Roark, H., Parmar, V., Click, C., Malohlava, M., Candel, A., Roark, H., Parmar, V., Bartz, A., Roark, H., Parmar, V., 2017. Gradient Boosting Machine with H2O. Https://Www.H2O.Ai/Resources/ 30.

Mladenović-Ranisavljević, I.I., Žerajić, S.A., 2018. Comparison of different models of water quality index in the assessment of surface water quality. Int. J. Environ. Sci. Technol. 15, 665–674. https://doi.org/10.1007/s13762-017-1426-8

Momenzadeh, M., Sehhati, M., Rabbani, H., 2019. A novel feature selection method for microarray data classification based on hidden Markov model. J. Biomed. Inform. 95, 103213. https://doi.org/10.1016/j.jbi.2019.103213

Muttil, N., Chau, K.W., 2007. Machine-learning paradigms for selecting ecologically significant input variables. Eng. Appl. Artif. Intell. 20, 735–744. https://doi.org/10.1016/j.engappai.2006.11.016

Naghibi, S.A., Hashemi, H., Berndtsson, R., Lee, S., 2020. Application of extreme gradient boosting and parallel random forest algorithms for assessing groundwater spring potential using DEM-derived factors. J. Hydrol. 589, 125197. https://doi.org/10.1016/j.jhydrol.2020.125197

Nives, Š.-G., 1999. Water quality evaluation by index in Dalmatia. Water Res. 33, 3423–3440. https://doi.org/10.1016/s0043-1354(99)00063-9

Nong, X., Shao, D., Zhong, H., Liang, J., 2020. Evaluation of water quality in the South-to-North Water Diversion Project of China using the water quality index (WQI) method. Water Res. 178. https://doi.org/10.1016/j.watres.2020.115781

Ogutu, J.O., Piepho, H.P., Schulz-Streeck, T., 2011. A comparison of random forests, boosting and support vector machines for genomic selection. BMC Proc. 5, 3–7. https://doi.org/10.1186/1753-6561-5-S3-S11

Pham, T.M.H., Sthiannopkao, S., Ba, D.T., Kim, K.W., 2011. Development of Water Quality Indexes to Identify Pollutants in Vietnam's Surface Water. J. Environ. Eng. https://doi.org/10.1061/(ASCE)EE.1943-7870.0000314.

Saffran, K., Cash, K., Hallard, K., 2001. CCME Water Quality Index 1.0 User's Manual. Can. Water Qual. Guidel. Prot. Aquat. Life 1–5.

Said, A., Stevens, D.K., Sehlke, G., 2004. An innovative index for evaluating water quality in streams. Environ. Manage. https://doi.org/10.1007/s00267-004-0210-y

Smith, D.G., 1990. A better water quality indexing system for rivers and streams. Water Res. 24, 1237–1244. https://doi.org/10.1016/0043-1354(90)90047-A

Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2018. Development of a water quality index for rivers in West Java Province, Indonesia. Ecol. Indic. 85, 966–982. https://doi.org/10.1016/j.ecolind.2017.11.049

Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2016. Development of river water quality indices—a review. Environ. Monit. Assess. https://doi.org/10.1007/s10661-015-5050-0

Tanha, J., Abdi, Y., Samadi, N., Razzaghi, N., Asadpour, M., 2020. Boosting methods for multi-class imbalanced data classification: an experimental review. J. Big Data 7. https://doi.org/10.1186/s40537-020-00349-y

Toner, P., Bowman, J., Clabby, K., Lucey, J., Mc, McGarrigle, M., Concannon, C., Clenaghan, C., Cunningham, P., J., D., O'Boyle, S., MacCárthaigh, M., Craig, M., Quinn, R., 2005. Water Quality in Ireland 2001-2003.

Touzani, S., Granderson, J., Fernandes, S., 2018. Gradient boosting machine for modeling the energy consumption of commercial buildings. Energy Build. 158, 1533–1543. https://doi.org/10.1016/j.enbuild.2017.11.039

Uddin, G., Nash, S., Olbert, A.I., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol. Indic. 122, 107218. https://doi.org/10.1016/j.ecolind.2020.107218

Uddin, M.G., Moniruzzaman, M., Quader, M.A., Hasan, M.A., 2018. Spatial variability in the distribution of trace metals in groundwater around the Rooppur nuclear power plant in Ishwardi, Bangladesh. Groundw. Sustain. Dev. 7. https://doi.org/10.1016/j.gsd.2018.06.002

Uddin, M.G., Nash, S., Olbert, A.I., Rahman, A., 2022. Development of a water quality index model - a comparative analysis of various weighting methods, in: Çiner, P.D.A. (Ed.), Mediterranean Geosciences Union Annual Meeting (MedGU-21). Istanbul, pp. 1–6.

Uddin, M.G., Stephen Nash, Olbert, A.I., 2020. Application of Water Quality Index Models to an Irish Estuary, in: Kieran Runae, V.J. (Ed.), Civil and Environmental Research. Civil and Environmental Research, Cork, Ireland, pp. 576–581.

Wang, X., Zhang, F., Ding, J., 2017. Evaluation of water quality based on a machine learning algorithm and water quality index for the Ebinur Lake Watershed, China. Sci. Rep. 7. https://doi.org/10.1038/s41598-017-12853-y

Wu, Z., Lai, X., Li, K., 2021. Water quality assessment of rivers in Lake Chaohu Basin (China) using water quality index. Ecol. Indic. 121. https://doi.org/10.1016/j.ecolind.2020.107021

Xia, X.H., Wu, Q., Mou, X.L., Lai, Y.J., 2015. Potential impacts of climate change on the water quality of different water bodies. J. Environ. Informatics 25, 85–98. https://doi.org/10.3808/jei.201400263

Zardari, N. ul H., Cordery, I., Sharma, A., 2010. An objective multiattribute analysis approach for allocation of scarce irrigation water resources. J. Am. Water Resour. Assoc. https://doi.org/10.1111/j.1752-1688.2009.00410.x

Zotou, I., Tsihrintzis, V.A., Gikas, G.D., 2019. Performance of Seven Water Quality Indices (WQIs) in a Mediterranean River. Environ. Monit. Assess. 191. https://doi.org/10.1007/s10661-019-7652-4

Zotou, I., Tsihrintzis, V.A., Gikas, G.D., 2018. Comparative Assessment of Various Water Quality Indices (WQIs) in Polyphytos Reservoir-Aliakmon River, Greece. Proceedings 2, 611. https://doi.org/10.3390/proceedings2110611

4. A novel approach for estimating and predicting uncertainty in water quality index model using machine learning approaches

This chapter was published in the Journal of **"Water Research"** on November 25, 2022. Details can be found at the following web resource: https://doi.org/10.1016/j.watres.2022.119422

4.1 Chapter highlights

- A novel approach was developed for quantifying uncertainty at each step of the WQI model.
- A comprehensive framework was provided on how to implement the developed approach.
- A range of statistical tools and techniques are used for estimating model uncertainty at each step and are then validated and predicted using state-of-the-art machine learning techniques.
- That was the first attempt to estimate model uncertainty at each stage of a WQI model using systematic framework.
- For the estimation of model uncertainty, eight WQI models were analyzed and compared to determine the best aggregation function(s) in terms of the model uncertainty.
- The indicator selection process contributed less than 1% of the uncertainty.
- The quantity of input indicators was found to have a significant impact on the model's input uncertainties.
- A significant amount of model uncertainty, around 13%, was associated with the sub-index functions; these could affect the model's reliability.
- The weighting component produces relatively low levels of uncertainty; it was less than 1%.
- The WQM and RMS models provided excellent performance in terms of reducing model uncertainty, those models contributed less than 2% uncertainty to the final assessment of water quality, whereas the widely used WQI models like SRDD, WJ, etc. produced more than 13% uncertainty.

- Prediction results also indicated that both weighted WQM and unweighted RMS models could be effective and reliable in order to reduce model uncertainty significantly.

4.2 Abstract

With the significant increase in WQI applications worldwide and lack of specific application guidelines, accuracy and reliability of WQI models is a major issue. It has been reported that WQI models produce significant uncertainties during the various stages of their application including: (i) water quality indicator selection, (ii) sub-index (SI) calculation, (iii) water quality indicator weighting and (iv) aggregation of sub-indices to calculate the overall index. This research provides a robust statistically sound methodology for assessment of WQI model uncertainties. Eight WQI models are considered. The Monte Carlo simulation (MCS) technique was applied to estimate model uncertainty, while the Gaussian Process Regression (GPR) algorithm was utilised to predict uncertainties in the WQI models at each sampling site. The sub-index functions were found to contribute to considerable uncertainty and hence affect the model reliability – they contributed 12.86% and 10.27% of uncertainty for summer and winter applications, respectively. Therefore, the selection of sub-index function needs to be made with care. A low uncertainty of less than 1% was produced by the water quality indicator selection and weighting processes. Significant statistical differences were found between various aggregation functions. The weighted quadratic mean (WQM) function was found to provide a plausible assessment of water quality of coastal waters at reduced uncertainty levels. The findings of this study also suggest that the unweighted root means squared (RMS) aggregation function could be potentially also used for assessment of coastal water quality. Findings from this research could inform a range of stakeholders including decision-makers, researchers, and agencies responsible for water quality monitoring, assessment and management.

Keyword: Water Quality Index; Gaussian Processes Regression; Monte Carlo Simulation; Uncertainty; Cork Harbour

4.3 Introduction

Uncertainty quantification (UQ) is an essential step in any experimental or computational assessment, as it determines how trustworthy the measured or computed data are; this also applies to water quality assessment. The water quality index (WQI) model is a widely used tool for evaluating water quality (WQ). This simple yet powerful tool facilitates the transformation of large quantities of often-complex intercorrelated WQ data into a single numerical value (Uddin et al., 2017; 2022). Its popularity has grown steadily in recent years as a result of its simple architecture, ease of application and straightforward result interpretation. The WQI model is comprises of four components: (1) WQ indicators selection, (2) sub-index (SI) function for converting different units to a uniform scale, (3) parameter weight value generation based on their relative importance, and (4) aggregation function for combining all three components and converting them into a single value (Uddin et al., 2022). To date, over 20 WQI models have been developed by states or organizations worldwide (Uddin et al., 2021) . One common and major drawback of these models is the model uncertainty problem.

There have been many studies that compare various WQI models and assess their predicative abilities. These studies mainly discuss the model structure and the effect of aggregation function on WQI scores. A small number go further and try to quantify the uncertainty introduced by the various steps of a WQI model. It is argued that there are many sources of model uncertainties and they occur at various stages of WQI modelling process (Abbasi and Abbasi, 2012; Uddin et al., 2021a). Juwana et al. (2016) and Sutadian et al. (2017) found that the sub-index functions and weight generation methods may contribute to the generation of model uncertainty; however, Uddin et al. (2022b) implied that the weighting procedure does not have significant effects on model uncertainty. Although recent research concludes that the aggregation function contributes to uncertainty generation (Juwana et al., 2016; Sutadian et al., 2018), no quantification of uncertainties at this step has yet been performed.

As expected, the structure of aggregation function in the WQI model has also an effect on the uncertainty (Abbasi and Abbasi, 2012; Smith, 1990). Smith (1990) and Lumb et al. (2011) conducted a comparative study of different WQI models, and found a significant variation in a use of unique WQ indicators among different aggregation functions. Uddin et al., (2022a) compared the performance of eight aggregation functions and found a significant statistical difference in WQI scores produced by these functions.

Model uncertainty, and directly linked to it model sensitivity, are the most fundamental features and characteristics of a model. The uncertainty refers to the result of measurement that reflects a lack of exact knowledge of the value of the measurand (BIPM et al., 2020). In order to understand the model's accuracy and reliability, it is important to estimate the uncertainty (Sankaran and Sarkar, 2009). Four types of uncertainties are typically evaluated in the models: structural, functional, parameter and data uncertainty (Ng and Perera, 2001; Sankaran and Sarkar, 2009; Wu et al., 2006). Uncertainties in WQI models are often related to various components of a model and its processes. Nonetheless, it is unclear how much of the total uncertainty is attributed to each component of the WQI model. Moreover, to the best of our knowledge, there is no specific framework for the estimation of the overall propagation of uncertainties in a WQI model.

In this context, the purpose of this study is to understand the generation of uncertainties along the cascade of WQI model processes, and accurately quantify how much uncertainty is conveyed by each component of the model. For the first time in this study, the individual and combined effects of inputs from steps (1) - (3) to the aggregation function are investigated.

A variety of methods can be reliably utilized for the quantification of model uncertainty. Two common techniques widely used are: (i) local and (ii) global approaches. The local technique is adopted to determine the sensitivity of the model's input parameters (Zhao et al., 2011). In contrast, the global method is suitable to estimate a range of possible parameter values in the parameter distribution (Jiang et al., 2018; Mishra, 2009). In this research, the Monte Carlo simulation (MCS) approach is employed to quantify the uncertainties in the WQI model by following the guide to the expression of uncertainty in measurement. GUM is the fundamental reference guide that provides an in-depth description of how to evaluate measurement uncertainty using the MCS method (Joint Committee For Guides In Metrology, 2008; Rodríguez et al., 1989). The MCS method is both systematic and comprehensive in assessing model uncertainty, and as such it is widely used (Jafari et al., 2016; Mishra, 2009).

Advanced artificial intelligence and machine learning (ML) techniques are also widely used to predict model uncertainty (Abdar et al., 2021; Tavazza et al., 2021). These techniques predict the confidence interval (CI) of measured values to determine how much data variation occurs in a dataset. Consequently, the model errors can be quantified and optimized using these techniques. In this study, the Gaussian Process Regression (GPR) ML algorithm was applied to predict WQI values with a 95% confidence interval. This was followed by a comparative analysis between the MCS and GPR results of model uncertainty to ultimately determine the model efficacy.

This paper is divided into four main sections. In the section 4.3, a brief overview of this study is provided. Section 4.4 discusses a new set of tools and techniques that are applied to estimate and predict model uncertainty. The analysis and findings are presented in section 4.5, and finally in section 4.6 conclusions are drawn from this research.

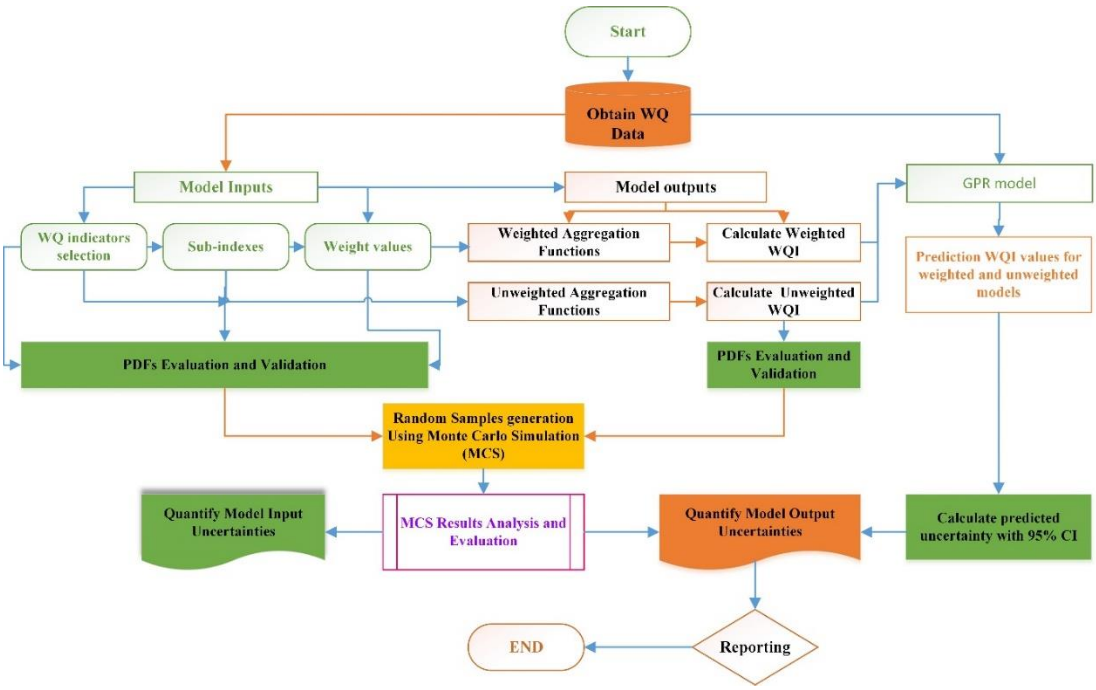


Figure 4.1. A schematic methodological framework of Monte Carlo Simulation for uncertainty analysis in WQI model.

4.4 Materials and methods

Eight widely used WQI models were used to calculate the WQIs, and the MCS technique was utilized to calculate the uncertainties. Several statistical tools, techniques, and ML approaches were used in this study to evaluate the MCS results. The methodology developed in this paper is presented graphically in Figure 4.1 and described in detail in the following subsections.

4.4.1 The application domain - Cork Harbour, Ireland

The proposed methodology was applied and tested in Cork Harbour, located on the south coast of Ireland (Figure 4.2). Cork Harbour was chosen as it was used for a previous WQI model study by the authors (Uddin et al., 2022a) and data were therefore already available. The Harbour, designated as a Special Protection Area (SPA), is Ireland's deepest and longest (17.72 km) surface water body (Hartnett and Nash, 2015; Nash et al., 2011). The area adjacent to the Harbour is one of Ireland's most economically promising zones. Cork Harbour receives large quantities of effluent from various sources each year, such as industries, domestic and municipal waste, which results in variable water quality throughout the harbour.

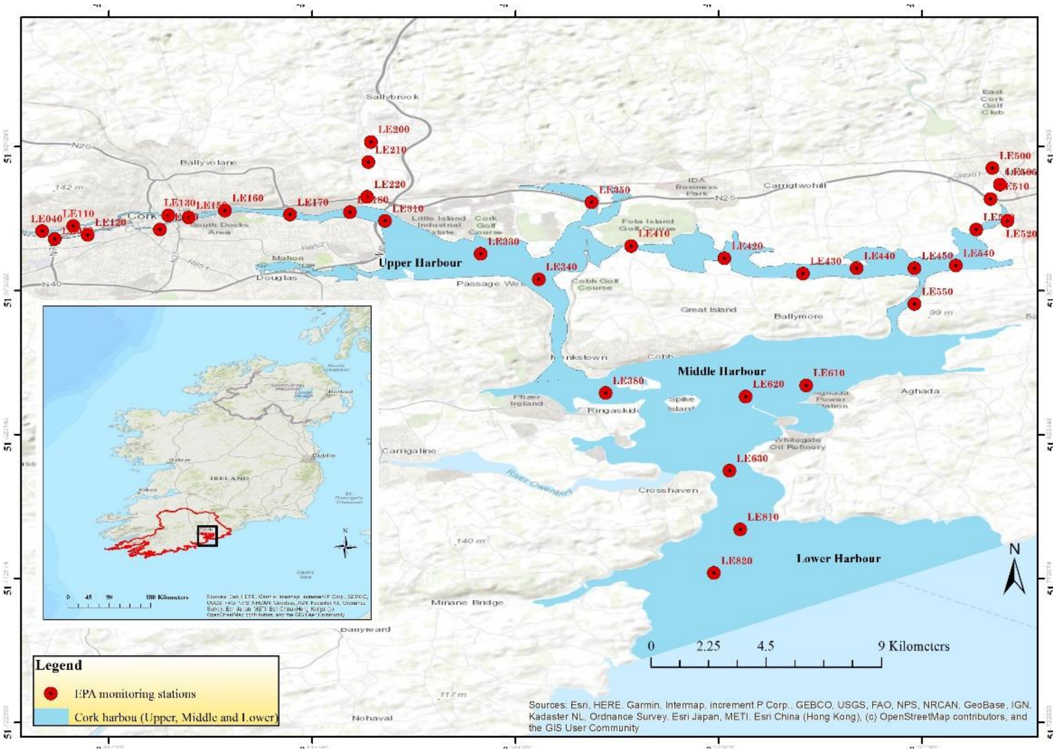


Figure 4.2. Cork Harbour and EPA's water quality monitoring sites.

4.3.2 Data collection

The Irish Environmental Protection Agency (EPA) collects monthly WQ data from monitoring sites in Irish waterbodies. The relevant water quality indicator data for Cork Harbour were obtained from https://www.catchments.ie/data/. Data for eleven water quality indicators including ammonia (AMN), transparency (TRAN), total organic nitrogen (TON), temperature (TEMP), dissolved oxygen (DOX), ammoniacal nitrogen (AMN), pH, salinity (SAL), molybdate reactive phosphorus (MRP), biological oxygen demand (BOD), and Chlorophyll a (CHL) from 29 monitoring sites were sampled at 1 m depth and at with these data being used in this study. The monitoring locations are presented in Figure 4.2. Water quality data from 29 out of 36 monitoring stations in Cork Harbour were obtained from the EPA for the period 2019 – 2020. The detailed water quality data are provided in Table 4.S1, and Table 4.S2 (Appendix 4) for the summer and winter periods, respectively.

4.3.3 WQI model

The WQI model of Uddin et al. (2022a) was used for the study as it was developed specifically for coastal waters and was tested using Cork Harbour. Like most WQI models, it involves four main stages: (1) selection of WQ indicators for inclusion, (2) calculation of sub-indices for each indicator using SI functions, (3) calculation of weightings for each indicator based on their influence on water quality, and (4) calculation of the final WQI using aggregation functions. The model was run for summer and winter periods. With regard to parameter selection, following Uddin et al. (2022a), seven water quality indicators were included for summer (CHL, DIN, AMN, TEMP, BOD, MRP and TRAN) and five were included for winter (DIN, TON, pH, DOX and TRAN).

The following SI functions were used to transfer various water quality data onto a uniform scale.

$$SI = (SI_u - SI_l) - \frac{(SI_u \times WQ_m)}{(STD_u - STD_l)} \ldots\ldots\ldots..(4.1)$$

$$SI = \frac{(WQ_{i_m} - STD_l)}{(STD_u - STD_l)} \times SI_u \ldots\ldots\ldots..(4.2)$$

$$SI = (SI_u - SI_l) - \frac{(WQ_{i_m} - STD_l)}{(STD_u - STD_l)} \ldots\ldots\ldots..(4.3)$$

SI_l and SI_u are the lower and upper limits of possible SI values (0 and 100, respectively). STD_l is lower threshold value, STD_u is the upper threshold value and WQ_m is the measured water quality parameter concentration. Parameter weighting was determined using the two-step process of Uddin et al., (2022a) involving XGBoost and the rank order centroid (ROC) methods.

Table 4.S3 and Table 4.S4 provide (Appendix 4) lists of the water quality indicators

included in the study, corresponding weight values and binary conditions for sub-indexes functions; these were all pre-determined by Uddin et al. (2022a). Like Uddin et al. (2022a), eight different aggregation function are tested here; four of these were weighted and four unweighted. Details of the aggregation functions can be found in Table 4.S5 (Appendix 4). Table 4.S6 provides the SI results obtained from the Table 4.2 SI functions and the binary rules for considered indicators. The outputs (WQI scores) from different aggregation functions are presented in Table 4.S1 and Table 4.S2 for summer and winter, respectively.

4.3.4 Model uncertainty

The Monte Carlo simulation (MCS) approach was used to quantify uncertainties at each stage of the WQI model application. The MCS technique is a widely recognised method for the quantification of all types of uncertainties in a system/model. Parametric and nonparametric MCS methods were utilised to generate target random samples and then to calculate the uncertainties for each model component. Figure 4.1 provides an overview of the experimental procedure and the following section provides a brief description of the MCS method. The four WQI model stages were divided into two categories for uncertainty analysis:

(1) Model input – including the selection, sub-indexing and weighting of water quality indicators, and
(2) Model output – including aggregation of the final indices.

4.3.4.1 Estimation of uncertainty in WQI model

The GUM methodology was used to implement the MCS method for the estimation of uncertainties in the model. Five common statistical measures of uncertainty were employed; these were: (1) the standard uncertainty (SU), (2) the expanded uncertainty (EU), (3) the combined uncertainty (CU), (4) the coverage factors (CF) and (5) the degree of freedom (df).

(i) Standard uncertainty

The standard uncertainty (SU) is widely used to estimate uncertainty in hydrological/hydraulic models (Liang et al., 2016; Liu et al., 2008; Rodríguez et al., 1989). It refers to the degree of data dispersion from the mean of observations

(Farrance and Frenkel, 2012). The method requires the definition of all input entities of the model - here the selected WQ indicators, sub-indexes and weight values. For the model error of an input variable I, the SU can be defined for each quantity as follows:

(i) Water quality indicator uncertainties; $SU_p = I(WQ_{p_i}) + \alpha_i$ ……… (4.12)

(ii) Sub-index (SI) uncertainties; $SU_{si} = I(SI_i) + \alpha_i$ ……………….. (4.13)

(iii) Weight uncertainties, $SU_w = I(w_i) + \alpha_i$ …………………….. (4.14)

(iv) Model output (aggregation functions) uncertainties;

(a) weighted model: $SU_{WQI_w} = WQI(WQ_{p_i}, SI_i, w_i) + \alpha_i$ ……………….. (4.15)

(b) unweighted model : $SU_{WQI_{uw}} = WQI(WQ_{p_i}, SI_i) + \alpha_i$ …… (4.16)

where, SU_p, SU_{si} and SU_w are the water quality indicators, sub-index and parameter weight values, respectively. $SU_{WQI_w}$is the weighted model output uncertainty and $SU_{WQI_{uw}}$ is the unweighted model output uncertainty. WQ_{p_i} is the ith value of the water quality indicator I. SI_i is the sub-index value and w_i is the weight value of i^{th} variable I. α is the variation between predicted and observed MCS values. The difference between predicted and observed variances are defined as follows:

$$\textit{Variance, } V(x) = V(\alpha_1) + V(\alpha_2) + \cdots + V(\alpha_n) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (4.17)$$

If all of the measured and observed random variations (α) are uncorrelated, then standard uncertainty can be defined as:

$$SU = s_{\bar{x}} = \sqrt{V(\bar{x})} = \frac{sd_{\bar{x}}}{\sqrt{N}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (4.18)$$

where, $SU_{\bar{x}}$is the standard uncertainty, $s_{\bar{x}}$ is the standard error of the mean value of each input components, and $sd_{\bar{x}}$ is the mean standard deviation of the random variations in the quantity being measured with the sample true mean. The $s_{\bar{x}}$ can be expressed as:

$$s_{\bar{x}} = \left(\frac{1}{N-1}\sum_{i=1}^{N}(x_i - \bar{x})^2\right)^{1/2} \ldots\ldots\ldots\ldots\ldots\ldots (4.19)$$

where, N is the number of random samples, x_i is the ith data value and $\bar{x}$ is the sample mean.

4.3.4.2 Combined uncertainty (CU)

In a model with multiple model components, each model component is a source of uncertainty. The combined uncertainty (CU) describes how the model result varies with changes in each model component (Meyer, 2007). In the case of the WQI model, the parameter selection, sub-indexing process and weighting technique all contribute to the input uncertainty. The CU is therefore a measure of the total magnitude of uncertainty associated with all inputs into the WQI model.

The quadrature Root Sum of the Squares (RSS) method is widely used to calculate the CU value in a model (Mishra, 2009). RSS is a measurement of the standard uncertainty for each variable, including the coefficient sensitivity. In this method, all PDFs are combined and converted into the normal distribution based on the central limit theorem (Paulo Roberto Guimarães Couto, 2016). In this study, RSS was used for quantifying CU as follows:

$$CU = \left[\sum_{i=1}^{n} [c_i\, SU(x_i)]^2\right]^{1/2} \quad \dots\dots\dots\dots\dots \; (4.20)$$

where, CU is the combined uncertainty, c_i is the sensitivity coefficient, and $SU(x_i)$ is the standard uncertainty of the ith water quality indicator. The sensitivity coefficient can be represented as follows:

$$C_i = \frac{\partial f(x_i)}{\partial x_i} = \frac{\partial y_i}{\partial x_i} \quad \dots\dots\dots\dots\dots.\dots\dots (4.21)$$

where, $\frac{\partial f(x_i)}{\partial x_i}$ is the changing value of the inputs of the WQI model (i.e. the model components water quality indicators, sub-indexes and weight values),and $\frac{\partial y_i}{\partial x_i}$ is the aggregation process of the WQI model that are changing by independent model input variables.

4.3.4.3 Expanded uncertainty (EU)

Expanded uncertainty is another statistical tool that can be used to quantify how much of the measurement's range can be assumed to cover a significant portion of the data distribution (Loucks, P. D., van Beek, 1981). It is anticipated to include a significant portion of the measured value distribution that can be reasonably linked to the model prediction (BIPM et al., 2020). Typically, the EU estimates are used to improve the level of confidence in the uncertainty of measured results. It usually expands the confidence interval by assuming the t-distribution function of the student t- test. The EU is calculated as follows:

$$EU = k \times\ U_c(y)(p\%) \dots \dots \dots \dots \dots \dots \dots \dots \dots (4.22)$$

where, y are the random input variables, and k is the coverage factor and U_c combine uncertainty of random data. The coverage factor can be defined as:

$$k = \ t_{v,1-\alpha/2} \dots \dots \dots \dots \dots \dots \dots \dots .. (4.23)$$

where v is the effective number of degree of freedom, $\alpha = 1 - P$, and t is the Student's t test (well known as t-test) variable. In this research, 95% confidence level (P) is used, v is calculated form the Welch–Satterthwaite equation that can be defined as:

$$v = \frac{\left(s_{\bar{x}}{}^2 + \sum_g b_{x,g}^2\right)^2}{\frac{s_x^4}{v_{s_x}}} + \sum\nolimits_g \frac{b_{x,g}^2}{v_{b_{x,g}}} \dots \dots \dots \dots . (4.24)$$

where, v_{s_x} is the variance of the measured data for N -1 number of degrees of freedom is = 28 (in this study), whereas $v_{b_{x,g}}$is the variance systematic error (Shaw, 2017) defined as:

$$v_{b_{x,g}} = \frac{1}{2U_{x,g}^2} \dots \dots \dots \dots \dots \quad (4.25)$$

where, $U_{x,g}$ is the relative uncertainty of $b_{x,g}$.

The uncertainty of the WQI model was calculated in a multi-step process as follows:

1. PDFs of all input components were generated.
2. Prior to performing the MCS, the *M* numbers of trials were set to define measurand and input entities in MCS. The trials *M* can be represented as follows:

$$M > \frac{10^4}{1-p} \dots \dots \dots \dots \dots \dots \dots \dots .. (4.25)$$

where, p is the coverage probability. For $p = 0.95$, the number of trials was $2e^5$. Commonly, higher number of trials is recommended in order to obtain greater convergence in the results.

3. After M trials, the N random values for α were estimated and applied to [equations (12) – (16)] calculate the SU_p, SU_{si} and SU_w , SU_{WQI_w} and $SU_{WQI_{uw}}$ values.
4. For completed M trials, the $SU_n(SU_p, SU_{si}$ and SU_w , SU_{WQI_w} , $SU_{WQI_{uw}}$) value calculated in step (3) was used to obtain the statistics of the parameter $s_{\bar{x}}$. Uncertainty can be treated as "stable" if there is a numerical tolerance that corresponds to the standard deviation of the output quantity; this tolerance should be less than two standard deviations of the input quantity. The standard uncertainty can be determined from $\times 10^i$, where i is the integer with a number of decimal places. The numerical tolerance can be expresses as:

$$\tau = \frac{1}{2} 10^i \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots. (4.26)$$

5. For the optimized MCS algorithm, the steps (3) and (4) are repeatedly run for M trails to generate the s_x value for each trail.
6. Finally, the p% coverage intervals for $s_{\bar{x}}$ values were evaluated, summarized and interpreted in the WQI model for the MCS output.

4.3.5 Prediction of WQI model uncertainty

4.3.5.1 Machine learning algorithms

ML technique is widely used for predicting unknown objects or analysis of the model performance (Elgeldawi et al., 2021; Haghiabi et al., 2018; Zhu et al., 2022). Recently, several studies have utilized this technique for estimating the model uncertainty with a 95% CI. In addition, a number of studies have utilized this technique for identifying the faults or biased nature of any model/system (Bode et al., 2020; Fernandes et al., 2022; Saufi et al., 2019; Yang et al., 2019). A few studies have utilized this technique for estimating water quality model uncertainty (Jiang et al., 2021; Khoi et al., 2022; Xu et al., 2022). In this study, the ML technique was utilized to quantify uncertainty in the WQI model because it focuses mostly on population variables that determine the prediction intervals. The calculations of uncertainty of each specific prediction can be fairly expensive computationally and usually requires an additional computational effort beyond the training of the model (Abdar et al., 2021; Tavazza et al., 2021).

4.3.5.1.1 ML models development processes

4.3.5.1.1.1 Data preparation

(a) Data standardization

Prior to develop the ML models, it is important to standardize the data for avoiding the model over-fitting problems. Usually, in ML technique, this approach used to convert various types of variables into uniform scale. In this research, data was standardized using the approach of Uddin et al., (2022c). Details of the methodology can be found in Uddin et al., (2022c).

(b) Preparing training and testing datasets

For the purposes of developing the ML models, dataset was divided into two sets (i) 70 % (20) of training and 30% (9) of testing. The detail input datasets are provided in Table 4.S1 and Table 4.S2 (Appendix 4) for summer and winter, respectively.

4.3.5.1.1.2 Development of ML models

After preparing datasets for training and testing, six ML-regression algorithms including (1) decision tree (DTs), (2) linear regression (LR) model, (3) Gaussian process regression (GPR) model, (4) support vector machines (SVMs), (5) neural network (NN), and (6) ensembles of tree model were trained and tested using training (20 monitoring sites) and testing (9 monitoring sites), respectively, whereas the model performance were evaluated during both training and testing phases. Details of the ML algorithms can be found in Uddin et al., (2022c).

The best-fit ML algorithm was selected from six ML techniques based on the trial-and-error analysis using the regression learner app with MATLAB R2021b (Bui et al., 2020). For obtaining the best-fit ML algorithm(s), many hyperparameter tuning techniques are used in ML studies, the grid search technique is one of them (Elgeldawi et al., 2021; Shekar and Dagnew, 2019; Uddin et al., 2022c). In this research, the grid search technique was utilized according to the methodology of Shekar & Dagnew, (2019) because, compared to other methods, this technique is effective in optimizing the model parameters. The present study was utilized the regression learner app with

MATLAB R2021b for the identification of optimal parameters of ML models using auto tuning approach. Table 1 provides the optimum hyperparameter values for the best-fit GPR model.

Based on the trial and error performance results of six ML models, the GPR ML model was found to produce the minimum training error and best fit for predicting WQI input dataset. Details of the GPR-ML algorithm can be found in Grbić et al., (2013). Table 4 provides the optimal parameters for the best-fitted GPR-ML in predicting various WQI model scores. The GPR, which incorporates Bayesian theory and statistical learning theory, is an effective method for solving complex regression problems such as high dimensionality and nonlinearity (Zhang et al., 2019). In terms of uncertainty analysis, a few studies have reveal that the GPR is different from traditional ML methods in that it automatically determines the prediction uncertainty when the model is fit (Rasmussen, 2003). Abdar et al., 2021 suggest that the GPR algorithm has a higher predictive accuracy than other algorithms and the technique has been successfully applied for predicting model uncertainty (i.e. Asadollah et al., 2021; Tavazza et al., 2021). Therefore, after obtaining the robust algorithm, the GPR-ML model was used for predicting WQI values with 95% of CI in order to estimate the model uncertainty. Once the WQI values and confidence intervals (CI) were predicted, the uncertainty was modelled using the inferential error (Cumming et al., 2007):

$$Inferential\ CI = M \pm t_{(n-1)} \times SE \quad \dots\dots\dots\dots\dots\dots \ (4.27)$$

where, M is the observation mean, $t_{(n-1)}$ is a critical value of t. SE is the standard error of observations.

4.3.5.2 Performance metrics

The cross validation approach is widely used to evaluate the ML model performance for relatively small dataset (Xiong et al., 2020). Following Uddin et al. (2022c), the 10-fold cross validation technique was utilized to evaluate prediction performance of the GPR model. The prediction performance was assessed using the standard error metrics: root mean square error (RMSE), mean absolute error (MAE), mean square error (MSE) and coefficient of determination (R^2), defined mathematically as:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.\ldots.(4.28)$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y_i}| \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(4.29)$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y_i})^2 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(4.30)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y_i})^2}{\sum_{i=1}^{n}(y_i - \hat{y})^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(4.31)$$

where y_i is the actual value of WQI , whereas$\hat{y}$ is the mean predicted WQI value for the ith monitoring site; n is the number of water quality monitoring sites.

Table 4.1. Optimized value for GPR model.

Model attributes	Optimized value	Hyperparameter search range
Signal standard deviation	10.8369	-
Basis function	Constant	Constant, Zero, Linear
Kernel function	Nonisotropic Squared Exponential	Nonisotropic Exponential, Nonisotropic Matern 3/2, Nonisotropic Matern 5/2, Nonisotropic Rational Quadratic, Nonisotropic Squared Exponential, Isotropic Exponential, Isotropic Matern 3/2, Isotropic Matern 5/2, Isotropic Rational Quadratic, Isotropic Squared Exponential
Kernel scale	0.25294	0.009433-9.433
Sigma	151.5629	0.0001-153.2569
Standardiz	false	true, false
Iterations	30	-

4.3.5.3 Model differences

Tukey's honestly significant difference post-hoc test (HSD) is a widely used statistical approach for differentiating the pairwise comparison among models/methods/datasets and was used here to compare the pair-wise WQI models (Goeman and Solari, 2021). The analysis of variance (ANOVA) using Welch's test was applied to validate the significance differences between WQI models. Recently, a number of studies have utilized this approach to compare the overall differences between outputs of models (Goeman and Solari, 2021; Rouder et al., 2016; Wang et al., 2017). HSD for each pair of mean values was estimated as follows

$$HSD = \bar{X}_i - \bar{X}_j \mp \frac{q}{\sqrt{2}} \sqrt{MS_e \left(\frac{1}{N_i} + \frac{1}{N_j}\right)} \quad \ldots\ldots\ldots\ldots\ldots\ldots..(4.32)$$

where $i \neq j$:, $\frac{q}{\sqrt{2}} \sqrt{MSE \quad \left(\frac{1}{N_i} + \frac{1}{N_j}\right)}$ is the margin of an error for the confidence intervals, q is the multiplier of the distribution, N is the number of samples within the group, MSE is the mean squared errors and, $\bar{X}_i$ and $\bar{X}_j$ are mean values for each group, respectively.

4.5. Results and discussion

4.5.1 Comparative assessment of water quality status

The ultimate aim of the WQI model is to assess the status of water quality using a classification scheme. The present study used the classification scheme of Uddin et al., (2022). Table 4.S7 contains more information about the classification system. Table 4.2 provides a comparison of the status of water quality using various WQI models. Tables S8 and S9, for the summer and winter seasons, respectively, show the overall water quality status at each monitoring site in Cork Harbour. From Table 4.2, it can see that relatively "good" water quality status was found in the summer season compared to the winter period. A significant difference was found in assessing water quality status for various WQI models. The results of WQI models indicate that the assessment results varied significantly due to the model architecture. Similar findings are reported to those of previous studies for Cork Harbour (Uddin et al., 2020; 2022)

4.5.2 Initialization of MCS run

The MCS run was initialized for 95% confidence level and 28 degree of freedom including coverage factor k = 2.05 (Meyer, 2007). The probability density function (PDF) of each input parameter is the essential requirement for MCS as they strongly influences the simulation results (Seifi et al., 2020). All input and output PDFs were verified using Kolmogorov-Smirnov test with p-value > 0.05. The MCS simulations were for M = $2 \times e^5$ trials. The parametric and non-parametric bootstrap tests were carried out to verify the estimated PDFs statistics (Shaw, 2017).

Table 4.2. Assessment of water quality in in Cork Harbour at monitoring site using different WQI models.

WQI methods	water quality classifications							
	summer				winter			
	Good	Fair	Marginal	Poor	Good	Fair	Marginal	Poor
(i) Weighted								
NSF	45% (13)	24% (7)	31% (9)	0	14% (4)	24% (7)	17% (5)	45% (13)
WQM	62% (18)	38% (11)	0	0	14% (4)	48% (14)	38% (11)	0
SRDD	28% (8)	34% (10)	7% (2)	31% (9)	10% (3)	10% (3)	5	17
WJ	41.5% (12)	17% (5)	0	41.5% (12)	14% (4)	14% (4)	10% (3)	18
(ii) Unweighted								
RMS	15	48% (14)	0	0	24% (7)	22	0	0
AM	9	20	0	0	6	41.5% (12)	11	0
Hanh	14% (4)	24	0	0	17% (5)	28% (8)	10% (3)	45% (13)
CCME	100% (29)	0	0	0	100% (29)	0	0	0

In total 29 monitoring sites were used in this assessment.

4.5.3 Sources of uncertainty in WQI model

4.5.3.1 Model input uncertainty

(i) Water quality indicators uncertainty

The results of the WQ indicators were evaluated graphically and statistically to quantify the input uncertainty of the WQI model. Figures (4.3 – 4.6) present the actual and MCS-simulated PDFs and cumulative distribution function (CDFs) of all WQI model input entities. All of the WQ indicators were found to be normally distributed during both seasons (Figure 4.3 and Figure 4.5). The uncertainties calculated for each water quality indicator are presented in Table 4.3. The PDF statistics and their corresponding confidence intervals for the MCS results are given in Table 4.S10 (Appendix 4).

From Figures 4.3 and 4.4, there was significant differences between the PDFs and CDFs of the actual and simulated concentrations of water quality indicators during the summer season. Large data variation was observed for CHL, DIN, TEMP, BOD, and TRAN whereas data consistency was found between actual and simulated for AMN and MRP. During winter (Figure 4.5 – 4.6), there was no significant difference found between the actual and simulated data at $p < 0.0001$, except for DOX.

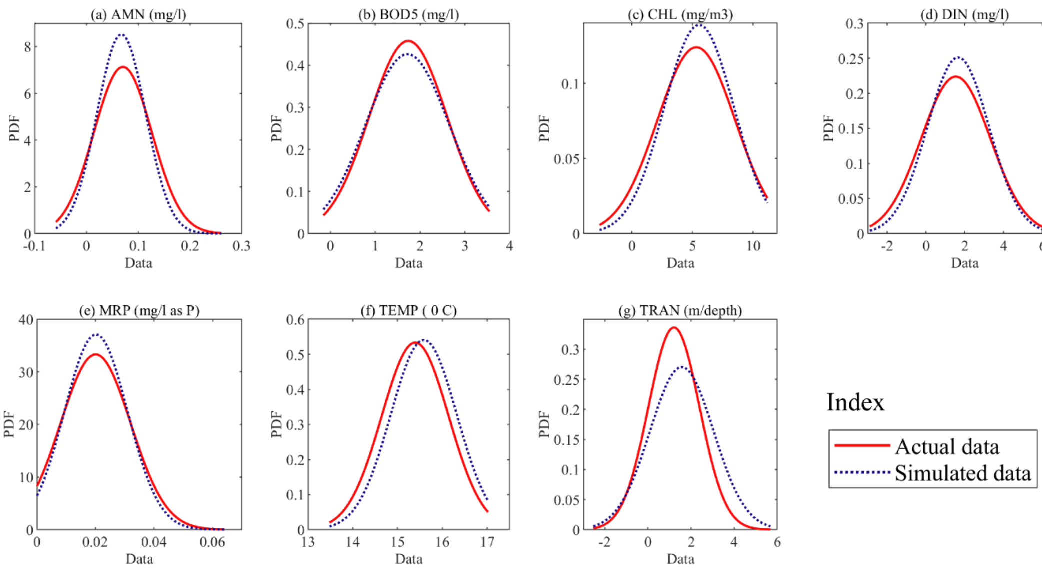


Figure 4.3. PDF plots of actual and simulated water quality indicators data in Cork Harbour for the summer period.

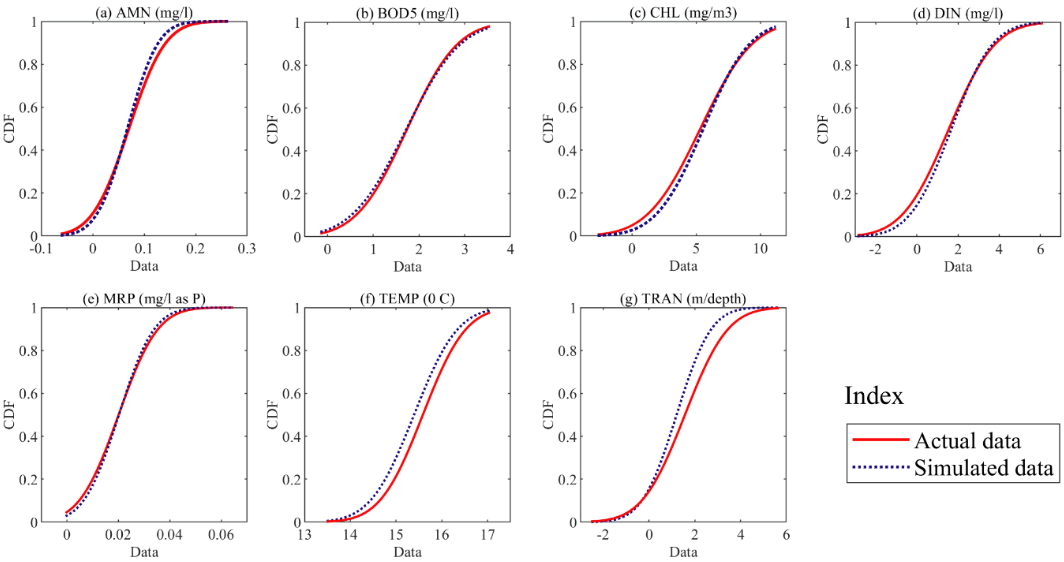


Figure 4.4. CDF plots of actual and simulated water quality indicators data in Cork Harbour for the summer period.

It can be concluded from the results of the CDFs and PDFs that five water quality indicators (CHL, BOD, DIN, TEMP, and TRAN) contribute to the generation of a small amount of uncertainty in the WQI model through the summer season. From Table 4.3, less than 1% of uncertainty was associated with all input indicators during both seasons. Seasonal intercomparison shows generally lower uncertainty for the winter period. The results of water quality indicator inputs indicate that the number of input variables plays a crucial role in producing the uncertainties in the WQI model.

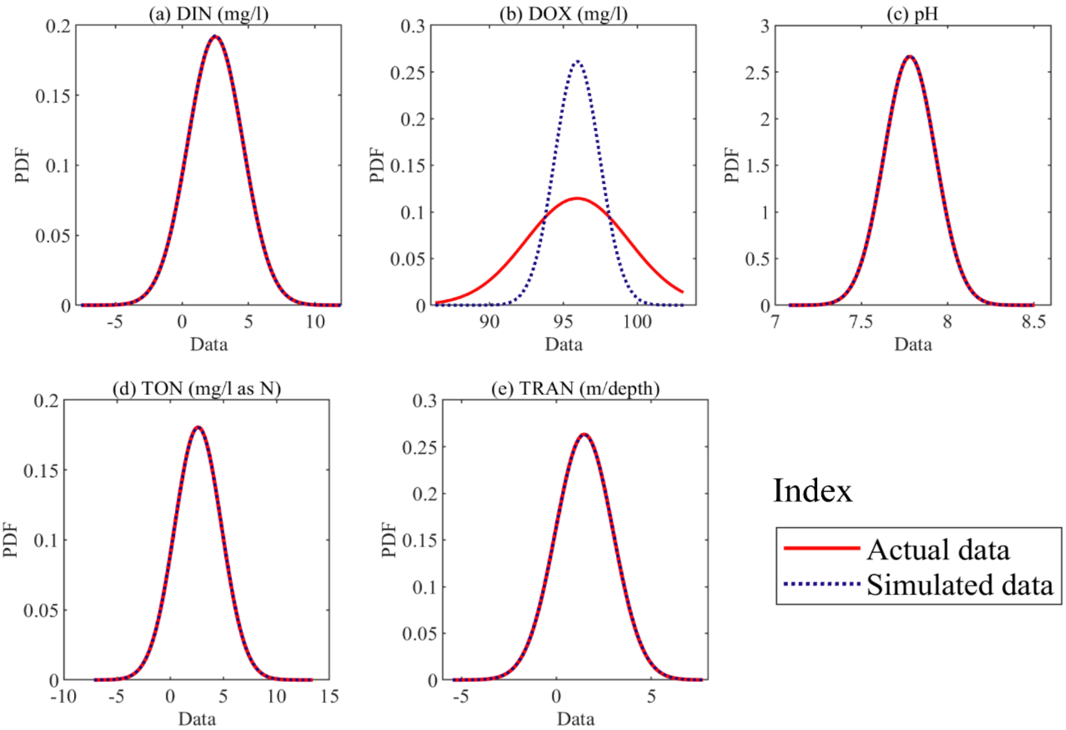


Figure 4.5. PDF plots of actual and simulated water quality indicators data in Cork Harbour over the winter season.

(ii) Sub-index uncertainty

Several studies argue that the sub-indexing process generates high levels of uncertainty in a WQI model, but the magnitudes of SI uncertainties have never been quantified. The MCS technique was used to calculate the levels of uncertainty generated during the sub-indexing process. The PDFs and CDFs of SI values are presented in Figure 4.7; Table 4.S10 provides the summary of MCS statistical results for distribution functions of sub-indexes. The associated uncertainties for each water quality indicator are presented in Table 4.3.The PDFs of sub-index functions for all indicators exhibit normal distribution for both seasons. During summer season, there was a significant difference found between the actual and simulated SI values for three parameters: DIN, AMN and TRAN (Figure 4.7a,b). Similar differences in SI were observed in winter season for four parameters: DOX, DIN, TON, and TRAN (Fig. 4.7c,d). There was a strong correlation found between the actual and simulated PDF and CDF of SI values for BOD, MRP, and CHL during summer and for DOX during winter. From Table 3, for summer, 7.07%, 5.34%, 4.49%, 4.42%, 3.81%, and 2.98% of SU were associated with the SI process for TRAN, AMN, DIN, CHL, MRP, and BOD, respectively. Interestingly there was no uncertainty produced by SI of TEMP. For winter, the SI of TRAN produced the highest SU values, whereas pH resulted in the lowest (Table 3).

Overall, the combined uncertainty values associated with the SI functions of the water quality indicators were 12.84% and 10.27% for summer and winter, respectively; thus, SI functions play an important role in generating uncertainty in the WQI model during both seasons. It can be concluded that the SI uncertainty varies depending on the spatiotemporal distribution of WQI model inputs.

Table 4.3. Estimating uncertainty for model inputs with 28 effective degree of freedom, 95% coverage probability and 2.05 coverage factor.

Input entities		summer		winter		
WQ paramters	SU[1]	EU[2]	CU[3]	SU	EU	CU
CHL	0.599	1.227				
AMN	0.011	0.021				
TEMP	0.137	0.281	***0.916***			
BOD	0.162	0.331				
MRP	0.002	0.004				
TRAN	0.268	0.549		0.282	0.577	
DIN	0.331	0.678		0.384	0.788	
TON				0.41	0.842	***0.812***
DOX				0.283	0.581	
pH				0.027	0.057	
Sub-indexing						
CHL	4.423	9.059				
AMN	5.34	10.94				
TEMP	0	0				
BOD	2.985	6.115	***12.836***			
MRP	3.819	7.823				
TRAN	7.076	14.49		7.412	15.18	
DIN	4.495	9.208		3.674	7.526	
TON				4.571	9.363	***10.27***
DOX				1.005	2.059	
pH				0.097	0.199	
Weighting	0.0228	0.0467	***0.183***	0.027	0.056	***0.205***
Combined input uncertainty			**13.936**			**11.29**

[1]*Standard uncertainty;* [2]*Expanded uncertainty;*[3]*Combine Uncertainty*

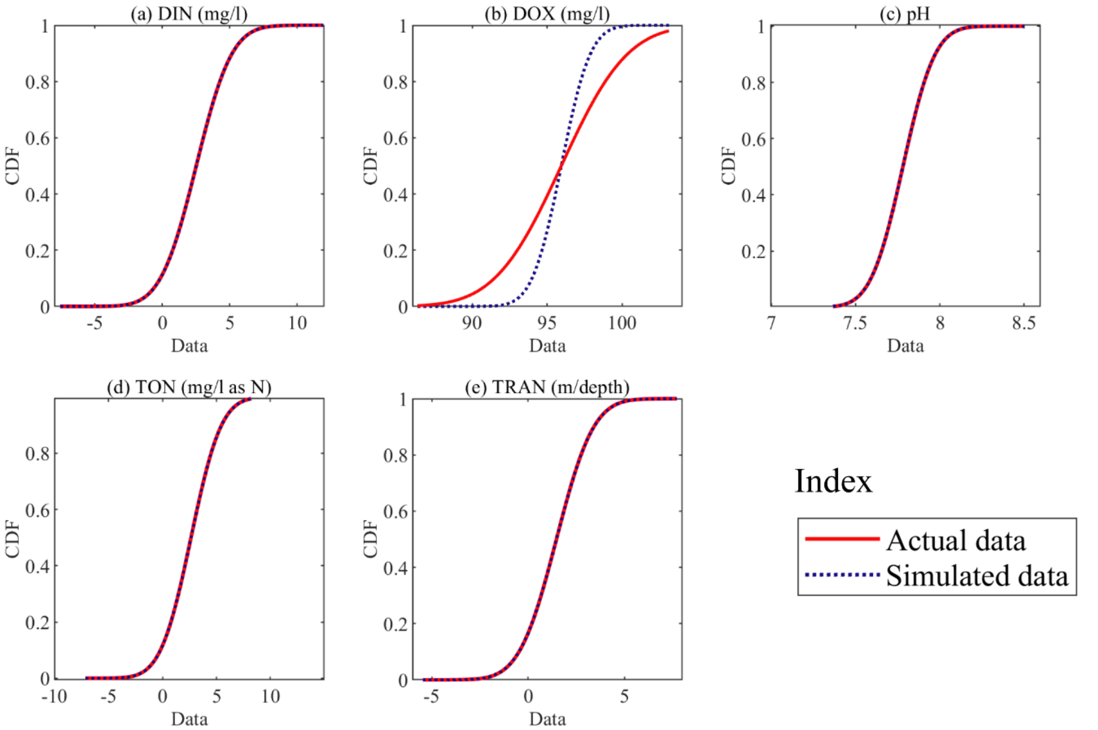


Figure 4.6. CDF plots of actual and simulated water quality indicators data in Cork Harbour over the winter period.

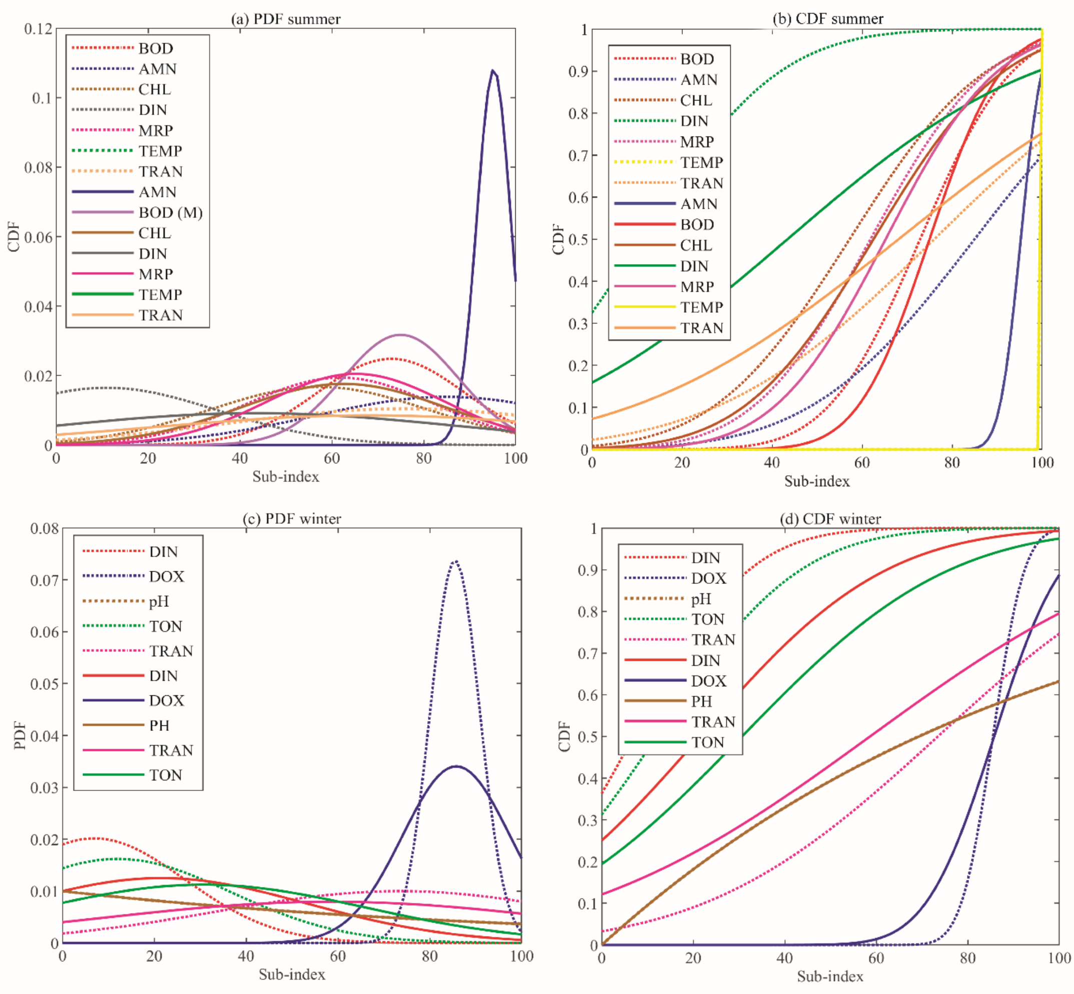


Figure 4.7**.** PDF and CDF plots of calculated and simulated sub-index values for (a,b) summer and (c,d) winter. Dashed lines are calculated SI values and solid lines are simulated values.

(iii) Parameter weighting uncertainty

Several studies argue that the weighting process generates a considerable amount of uncertainty that contributes to the final WQI score (Seifi et al., 2020; Sutadian et al., 2017, 2016; Uddin et al., 2021). Once again, the MCS approach was utilized to estimate the uncertainties generated in the weighting process. Figure 4.8 presents the PDFs and CDFs of the actual and simulated weight values for summer and winter. Table 4.3 provides the uncertainty results obtained from the MCS analysis of the weight values. Detailed PDFs statistics and uncertainty intervals are presented in Table 4.S10 (Appendix 4).

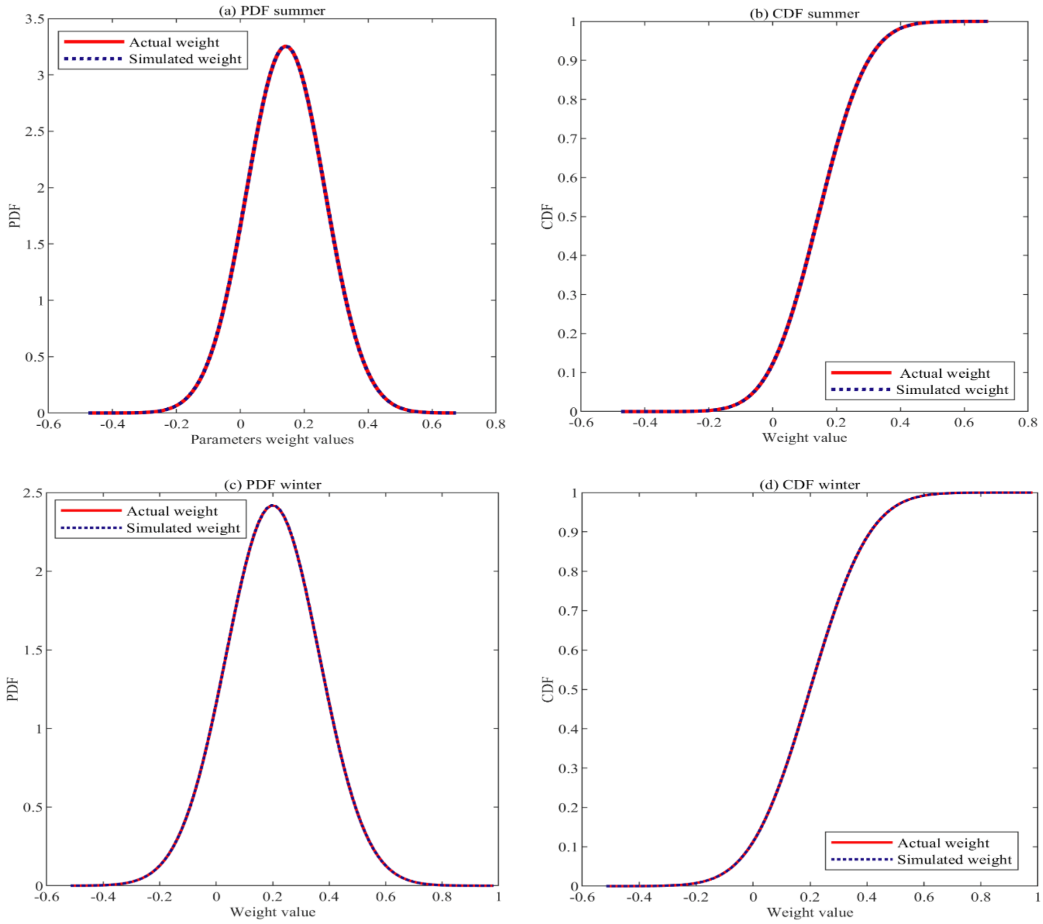


Figure 4.8. PDF and CDF plots of estimated and simulated indicators weight values with 95% confidence interval of the probability.

The indicator weight values were found to have a normal distribution for both seasons. No weight variations were found between the actual and simulated values for either season. It can be seen from Table 4.3 that less than 1% of uncertainty is attributed to the weighting process. These findings suggest that the weighting process of Uddin et al., (2022b) does not significantly contribute to uncertainty generation in the WQI model. This is in line with the findings of Uddin et al., (2022a). Unlike the findings of this study, a few studies have revealed that the weight values can contribute a considerable amount of uncertainty in a WQI model (Sutadian et al.,2018).

(a) Impact assessment of input components on the WQI model

Table 4.3 provides the uncertainty results obtained from the MCS analysis for each input component of the WQI model. Comparing the two seasons, it can be seen that during summer the uncertainty levels of 0.92%, 12.82% and 0.18% were attributed to the water quality indicators, sub-index functions and parameter weight values, respectively. The total uncertainty of the three inputs together is 13.94% (at 95% confidence level) for summer season. For winter, the uncertainties of 0.81%, 10.27%, and 0.21% were attributed to the three processes with a total uncertainty level of 11.29%, which is marginaly lower than the summer score. As for summer, the sub-index function uncertainty level has the most significant impact on the WQI score. Interestingly, and perhaps surprisingly, this study demonstrates that water quality indicators and weight values have no significant impacts on the model score. To our knowledge this is the first research study that quantifies uncertainties at each step of WQI modelling.

4.5.3.2 Model output uncertainty

The aggregation process is the final step of the WQI model. It is used to aggregate the sub-indices into a single overall WQI score. Eight different aggregation functions were assessed to quantify the uncertainties that they contributed to the WQI score.

The PDFs and CDFs for calculated and simulated results of the eight different aggregation functions (4 weighted and 4 unweighted) are presented in Figures 4.9 and 10, respectively. The probability distribution of all aggregation functions were normal during both seasons. Table 4.S11 provides the detailed statistics of MCS. For weighted functions, Significant differences were found between the calculated and simulated

WQI values for the SRDD and WJ models over the study period while lower differences were observed between the calculated and simulated WQI values for the NSF and WQM models during both seasons.

For unweighted functions, in general there were no significant data variation between the calculated and simulated WQIs ($p < 0.0001$). The Hanh model exhibits slightly higher differences than the AM and RMS models, but the CCME model shows very small differences (Fig. 9c, 10cd). The performance of the CCME function could be attributed to its architecture, which differs significantly from the others. Lumb et al. (2011) and Uddin et al. (2022a) found that the CCME model has eclipsing issues linked to overestimation.

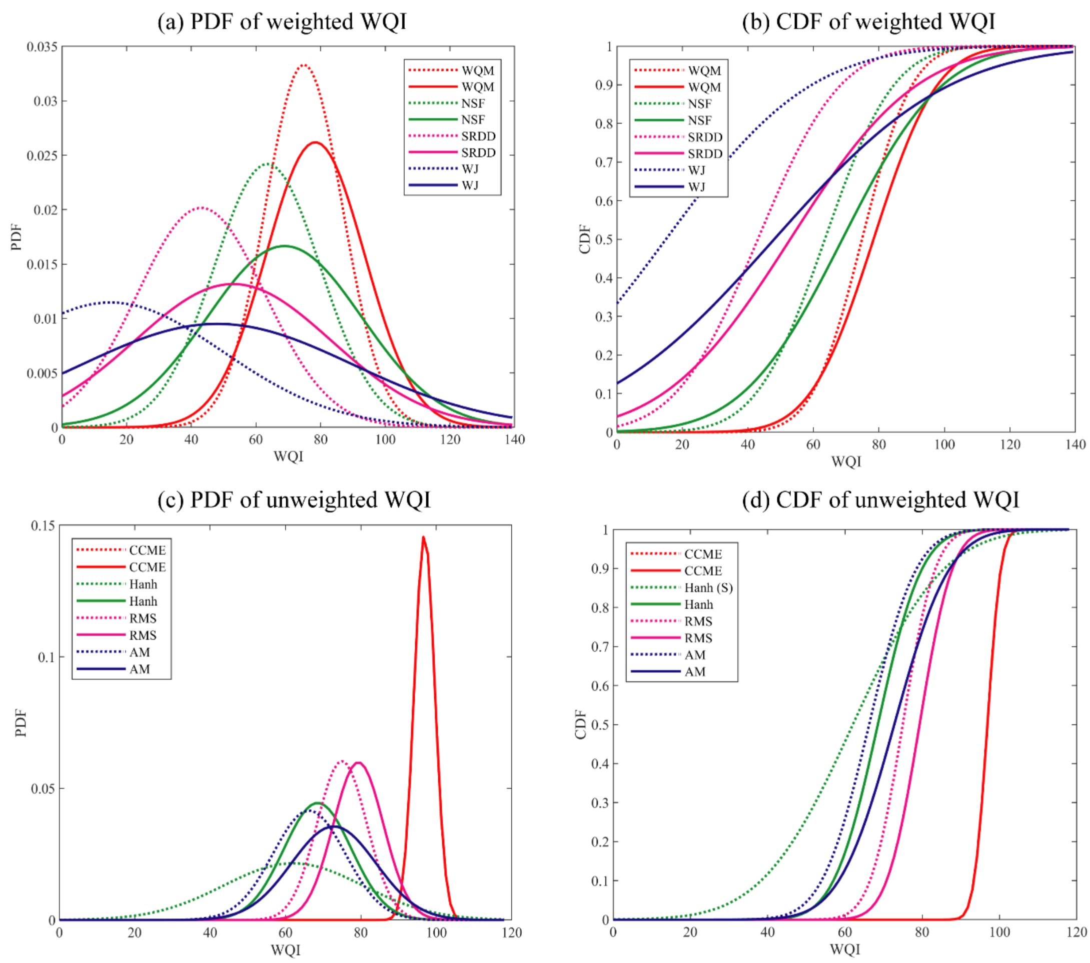


Figure 4.9. PDF and CDF plots of calculated and simulated WQI values for different aggregation functions of WQI models over the summer season in Cork Harbour, including 95% confidence level of the probability functions; solid line represents the calculated WQI values and dotted line illustrated for the simulated WQI values.

Figure 4.11 presents the results of the standard, expanded, and combined uncertainty produced by the eight aggregation functions. For the weighted methods, the WJ and the SRDD functions contributed the highest uncertainty to final WQI scores during both seasons while the WQM model contributed the lowest level of uncertainty.

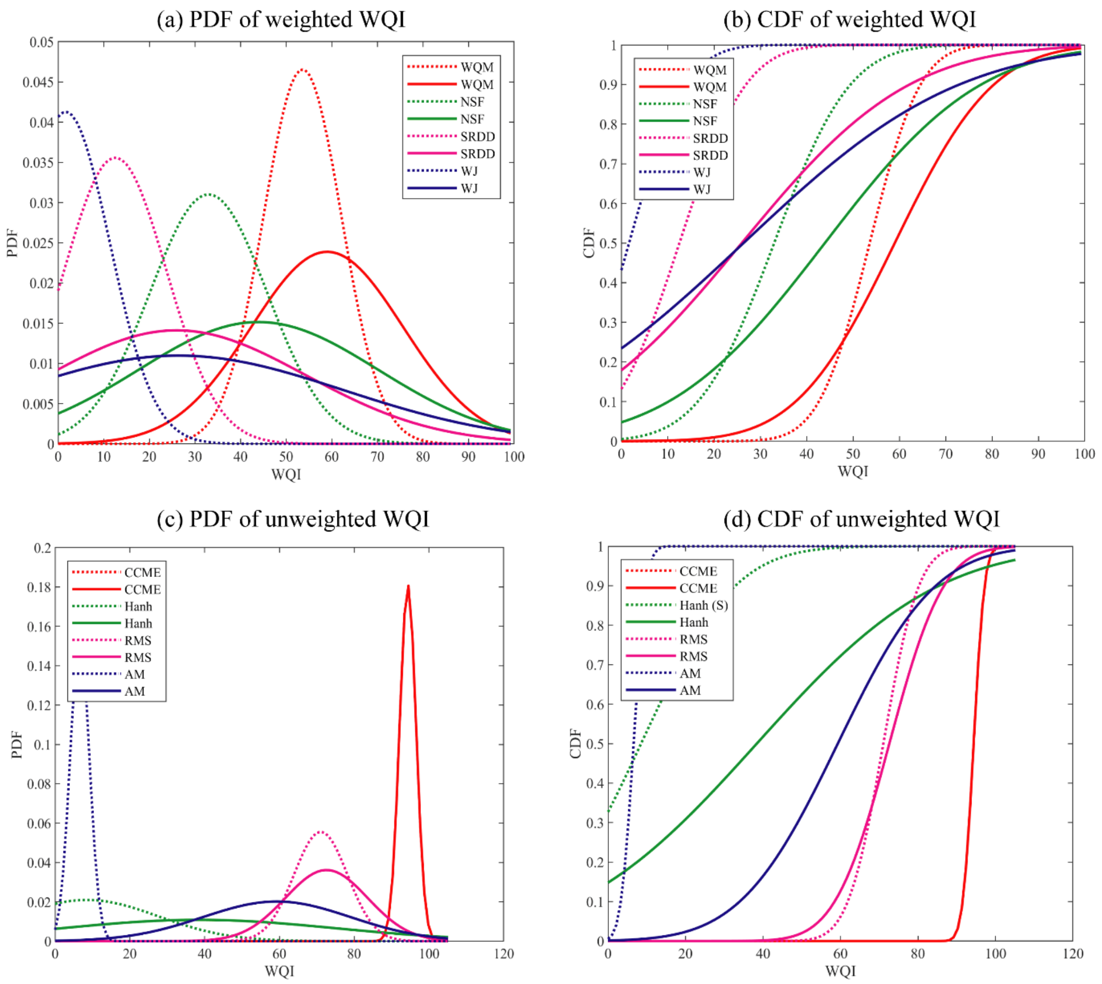
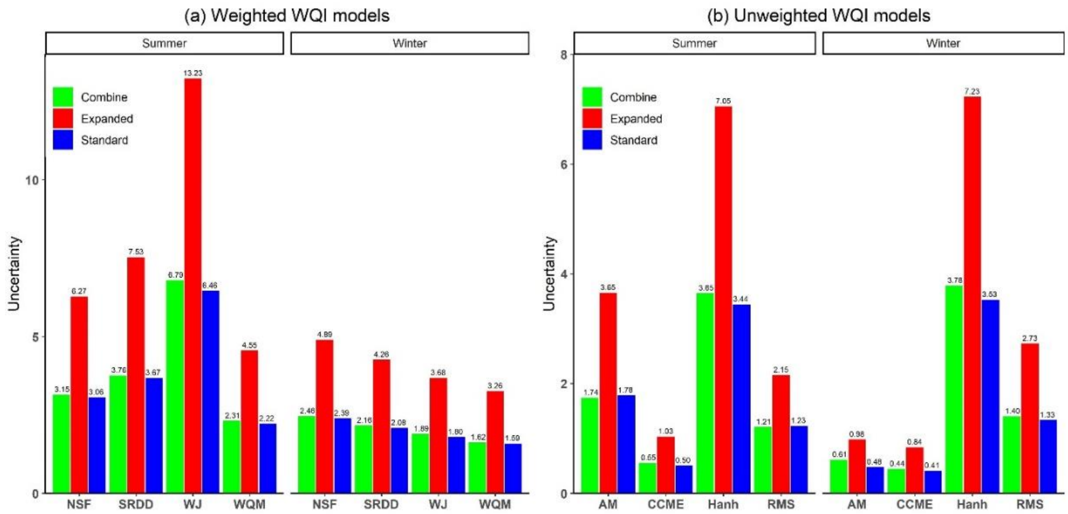


Figure 4.10. PDF and CDF plots of calculated and simulated WQI values for different aggregation functions of WQI models over the winter season in Cork Harbour, including 95% confidence level of the probability functions; where solid line represents the calculated WQI values and dotted line illustrated for the simulated WQI values.

During summer, the highest and lowest SU values were produced by the WJ and the WQM models, respectively (6.46 % versus 2.22%). By comparison, during winter, the highest and lowest SU were produced by the NSF and WQM models, respectively (2.39 % and 1.59%) (Figure 4.11a). The WJ model exhibits the highest expanded uncertainty range, while the WQM model had the lowest. The expanded uncertainty results indicate that the WJ model could generate a larger data variation than other models. The WJ model exhibits a particularly high sensitivity to inputs during the summer season. This implies that the variations in model inputs result in a significant variation in model outputs. A well-balanced combined uncertainty in the input variables of 2.31% and 1.62% were found for the WQM model through the summer and winter, respectively. For the unweighted models, the CCME and Hanh models recorded the lowest and highest levels of uncertainty during both seasons, respectively (Figure 4.11b). Similar results for the CCME model were reported in literature (Ahmed et al., 2021; Davies, 2006; Gupta et al., 2003; Lumb et al., 2011; Wu et al., 2021; Zotou et al., 2019)



.

Figure 4.11. Uncertainty of different WQI models with 95% coverage probability and 2.05 coverage factor.

There is a significant seasonal difference in the uncertainties between the models with generally lower uncertainty levels observed during the winter season. This could be attributed to a variety of reasons, including the number of lower number of WQ variables used in winter, ambiguity of the sub-index functions, sample sizes, and the eclipsing problem of the model aggregation process (Gupta et al., 2003; Seifi et al., 2020; Sutadian et al., 2018; Uddin et al., 2021; 2022a). A comparison of uncertainty levels generated by the weighted and unweighted models shows that the unweighted models produce lower uncertainties. Ignoring the CCME model because of its aforementioned problems, the weighted WQM and unweighted RMS models are recommended for use because they produced the lowest levels of uncertainty. The results of the MCS are in line with those of earlier studies (Carsten Von Der Ohe et al., 2007; Gupta et al., 2003; Lumb et al., 2011; Mladenović-Ranisavljević and Žerajić, 2018; Wu et al., 2021; Zotou et al., 2019).

4.5.4 Predicting uncertainty

The GPR model was utilized for predicting WQI model uncertainty. Table 4.4 provides the 10-fold cross validation results of the GPR prediction model for the eight WQI models and for summer and winter. For the weighted models, the lowest prediction error was produced for the WQM model, while for the unweighted models the lowest error was for the CCME and RMS models.

Table 4.4. 10-fold cross validation results of GPR prediction model.

WQI Models	Summer			Winter		
	RMSE	MSE	MAE	RMSE	MSE	MAE
NSF	6.018	36.022	4.296	0.390	0.152	0.342
WQM	**4.094**	**16.763**	**2.855**	**0.266**	**0.071**	**0.183**
SRDD	7.622	58.087	6.041	1.296	1.679	0.594
WJ	16.010	373.270	14.508	9.709	94.274	4.462
CCME	**1.331**	**1.772**	**0.967**	**0.643**	**0.458**	**0.440**
Hanh	3.067	9.404	2.465	6.448	41.580	2.224
AM	3.623	13.132	2.794	0.276	0.074	0.247
RMS	**1.887**	**3.561**	**1.526**	**0.532**	**0.282**	**0.306**

**Bold values indicates the higher accuracy of prediction model.*

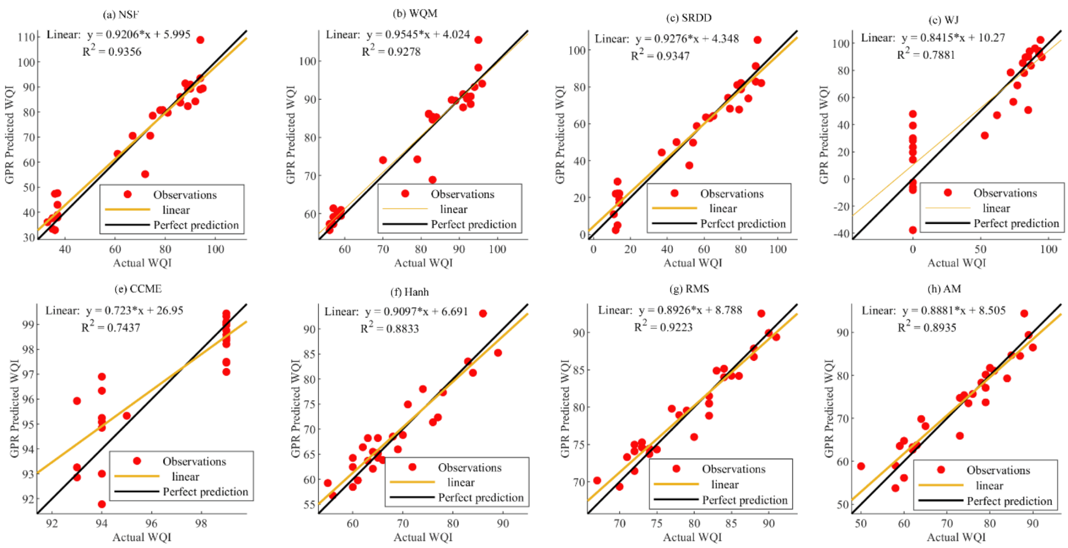


Figure 4.12 Scatter plots of GPR predicted and actual (calculated) WQI values of different WQI models for the summer season.

Figure 4.12 and Figure 4.13 present linear regression analyses of the GPR predicted scores and those calculated (actual) using the WQI models. Generally there is a good fit of the GPR model for both seasons. For the purposes of assessing the predictors' effect on the model response, the present study utilized the coefficient of determination according to the approach of Uddin et al., (2022a). For the determination of R^2, the present study used twenty-nine samples of water quality data. The coefficient of determination was found to be less than 0.8 only for the WJ and CCME models during the summer season.

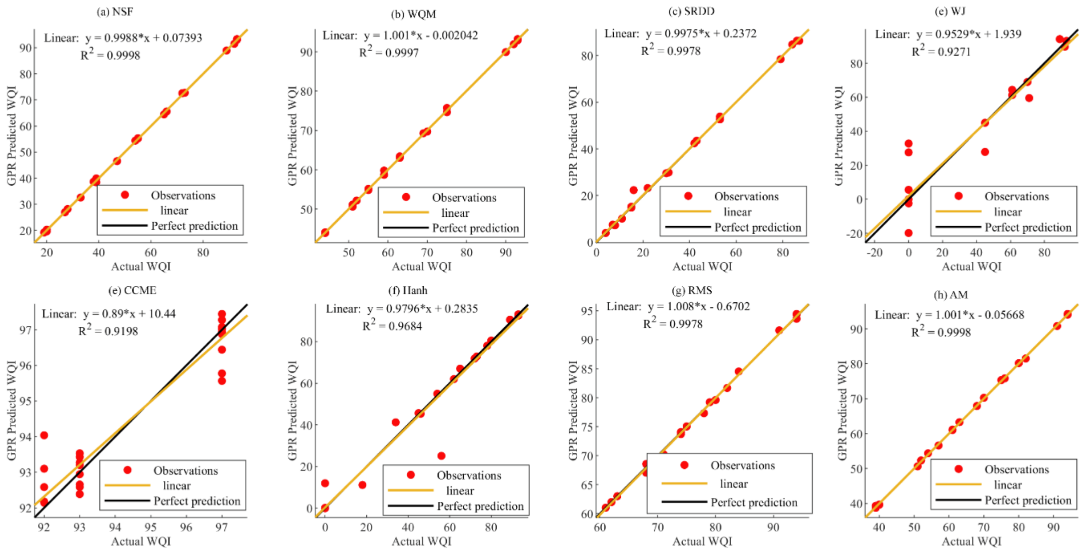


Figure 4.13. Scatter plots of GPR predicted and actual (calculated) WQI values of different WQI models for the winter season.

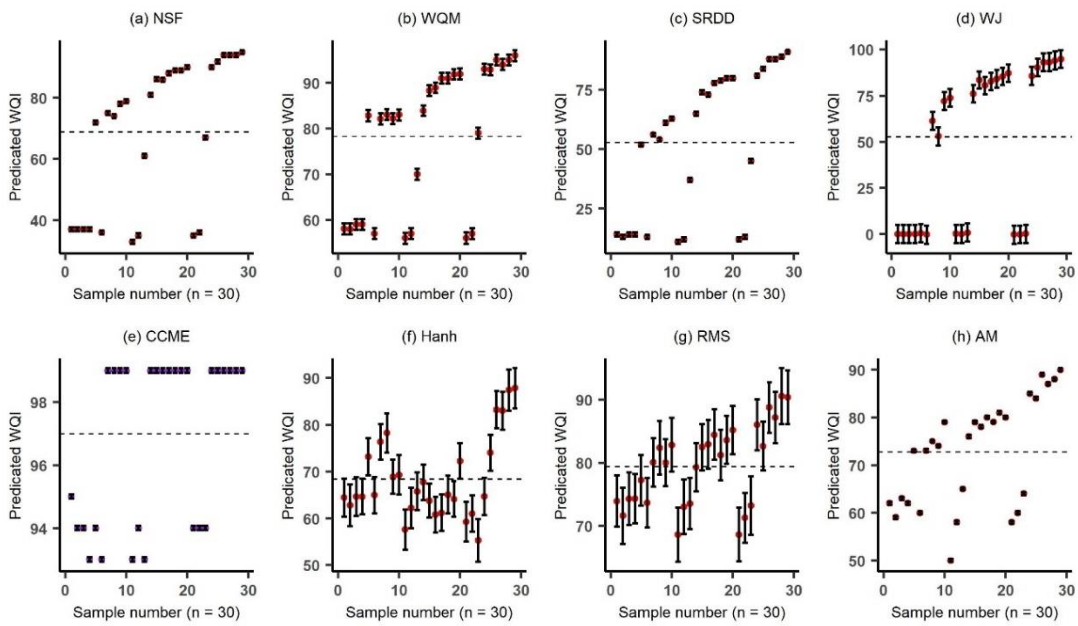


Figure 4.14. GPR-predicted WQI values for summer in Cork Harbour. 95% CI bars are shown with various individual GPR means for monitoring site, whereas *n*=29. A population mean is marked by the black dashed line.

Figures 4.14 and 4.15 show the GPR-predicted WQI values, SE and 95% CI for each sampling location in Cork Harbour for summer and winter, respectively. Table 4.5 provides the results obtained from the t-test analysis of GPR predicted WQI values for the different WQI aggregation functions. The t-test results indicate that the WQI values predicted for the WQM are noticeably different from the calculated values, when compared to the other weighted functions. In addition, lower SE and SD were found for the WQM function than for the other three weighted functions (Table 4.5). For unweighted functions, similar trends were found for the CCME and the RMS models. They also exhibited lower SE and SD values. The results of the predicted uncertainty analysis showed that the WQM and the RMS prediction models could be effective for estimating WQI values in terms of model uncertainty. The findings of prediction uncertainty agree with Uddin et al. (2022a) which found that the SRDD, WJ and CCME models were highly influenced by eclipsing and ambiguity problems.

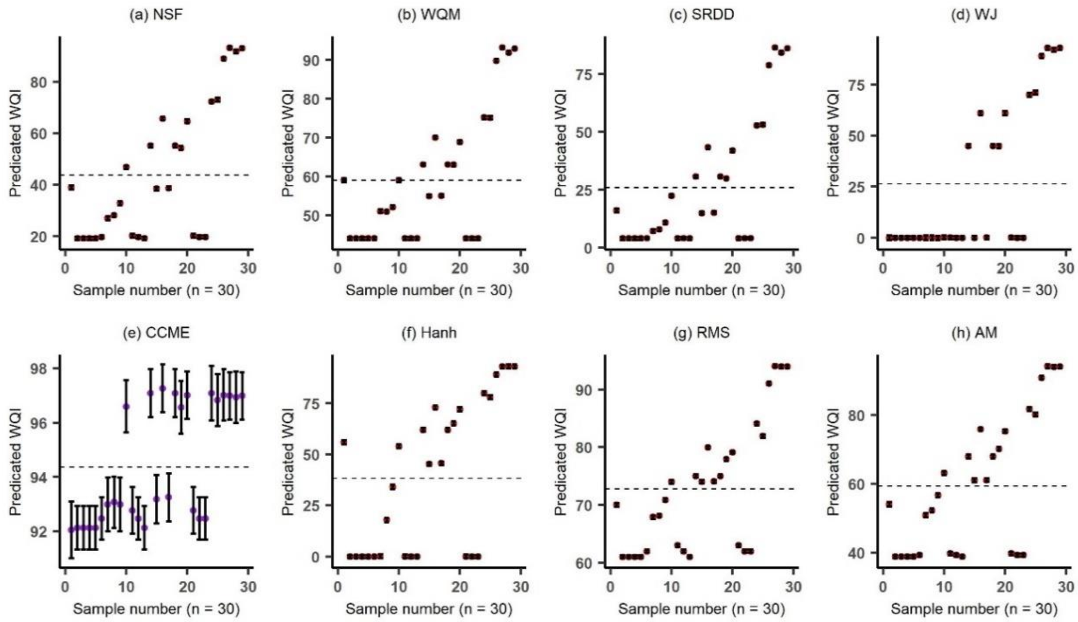


Figure 4.15. GPR-predicted WQI values for winter in Cork Harbour. 95% CI bars are shown with various individual GPR means for monitoring site, whereas *n*=29. A population mean is marked by the black dashed line.

Throughout the study period (summer and winter), there was no significant difference between the predicted and actual WQI mean, SE, or uncertainty intervals. As can be seen in Figure 16, there was a strong statistically significant difference among the WQI models at p < 0.0001 in this research. During both seasons, the WQM model had the most consistent WQI variation with the lowest uncertainty and SE trend (Table 5). Similarly, the NSF model had lower SE and shorter intervals than the SRDD and WJ models, which exhibited stronger effects of uncertainty. In terms of seasonal variability of WQI model uncertainty, a significant statistical difference (p < 0.0001) was found for the WQI models between summer and winter seasons (Fig. 16).

Table 4.5. t-statistics of GPR predicted WQI values for df = 9999, at 95% confidence level, where p < 0.0001.

WQI models	Summer				Winter			
	t-value	Mean	SE	SD	t	Mean	SE	SD
NSF	417	63.62	0.152	15.27	292	33	0.11	11.34
WQM	**669**	75.0	0.11	11.2	**767**	53.7	0.07	6.99
SRDD	242	43.11	0.18	17.78	134	12.56	0.1	9.4
WJ	47	15.0	0.31	30.95	21	1.73	0.083	8.3
CCME	**9.24E+07**	96.86	0	1.04	**1.25E+06**	94.35	0.0	0.08
Hanh	369.6	62.21	0.17	16.83	52.66	9.05	0.18	17.19
RMS	**1242**	75.0	0.06	6.03	**1082**	71.021	0.07	6.6
AM	**761**	66.32	0.08	8.71	**4304**	58.98	0.01	1.37

**Bold values indicates the higher data variation.*

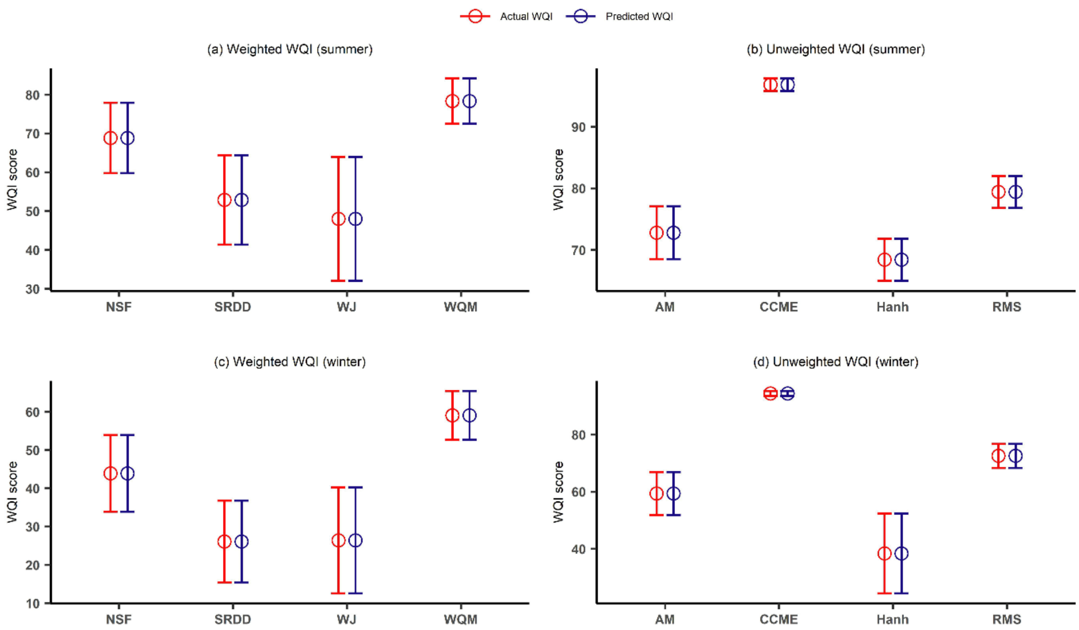


Figure 4.16. WQI score means with 95% CI bars for weighted and unweighted WQI models when n is 29, p < 0.0001. "Overlap" refers to the fraction of the average CI

error bar arm, i.e., the average of the various WQI model arms. [see Cumming et al., (2007) for the details of CI overlap rule].

Overall, the model intercomparison for GPR-predicted WQI mean, SE, and CI implies that the WQM is the most effective model for assessing coastal water quality in terms of reducing model uncertainty. The ranking of WQI models in terms of generated uncertainty levels, from highest to lowest, is as follows based on the MCS and GPR analyses:

(a) Weighted WQI models: WJ > SRDD > NSF > WQM

(b) Unweighted WQI models: Hanh > AM > RMS > CCME

4.5.5 WQI model intercomparison

The Tukey's HSD approach was used for pair-wise analysis to intercompare WQI models. Figure 4.17 presents differences between the model means for all combinations of model pairs. There was very little difference between the weighted WQM model and unweighted RMS model for summer period; this is also confirmed by the box plot statistics in Figure 4.18a. A small difference was also found for the NSF-Hanh model pair. The largest differences in means were found during the winter period, and this is also confirmed by the boxplot statistics. There was a significant difference (F value for summer = 7127 and winter F = 38675 at $p < 0.0001$ respectively) in pairwise comparison ($p < 0.0001$) between weighted and unweighted WQI models.

In terms of individual models, the WQM is significantly better than other WQI models during both the summer and the winter period; it was clearly presented in Figure 4.18 data obtained from the HSD Tukey test. However, the CCME shows an identical statistical pattern to the other models over the study period (Ahmed et al., 2021; Davies, 2006; Pang et al., 2021). As this study shows that the CCME aggregation function is a source of large uncertainty in the WQI model, and given that it has been shown to be highly susceptible to model eclipsing and ambiguity problems (Uddin et. al., 2022a), the CCME model is not recommended for water quality assessment (Gupta et al., 2003; Lumb et al., 2011; Mladenović-Ranisavljević and Žerajić, 2018). Based on the HSD and uncertainty results, the WQM model appears to be a reliable tool that performed better than other WQI models in this study. This agrees with the findings of Uddin et al. (2022a).

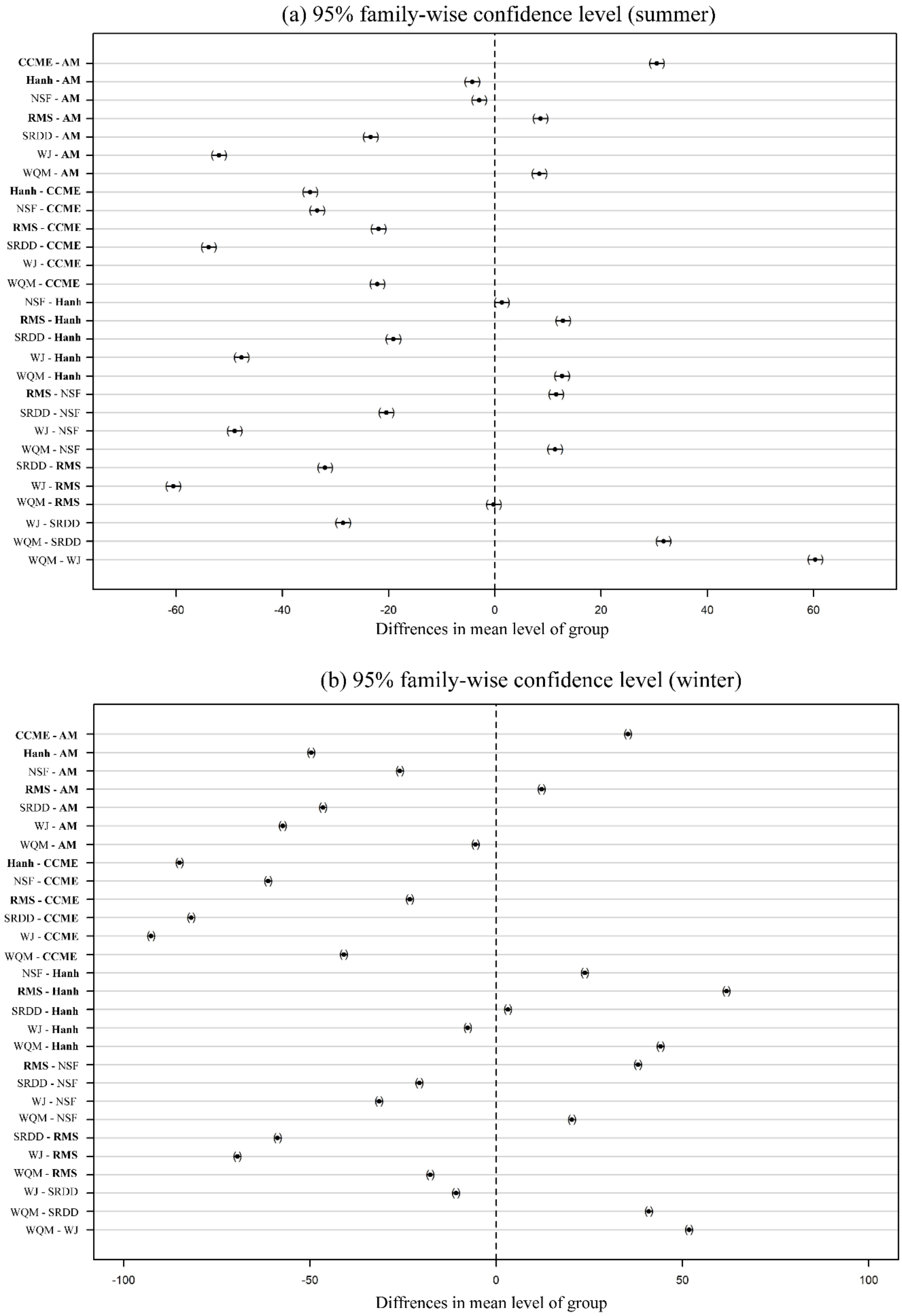


Figure 4.17. Pair-wise comparison between the WQI models with 95% CI from Tukey's HSD. The vertical dashed line indicates the point where the difference

between the means is equal to zero or the similarity of model statistics where Unweighted WQI models are in bold.

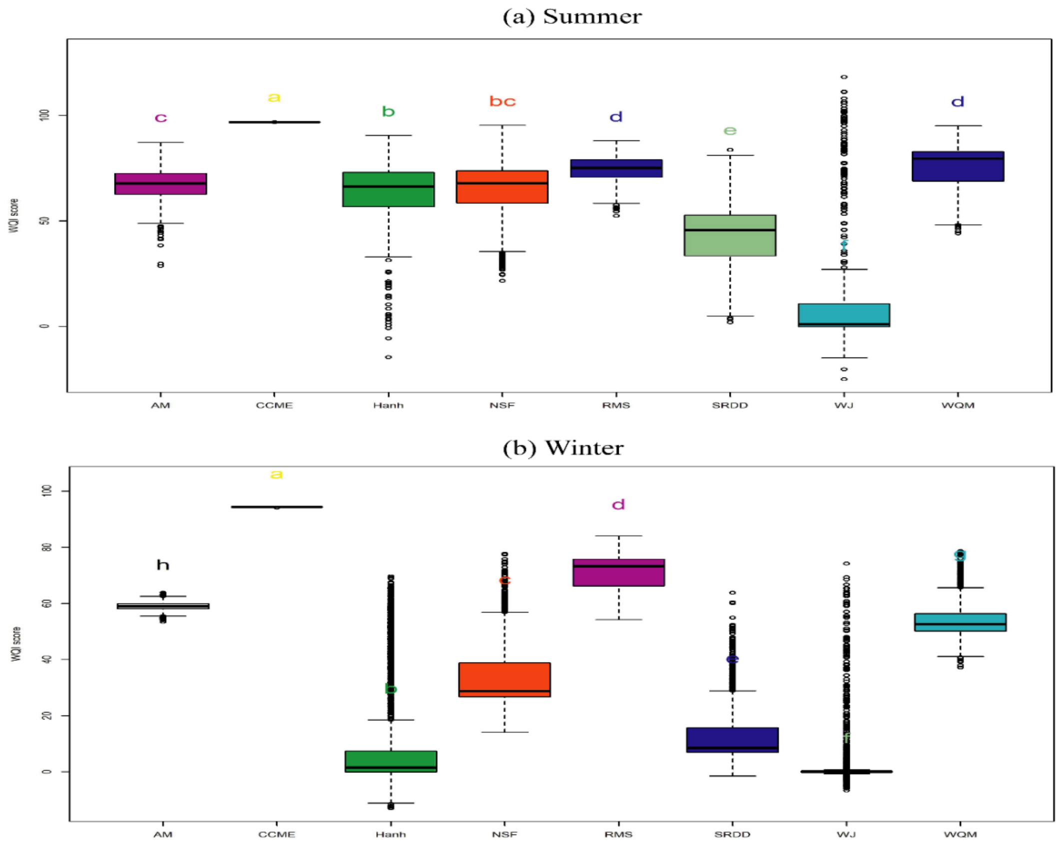


Figure 4.18. Box plots of WQI models by group with Tukey's HSD compact letter.

4.5.6 Validation of uncertainty results Summary of statistics

As assessment of the ML predicted scores versus the WQI calculated scores is presented in the Taylor diagrams of Figure 4.19. The diagram helps to visually and numerically evaluate model performance using three statistical properties namely: the centred root-mean-square deviation (RMSD), the standard deviation (SD) and the correlation (Calim et al., 2018). The statistics of the calculated and simulated WQI values in Cork Harbour for summer and winter periods are presented in Figure 4.19. For the summer period the Hanh, WQM and AM models show the smallest discrepancies and display correlation coefficients of over 95%. In winter, all WQI models cluster around very low SD (<5), low RMSD (<10) and correlation coefficients over 0.8. The CCME model, with correlation coefficients close to 1.0 and near zero RMSD and SD, again shows low discrepancies in WQI scores, but the eclipsing and ambiguity problems have to be emphasized again. With respect to aggregation function, it can be seen from the Taylor statistics that the unweighted WQI models outperform the weighted WQI models.

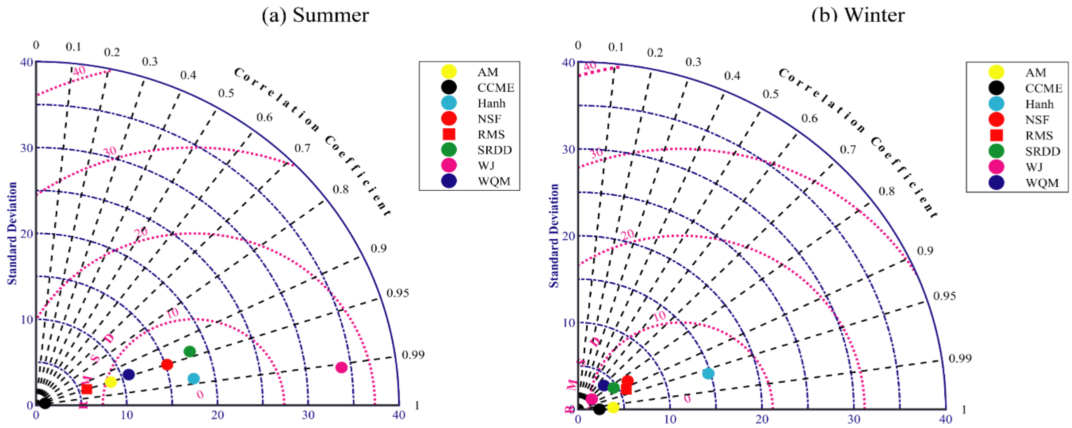


Figure 4.19 Taylor diagram statistics for different WQI models.

Overall, the Taylors diagram statistics are consistent with the findings of the MCS and GPR analyses, and reinforce the conclusion that the weighted WQM and unweighted RMS produce lowest uncertainties over the study period. In addition, compared to the weighted methods, the WQM model could be more effective and robust in assessing coastal water quality in terms of the model uncertainty problem.

4.6. Conclusion

This study is the first attempt to improve the theoretical and experimental understanding of uncertainty in a WQI model. Many researchers argue that uncertainty is produced throughout the various stages of WQI modelling. Most of the recent studies imply that the processes of model indicators selection and sub-indexing play a significant role in generating uncertainty in a WQI model. Some studies suggest that the weighting process also has an effect on the WQI model's efficiency and accuracy. To date, several studies have been conducted which try to evaluate WQI model uncertainty by comparing very generalized statistical measures, but the present study is the first effort to estimate model uncertainty by taking the effect of the individual model stages into account. In this research, a comprehensive quantification of model uncertainty at each step of the WQI model was conducted to understand the individual and combined effects of each contributor of uncertainty in the model. The MCS technique was applied to estimate the WQI model uncertainty, while the GPR algorithm was utilized to predict uncertainties. The major findings of this study can be summarized as follows:

- The values of the selected water quality indicators generated less than 1% of the total model uncertainty; however, the number of input indicators was found to have a significant impact on the model's input uncertainties.
- Sub-index functions were found to contribute significantly to the WQI model uncertainties, and hence affect the model reliability. Therefore, the determination of sub-index functions needs to be taken with care.
- The weighting component produces relatively low levels of uncertainties.
- Significant statistical differences were found between the eight aggregation functions tested. The weighted quadratic mean (WQM) function was found to provide a plausible assessment of the WQ of coastal waters at reduced uncertainty levels. The findings of this study also suggest that the unweighted root mean squared (RMS) aggregation function could also be potentially used for assessment of coastal WQ.
- Finally, the WQM and RMS models were found to exhibit a higher prediction accuracy and these WQI models could be effective and reliable tools to provide low-uncertainty assessment of water quality status.

This research provides a robust statistically sound methodology for assessment of WQI model uncertainties. A set of statistical tools in this method can be used to identify sources of uncertainty, quantify them and evaluate their impact on the overall model performance. Therefore, the finding of this research could aid a range of stakeholders including decision-makers, researchers, and agencies responsible for water quality monitoring, assessment and management. The methodology was only tested for one domain application. For its further improvement and validation it should be applied to various types of waterbodies.

4.7 Declaration of competing interest

The authors state that they did not experience competing financial interests or personal relationships that could have been influenced by the work reported in this paper.

4.8 Acknowledgement

The authors gratefully acknowledge the editor's and anonymous reviewers' contributions to the improvement of this paper. This research was funded by the Hardiman Research Scholarship of the National University of Ireland, Galway, which funded the first author as part of his PhD program. The authors would like to thank the Environmental Protection Agency of Ireland for providing water quality data. The authors also would like to acknowledge support from MaREI, the SFI Research Centre for Energy, Climate, and Marine research. The authors sincerely acknowledge Charles Sturt University for providing all necessary supports to this PhD project through the excellent international co-supervision. Moreover, the authors also sincerely acknowledge the Eco HydroInformatics Research Group (EHIRG), School of Engineering, College of Science and Engineering, University of Galway, Ireland for providing computational laboratory facilities to complete this research.

4.9 References

Abdar, M., Pourpanah, F., Hussain, S., Rezazadegan, D., Liu, L., Ghavamzadeh, M., Fieguth, P., Cao, X., Khosravi, A., Acharya, U.R., Makarenkov, V., Nahavandi, S., 2021. A review of uncertainty quantification in deep learning: Techniques, applications and challenges. Inf. Fusion 76, 243–297. https://doi.org/10.1016/j.inffus.2021.05.008

Ahmed, M., Mumtaz, R., Zaidi, S.M.H., 2021. Analysis of water quality indices and machine learning techniques for rating water pollution: A case study of Rawal Dam, Pakistan. Water Supply 21, 3225–3250. https://doi.org/10.2166/ws.2021.082

Asadollah, S.B.H.S., Sharafati, A., Motta, D., Yaseen, Z.M., 2021. River water quality index prediction and uncertainty analysis: A comparative study of machine learning models. J. Environ. Chem. Eng. 9, 104599. https://doi.org/10.1016/j.jece.2020.104599

BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, OIML, 2020. GUM modeling: Guide to the expression of uncertainty in measurement - Part 6: Developing and using measurement models JCGM GUM-6, 1–103.

Bui, D.T., Khosravi, K., Tiefenbacher, J., Nguyen, H., Kazakis, N., 2020. Improving prediction of water quality indices using novel hybrid machine-learning algorithms. Sci. Total Environ. 721, 137612. https://doi.org/10.1016/j.scitotenv.2020.137612

Bode, G., Thul, S., Baranski, M., Müller, D., 2020. Real-world application of machine-learning-based fault detection trained with experimental data. Energy 198. https://doi.org/10.1016/j.energy.2020.117323

Calim, M.C., Nobre, P., Oke, P., Schiller, A., Siqueira, L.S.P., Castelão, G.P., 2018. A new tool for model assessment in the frequency domain – Spectral Taylor Diagram : application to a global ocean general circulation model with tides. Geosci. Model Dev. https://doi.org/10.5194/gmd-2018-5

Carsten Von Der Ohe, P., Prüß, A., Schäfer, R.B., Liess, M., de Deckere, E., Brack, W., 2007. Water quality indices across Europe - A comparison of the good ecological status of five river basins. Journal of Environmental Monitoring 9, 970–978. https://doi.org/10.1039/b704699p

Cumming, G., Fidler, F., Vaux, D.L., 2007. Error bars in experimental biology. J. Cell Biol. 177, 7–11. https://doi.org/10.1083/jcb.200611141

Davies, J.M., 2006. Application and tests of the canadian water quality index for assessing changes in water quality in lakes and rivers of central North America. Lake Reserv Manag 22, 308–320. https://doi.org/10.1080/07438140609354365

Ekici, S., Unal, F., Ozleyen, U., 2019. Comparison of different regression models to estimate fault location on hybrid power systems. IET Gener. Transm. Distrib. 13, 4756–4765. https://doi.org/10.1049/iet-gtd.2018.6213

Elgeldawi, E., Sayed, A., Galal, A.R., Zaki, A.M., 2021. Hyperparameter tuning for machine learning algorithms used for arabic sentiment analysis. Informatics 8, 1–21. https://doi.org/10.3390/informatics8040079

Fernandes, M., Corchado, J.M., Marreiros, G., 2022. Machine learning techniques applied to mechanical fault diagnosis and fault prognosis in the context of real industrial manufacturing use-cases: a systematic literature review. Applied Intelligence. https://doi.org/10.1007/s10489-022-

03344-3
Galal Uddin, M., Moniruzzaman, M., Khan, M., 2017. Evaluation of Groundwater Quality Using CCME Water Quality Index in the Rooppur Nuclear Power Plant Area, Ishwardi, Pabna, Bangladesh. Am. J. Environ. Prot. https://doi.org/10.12691/env-5-2-2
Grbić, R., Kurtagić, D., Slišković, D., 2013. Stream water temperature prediction based on Gaussian process regression. Expert Syst Appl 40, 7407–7414. https://doi.org/10.1016/j.eswa.2013.06.077
Gupta, A.K., Gupta, S.K., Patil, R.S., 2003. A comparison of water quality indices for coastal water. J Environ Sci Health A Tox Hazard Subst Environ Eng 38, 2711–2725. https://doi.org/10.1081/ESE-120024458
Goeman, J.J., Solari, A., 2021. Comparing Three Groups _ Enhanced Reader.pdf. Am. Stat. https://doi.org/https://doi.org/10.1080/00031305.2021.2002188
Haghiabi, A.H., Nasrolahi, A.H., Parsaie, A., 2018. Water quality prediction using machine learning methods. Water Quality Research Journal 53, 3–13. https://doi.org/10.2166/wqrj.2018.025
Jafari, F., Javadi, S., Golmohammadi, G., Mohammadi, K., Khodadadi, A., Mohammadzadeh, M., 2016. Groundwater risk mapping prediction using mathematical modeling and the Monte Carlo technique. Environ. Earth Sci. 75, 1–11. https://doi.org/10.1007/s12665-016-5335-9
Jiang, Y., Li, C., Sun, L., Guo, D., Zhang, Y., Wang, W., 2021. A deep learning algorithm for multi-source data fusion to predict water quality of urban sewer networks. J Clean Prod 318. https://doi.org/10.1016/j.jclepro.2021.128533
Joint Committee For Guides In Metrology, 2008. Evaluation of measurement data — Guide to the expression of uncertainty in measurement. Int. Organ. Stand. Geneva ISBN 50, 134. https://doi.org/10.1373/clinchem.2003.030528
Juwana, I., Muttil, N., Perera, B.J.C., 2016. Uncertainty and sensitivity analysis of West Java Water Sustainability Index - A case study on Citarum catchment in Indonesia. Ecol. Indic. 61, 170–178. https://doi.org/10.1016/j.ecolind.2015.08.034
Khoi, D.N., Quan, N.T., Linh, D.Q., Nhi, P.T.T., Thuy, N.T.D., 2022. Using Machine Learning Models for Predicting the Water Quality Index in the La Buong River, Vietnam. Water (Switzerland) 14. https://doi.org/10.3390/w14101552
Liang, S., Jia, H., Xu, C., Xu, T., Melching, C., 2016. A Bayesian approach for evaluation of the effect of water quality model parameter uncertainty on TMDLs: A case study of Miyun Reservoir. Sci. Total Environ. 560–561, 44–54. https://doi.org/10.1016/j.scitotenv.2016.04.001
Liu, Y., Yang, P., Hu, C., Guo, H., 2008. Water quality modeling for load reduction under uncertainty: A Bayesian approach. Water Res. 42, 3305–3314. https://doi.org/10.1016/j.watres.2008.04.007
Loucks, P. D., van Beek, E., 1981. Water resource systems planning and analysis - An introduction to Methods, Models, and Applications, Advances in Water Resources.
Lumb, A., Sharma, T.C., Bibeault, J.-F., Klawunn, P., 2011. A Comparative Study of USA and Canadian Water Quality Index Models. Water Qual Expo Health 3, 203–216. https://doi.org/10.1007/s12403-011-0056-5
Meyer, V.R., 2007. Measurement uncertainty. J. Chromatogr. A 1158, 15–24. https://doi.org/10.1016/j.chroma.2007.02.082
Mishra, S., 2009. Uncertainty and sensitivity analysis techniques for hydrologic modeling. J. Hydroinformatics 11, 282–296. https://doi.org/10.2166/hydro.2009.048
Mladenović-Ranisavljević, I.I., Žerajić, S.A., 2018. Comparison of different models of water quality index in the assessment of surface water quality. International Journal of Environmental Science and Technology 15, 665–674. https://doi.org/10.1007/s13762-017-1426-8
Ng, A.W.M., Perera, B.J.C., 2001. Uncertainty and sensitivity analysis of river water quality model parameters. Prog. Water Resour. 48, 175–184.
Pang, M., Xu, R., Hu, Z., Wang, J., Wang, Y., 2021. Uncertainty and sensitivity analysis of input conditions in a large shallow lake based on the latin hypercube sampling and morris methods. Water (Switzerland) 13. https://doi.org/10.3390/w13131861
Rodríguez, E., Arqués, J.L., Rodríguez, R., Nuñez, M., Medina, M., Talarico, T.L., Casas, I.A., Chung, T.C., Dobrogosz, W.J., Axelsson, L., Lindgren, S.E., Dobrogosz, W.J., Kerkeni, L., Ruano, P., Delgado, L.L., Picco, S., Villegas, L., Tonelli, F., Merlo, M., Rigau, J., Diaz, D., Masuelli, M., 1989. Monte Carlo Simulations Applied to Uncertainty in Measurement. Intech 32, 137–144.
Rouder, J.N., Engelhardt, C.R., McCabe, S., Morey, R.D., 2016. Model comparison in ANOVA. Psychon. Bull. Rev. 23, 1779–1786. https://doi.org/10.3758/s13423-016-1026-5
Sankaran, M., Sarkar, S., 2009. Uncertainty analysis methods. Issues Quant. Qual. risk Model. with Appl. import risk Assess. ACERA Proj. 1–26.
Saufi, S.R., Ahmad, Z.A. bin, Leong, M.S., Lim, M.H., 2019. Challenges and opportunities of deep learning models for machinery fault detection and diagnosis: A review. IEEE Access.

https://doi.org/10.1109/ACCESS.2019.2938227
Seifi, A., Dehghani, M., Singh, V.P., 2020. Uncertainty analysis of water quality index (WQI) for groundwater quality evaluation: Application of Monte-Carlo method for weight allocation. Ecol. Indic. 117, 106653. https://doi.org/10.1016/j.ecolind.2020.106653
Shekar, B.H., Dagnew, G., 2019. Grid search-based hyperparameter tuning and classification of microarray cancer data. 2019 2nd International Conference on Advanced Computational and Communication Paradigms, ICACCP 2019. https://doi.org/10.1109/ICACCP.2019.8882943
Shaw, B.D., 2017. Uncertainty Analysis of Experimental Data with R. Chapman and Hall/CRC, Boca Raton : CRC Press, 2017. https://doi.org/10.1201/9781315366715
Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2018. Development of a water quality index for rivers in West Java Province, Indonesia. Ecol. Indic. https://doi.org/10.1016/j.ecolind.2017.11.049
Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2017. Using the Analytic Hierarchy Process to identify parameter weights for developing a water quality index. Ecol. Indic. 75, 220–233. https://doi.org/10.1016/j.ecolind.2016.12.043
Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2016. Development of river water quality indices—a review. Environ. Monit. Assess. https://doi.org/10.1007/s10661-015-5050-0
Tavazza, F., Decost, B., Choudhary, K., 2021. Uncertainty prediction for machine learning models of material properties. ACS Omega 6, 32431–32440. https://doi.org/10.1021/acsomega.1c03752
Uddin, M.G., Nash, S., Olbert, A.I., 2021a. A review of water quality index models and their use for assessing surface water quality. Ecol. Indic. https://doi.org/10.1016/j.ecolind.2020.107218
Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022a. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment. Water Res. 219, 118532. https://doi.org/10.1016/j.watres.2022.118532
Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022b. Development of a water quality index model - a comparative analysis of various weighting methods, in: Çiner, P.D.A. (Ed.), Mediterranean Geosciences Union Annual Meeting (MedGU-21). Istanbul, pp. 1–6.
Uddin, M.G. and Nash, S., Rahman, A., Diganta, M. T. M., Olbert, A.I., 2022c. Robust Machine Learning Algorithms for Predicting Coastal Water Quality Index. Available at SSRN: https://ssrn.com/abstract=4135697 or http://dx.doi.org/10.2139/ssrn.4135697
Wang, L., Del Fiol, G., Bray, B.E., Haug, P.J., 2017. Generating disease-pertinent treatment vocabularies from MEDLINE citations. J. Biomed. Inform. 65, 46–57. https://doi.org/10.1016/j.jbi.2016.11.004
Wu, Z., Lai, X., Li, K., 2021. Water quality assessment of rivers in Lake Chaohu Basin (China) using water quality index. Ecol Indic 121. https://doi.org/10.1016/j.ecolind.2020.107021
Wu, J., Zou, R., Yu, S.L., 2006. Uncertainty analysis for coupled watershed and water quality modeling systems. J. Water Resour. Plan. Manag. https://doi.org/10.1061/(ASCE)0733-9496(2006)132:5(351)
Xiong, Z., Cui, Y., Liu, Z., Zhao, Y., Hu, M., Hu, J., 2020. Evaluating explorative prediction power of machine learning algorithms for materials discovery using k-fold forward cross-validation. Comput. Mater. Sci. 171, 109203. https://doi.org/10.1016/j.commatsci.2019.109203
Xu, X., Lai, T., Jahan, S., Farid, F., Bello, A., 2022. A Machine Learning Predictive Model to Detect Water Quality and Pollution. Future Internet 14, 324. https://doi.org/10.3390/fi14110324
Yang, C., Liu, J., Zeng, Y., Xie, G., 2019. Real-time condition monitoring and fault detection of components based on machine-learning reconstruction model. Renew Energy 133, 433–441. https://doi.org/10.1016/j.renene.2018.10.062
Zhang, Z., Ye, L., Qin, H., Liu, Y., Wang, C., Yu, X., Yin, X., Li, J., 2019. Wind speed prediction method using Shared Weight Long Short-Term Memory Network and Gaussian Process Regression. Appl. Energy 247, 270–284. https://doi.org/10.1016/j.apenergy.2019.04.047
Zhu, M., Wang, J., Yang, X., Zhang, Y., Zhang, L., Ren, H., Wu, B., Ye, L., 2022. A review of the application of machine learning in water quality evaluation. Eco-Environment & Health 1, 107–116. https://doi.org/10.1016/j.eehl.2022.06.001
Zotou, I., Tsihrintzis, V.A., Gikas, G.D., 2019. Performance of Seven Water Quality Indices (WQIs) in a Mediterranean River. Environ Monit Assess 191. https://doi.org/10.1007/s10661-019-7652-4

5. Performance analysis of the water quality index model for predicting water state using machine learning techniques

This chapter was published in the Journal of **“Process Safety and Environmental Protection”** on November
30, 2022. Details can be found at the following web resource:
https://doi.org/10.1016/j.psep.2022.11.073

5.1 Chapter highlights

- A novel approach was developed for assessing the WQI model's performance in order to correct multi-class classification using a newly developed coastal water classification scheme incorporating ML approaches.
- Existing WQI systems’ classification problems (metaphoring problems) have addressed using ML techniques.
- Seven WQI models, including four widely used (NSF, SRDD, WJ, Hanh) and three newly proposed (WQM, RMS, and AM), were assessed and compared in terms of their performance.
- To the best of the author's knowledge, it was the first study to analyze the WQI model performance using multiclass classifiers.
- Improved ML algorithm(s) for predicting coastal water quality most accurately by comparing a range of classifiers
- XGBoost and KNN algorithms outperformed in order to correctly classify water quality
- XGBoost can be classified in most water quality classes 100% correctly, except the "poor" class.
- Weighted WQM and unweighted RMS models could be effective for avioding the metaphoring problems.
- Results of this research indicate that both models are superior to others for the correct classification of coastal water quality.

5.2 Abstract

Existing water quality index (WQI) models assess water quality using a range of classification schemes. Consequently, different methods provide a number of interpretations for the same water properties that contribute to a considerable amount of uncertainty in the correct classification of water quality. The aims of this study were to evaluate the performance of the water quality index (WQI) model in order to classify coastal water quality correctly using a completely new classification scheme. Cork Harbour water quality data was used in this study, which was collected by Ireland's environmental protection agency (EPA). In the present study, four machine-learning classifier algorithms, including support vector machines (SVM), Naïve Bayes (NB), random forest (RF), k-nearest neighbor (KNN), and gradient boosting (XGBoost), were utilized to identify the best classifier for predicting water quality classes using widely used seven WQI models, whereas three models are completely new and recently proposed by the authors. The KNN (100% correct and 0% wrong) and XGBoost (99.9% correct and 0.1% wrong) algorithms were outperformed in predicting the water quality accurately for seven WQI models. The model validation results indicate that the XGBoost classifier outperformed, including accuracy (1.0), precision (0.99), sensitivity (0.99), specificity (1.0), and F1 (0.99) score, in order to predict the correct classification of water quality. Moreover, compared to WQI models, higher prediction accuracy, precision, sensitivity, specificity, and F1 score were found for the weighted quadratic mean (WQM) and unweighted root mean square (RMS) WQI models, respectively, for each class. The findings of this study showed that the WQM and RMS models could be effective and reliable for assessing coastal water quality in terms of correct classification. Therefore, this study could be helpful in providing accurate water quality information to researchers, policymakers, and water research personnel for monitoring using the WQI model more effectively.

Keyword: water quality index; coastal water quality classification; model uncertainty; classification algorithm; Cork Harbour

5.3 Introduction

The management policy of water resource is a critical and systematic process that is associated with diverse components like as policy, law and regulations, institutional framework, advanced analytical facilities, skilled labour, well organization infrastructures, financial freedom etc. A number of framework used to implement the management policy for restoring good water quality status. The monitoring program is the most widely used approach for assessing water quality on a priority basis. Mainly, it aims is to obtain quantitative information on the physical, chemical and biological attributes of water statistical approaches (Strobl and Robillard, 2008). Whereas it has required specific resource requirements, it is particularly important to have access to technical and financial resources (Steele, 1987). The Water Framework Directive (WFD) is a useful tool that provides detailed guidelines for maintaining good water quality and a healthy aquatic ecosystem (Gikas et al., 2020). However, it has suggested a set of water quality measures for evaluating rivers and streams. In that case, it is frequently impractical and exceedingly costly for all parties involved, particularly those with minimal resources.

To date, many tools and technique have developed for assessing water quality. Water quality index model is one of them, its allows converting a vast water quality information into single numerical values more simplified way than traditional approaches (Gupta and Gupta, 2021; Uddin et al., 2021). In recent, this tool has been widely used for assessing water quality (surface and ground) due to its easy mathematical operators (Gupta and Gupta, 2021; Uddin et al., 2020, 2017). A number of WQIs have established by various countries/organizations in order to specific goals such as ground water quality index, surface quality water index etc. (Uddin et al., 2022c). This technique has been criticized for a number of reasons, including (i) uncertainty issues, (ii) model reliability, (iii) transparency, and (iv) model sensitivity. Recently, several studies have revealed that WQI model produced a considerable uncertainty to the final score due to its archetectural problem (Juwana et al., 2016; Sutadian et al., 2018; Uddin et al., 2021). Moreover, recently many researchers has revealed that the water quality index model does not express actual state of water quality due to the entire WQI index model's uses a variety of classification schemes (Uddin et al., 2021). Those are recommended for the interpretation of WQI score using many qualitative measures, including "excellent," "good," "bad," "very bad", “poor”, marginal, higher, lower etc. Consequently, different methods provide a number of interpretations for the similar water properties that contribute to considerable uncertainty in the correct classification of water quality. These types of problems can be addressed as “metaphoring problems” of classification. Concerns regarding these problems are growing as the WQI model is becoming more widely used gradually. According to recent studies, the current WQI model provides ambiguous information to the water resources manager as a result of these issues, causing waterbodies to fail to respond as quickly as required (Uddin et al., 2022a). As a response of above circumstance, it should be refined into a unique scale for determining the proper water quality classification.

Therefore, in order to obtain the WQI values, the present study used seven WQI models, including four weighted (NSF, SRDD, WJ, and WQM) and three unweighted (RMS, Hanh, and AM). Details of the various WQI models can be found in Uddin et al., (2021) and (2022a). WQI values were obtained according to the improved WQI methodology of Uddin et al. (2022a). Details of the methodology can be found in Uddin et al. (2022a). As discussed earlier, the ultimate goal of the WQI model is to classify the water quality using a classification scheme (Najafzadeh et al., 2021; Uddin et al., 2021). Typically, the WQI model's final output is a numerical value that is well known as an index score, the index score ranges from 0 to 100, with 0 indicating "worst" water quality and 100 "good" (Najafzadeh et al., 2021; Uddin et al., 2021). Moreover, many recent studies have revealed that a significant amount of uncertainty has been produced in the WQI system due to inappropriate classification schemes. Consequently, the traditional classification techniques can provide inconsistent results in the final assessment of water quality for similar groups of water quality indicators (Uddin et al., 2022a; 2021). In addition, recently a number of studies have reported that the widely used classification scheme "One Out-All Out" of the water framework directive also received much more criticism for the same problem (Latinopoulos et al. 2021; Prato et al. 2014). Therefore, in order to avoid this inaccurate assessment and optimize the metaphoring problems of existing classification systems, the authors have proposed a universal classification scheme (see Table 5.3) for assessing coastal and transitional water quality in an earlier study (Uddin et al. 2022a). Uddin et al., (2022a) have revealed that the results of water quality using the universal scheme could be effective in reflecting accurate scenarios of water quality. Details of the classification scheme and developing methodology can be found in Uddin et al. (2022a). In this research, this classification scheme was utilized to obtain the state of water quality in Cork Harbour. After obtaining the water quality classes, the WQI models performance were evaluated utilizing various machine learning classifier algorithms. For the purposes of predicting classification of water quality, recently advanced machine-learning algorithms has been widely used to reduce the model uncertainty (Islam Khan et al., 2021; Kaur et al., 2021; Malek et al., 2022; Najafzadeh et al., 2019; Najafzadeh and Ghaemi, 2019). Recently, a few studies have utilized the machine learning technique in order to assess the WQI model's reliability in terms of predicting the correct classification of water quality (Islam Khan et al., 2021; Najafzadeh et al., 2021). Up to date, most machine learning algorithms has developed for the solution of binary classification (Allwein, 2000; Babbar and Babbar, 2017). As a result, several studies have evaluated WQI models using binary classes (Islam Khan et al., 2021; Malek et al., 2022); even though most WQI models in the literature suggest using multiple classification schemes to evaluate water quality (Uddin et al., 2021; 2022e). In order to solve the multiclass problem, many researchers have developed a number of classifier algorithms using state-of-the-art machine learning technique (Bourel and Segura, 2018; Chamasemani, 2011; Tiyasha et al., 2021). For the purposes of the multiclass problem analysis, most commonly used algorithms are support vector machines (SVM), Naïve Bayes (NB), random forest, decision trees, logistic regression, k-nearest neighbor (KNN), and gradient boosting (XGBoost) classifiers (Uddin et al., 2022b). A few studies have reported that the multiple-kernel support vector regression algorithm and random forest could enhance the model's performance for predicting water quality using the WQI model (Najafzadeh and Ghaemi, 2019; Najafzadeh et al., 2021; Najafzadeh and Niazmardi, 2021). In order to predict water quality classification, recently, several studies have utilised machine learning techniques to assess the performance of water quality model in terms of binary classification of water quality (Asadollah et al., 2021; Cheryl A. Brown and Nelson, 2010; Danades et al., 2017; Savira and Suharsono, 2013). The present study utilized four classifier algorithms (including NB, SVM, KNN and XGBoost) for predicting multi-class classification of coastal water quality incorporating water quality index model. These classifiers were selected based on the initial assessment of six classifiers algorithms (see Table 5.4). Because, recently, several studies have revealed that the SVM, NB, random forest, KNN, and XGBoost classifiers are effective for the prediction of correct classification in assessing water quality (Danades et al., 2017; Dezfooli et al., 2018; Islam Khan et al., 2021; Kurt et al., 2008; Muhammad et al., 2015; Najafzadeh and Niazmardi, 2021; Prakash et al., 2018; Shakhari and Banerjee, 2019). To the best of the authors' knowledge, this study represents the first effort to evaluate the performance of a WQI model using a multi-class classifier algorithm. In order to evaluate prediction performance of classifier model(s), most studies have utilized widely the receiver operating characteristic (ROC) curves and confusion matrix to compare the model sensitivity, accuracy and efficiency in terms of multi-class classification [in that case it was considered the classification of water quality by using WQI model] (Morrison et al., 2003; Savira and Suharsono, 2013). For the development of the ROC curve(s), the present study used four classifier algorithms (NB, SVM, KNN, and XGBoost) , whereas the confusion matrix analysis technique was used for evaluating the performance of WQI model in terms of the correct classification of coastal water quality in Cork Harbour (Fawcett, 2006; Gonçalves et al., 2014).

As mentioned in earlier sections above, considering the limitations of exiting WQI model according to the findings in the literature (Uddin et al., 2021), in recent years, the authors have carried out several studies in terms of investigating the appropriate technique for selecting crucial indicators (Uddin et al., 2022a; 2022c; 2022f), developed three new sub-index functions for transferring various indicators concentration into the uniform scale (Uddin 2022a), proposed a comprehensive weighting technique incorporating machine learning and statistical based rank order centroid approaches (Uddin et al., 2022a) , proposed new two aggregation functions to reduce the model uncertainty (Uddin et al., 2022a), brand new classification scheme for assessing the state of coastal waters (Uddin et al., 2022a), sources of uncertainty and estimation them using machine learning approach (Uddin et al., 2022d). An effort to improve the method and develop a tool that can be used by environmental regulators to abate water pollution. After conducting the aforementioned studies, this study propose a more accurate algorithm for predicting and classifying coastal and transitional water quality using the brand new classification scheme in order to reduce the inconsistence of the final assessment of water quality. That could be effective for improving the WQI model performance in terms of model reliability and consistence of the assessment results.

However, the aims of this study were to assess WQI model(s) performance in order to correct classification using machine learning approaches incorporating a brand new classification scheme for the assessment of coastal and transitional water quality. The goal(s) of the study were obtained as follows:

(i) Archiving WQI score for coastal water quality using recently developed improved WQI approaches (Uddin et al., 2022a) and then determine the water quality classes was utilized the coastal water quality classification scheme (Table 5.3) .

(ii) Once the dataset was obtained, four commonly used predictive classifier models were utilized in this research to identify the best predictive model by comparing them incorporating seven WQI models.

(iii) After that, the best predictive model was applied to predict water quality class for each WQI model.

(iv) Finally, WQI models performance were evaluated using performance metrics (i.e., roc technique and confusion matrix) of machine learning predictive model.

This paper has been divided into five main sections. In the section 5.3, a brief overview of this study are provided in this section. The section 5.4 to 5.5, discussed a new set of tools and techniques that are being applied to assess model performance. Results and findings are presented in the section three. Section 5.6 discussed how to identify the appropriate WQI model using model performance metrics, Section 5.7 evaluated the various WQI models performance, and section 5.8 presents the conclusions and implications of findings the research.

5.4 Materials and methods

5.4.1 Application domain: Cork Harbour

In this research, the proposed framework was employed in Cork Harbour a case study approaches for assessing the coastal water quality in order to correct classification. Cork Harbour located on the southwest coast of Ireland is the largest natural harbour in Ireland. Cork Harbour is heavily populated and industrialized. Cork City located at the mouth of the River Lee is home to a population of approximately 125,000. When its immediate suburbs are included, the population rises to approximately 200,000 (Hartnett and Nash, 2015). The city is the industrial hub of the Irish southwest region and the surrounding hinterlands are subject to relatively intense agricultural activities which impact water quality in the region. Additionally, effluent discharges (Figure 5.1) from seven effluents treatment plants (ETPs) in the catchment area further impact water quality in the Harbour (EPA, 2016).

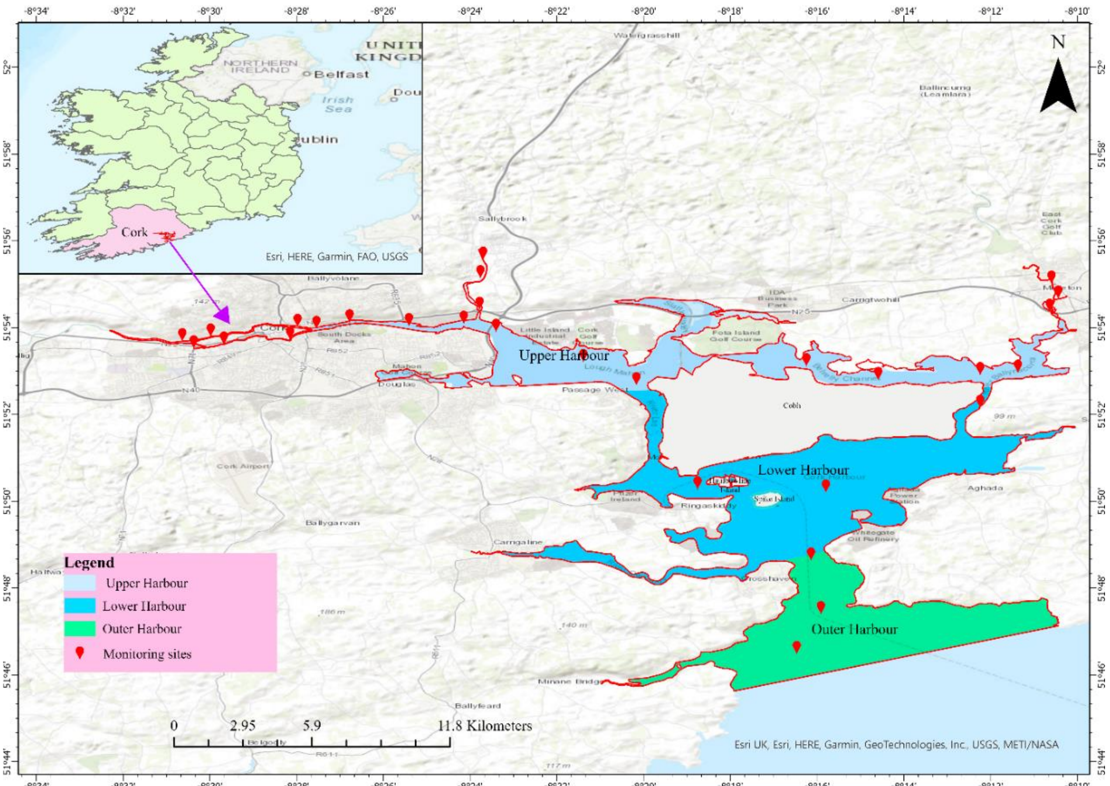


Figure 5.1. Model application domain and water quality monitoring sites in Cork Harbour, Ireland.

5.4.2 Data obtaining process

5.4.2.1 Description of water quality data

For the purposes of this study, the present study was used the water quality monitoring data in year 2019. Typically, the Irish Environmental Protection Agency (EPA) monitors the water quality of the Harbour at 32 monitoring stations. Water samples were taken from one-meter depth below water surface at approximately high and low tides over the year. In this research 29 monitoring sites were considered based on the indicators data availability and coverage of the full extents of the Cork Harbour. Details of monitoring sites and water quality indicators at each monitoring site are given, respectively Figure 5.1 and Table 5.S1 in Appendix 5. To perform this study, in total, average concentration of ten water quality indicators from the 2019 monitoring dataset were used: water temperature (TEMP), pH, dissolved oxygen (DOX), total organic nitrogen (TON), ammoniacal nitrogen (AMN), molybdate reactive phosphorus (MRP), biological oxygen demand (BOD5), transparency (TRAN), *Chlorophyll a* (CHL) (as a measure of algae), and dissolved inorganic nitrogen (DIN). Details of the water quality indicators data for Cork Harbour are available at https://www.catchments.ie/data/. Table 5.1 provides the details the statistical summary of water quality indicators and their guideline values for coastal water quality.

Table 5.1 A statistical summary and guideline values of water quality indicators for coastal water quality.

Parameter	unit	Standard threshold (Uddin et al., 2022a)		Statistical summary
		Lower	Upper	
CHL[(i)]	mg/m^3	0.0	14.2	5.32 ± 3.22
DOX[(i)]	% sat	72	128	107.90 ± 15.18
MRP[(i)]	µg/l as P	0.0	0.057	0.02 ± 0.01
DIN[(i)]	mg/l	0.0	1.208	1.54 ± 1.78
AMN[(ii)]	mg/l	0	1.5	0.07 ± 0.06
BOD5[(ii)]	mg/l	0	7	1.74 ± 0.87
pH[(iii)]	-	5	9	8 ± 0.23
TEMP[(ii)]	^{0}C	-	25	15.59 ± 0.74
TON[(iv)]	mg/l as N	0.0	2	1.48 ± 1.79
TRAN[(v)]	m/depth	>1	-	1.57 ± 1.48

(vi) ATSEBI standards, determine the standard values based on median value of Salinity (see details Toner et al., (2005)*, pp. 72 – 76).*

(vii) EPA, Ireland (2001), recommended values for the surface water/freshwater/river water/aquatic life.

(viii) Estuary Monitoring Manual for pH and Alkalinity, EPA,USA

(ix) The European Communities (Quality of surface water intended for the abstraction of drinking water) regulations, 1989 (S.I. No. 294/1989).

(x) Bathing Water Quality Regulations 2008, (S.I. No. 79/2008).

5.4.2.2 Importance of water quality indicators

Existing WQI models have utilized a range of statistical approaches for selecting the crucial water quality indicators (Uddin et al., 2021; 2022a; 2022b, 2022c). Recently, several studies have revealed that the existing techniques not effective in order to select important indicators (Sutadian et al., 2018 ; Uddin et al., 2022a). For the purposes of selecting relative importance indicators, authors have proposed an improved method in their earlier studies (Uddin et al., 2022a). Therefore, crucial water quality indicators were selected in this study according the methodology of Uddin et al., (2022a). Details the XGBoost can be found in Uddin et al., (2022a). Seven water quality indicators out of ten were found to be important for obtaining the goals of this research. Figure 5.6 presents the important water quality indicators and their relationships.

5.4.2.3 Water quality index (WQI)

A range of techniques and tools are used to assess water quality for the management of water resources. The WQI model is one of them. This technique is widely used for the assessment of water quality, i.e., surface water, groundwater, etc. It allows converting huge amounts of water quality information into a single numerical value that is well known as the index score (Parween et al., 2022; Uddin et al., 2021; 2022a). Since the development, its application has increased recently due to its ease of use and simple mathematical operators compared to other hydrological tools (Uddin et al., 2021; 2022a). In addition, this technique have received much criticism due to the model eclipsing and ambiguity problem that are described in detail in our recent study (Uddin et al., 2021).

Table 5.2 Selected seven WQI models aggregation functions and their properties according to Uddin et al., 2022a.

Types of functions	WQIs Models	Aggregation functions
(a) Weighted models	Weighted Quadratic Mean (WQM)	$WQM = \sqrt{\sum_{i=1}^{n} w_i\, s_i^2}$ ……………. (5.1)
	NSF index [Weighted Arithmetic Mean (WAM)]	$NSF = \sum_{i=1}^{n} s_i w_i$ ……………… (5.2)
	SRDD index (modified additive function)	$SRDD = \frac{1}{100}\left(\sum_{i=1}^{n} S_i W_i\right)^2$ …… (5.3)
	West Java WQI [Weighted Geometric Mean (WGM)]	$WJ = \prod_{i=1}^{n} {s_i}^{w_i}$ ………..…..…. (5.4) where s_i is the SI value for indicator *i*; w_i is weight value of respective variables and *n* is the number of indicators.
(b) unweighted models	Arithmetic Mean (AM)	$AM = \frac{1}{n}\sum_{i=1}^{n} s_i$ ……….. (5.5)
	Root Mean Squared (RMS)	$RMS = \sqrt{\frac{1}{n}\sum_{i=1}^{n} s_i^2}$ …………. (5.6)
	Hanh index	$WQI_b = \left[\frac{1}{n}\sum_{i=1}^{n} q_i \times \frac{1}{n} q_j \times q_k\right]^{1/3}$ ………… (5.7) Where, WQI_b is the basic water quality index; q_i is the subindex value of the organic; q_j is the inorganic substance; q_k is the subindex value of the biological or bacterial groups components; n is the number of components each group

For the purposes of reducing model uncertainty, Uddin et al. (2022a) recently have proposed an enhanced and comprehensive WQI approach for computing WQI scores in order to assess the coastal and transitional water quality. In this research the WQI values were computed using the improved WQI methodology of Uddin et al., (2022a). The details of the procedure can be found in Uddin et al., (2022a). This approach is shown to be more reliable than that used in existing methods because it is the most up-to-date method for computing WQI, and it may be an effective tool to avoid model uncertainty and ambiguity (Uddin et al., 2022b). For the purposes of calculating WQI values, 10,000 random samples were generated using the Monte Carlo simulation technique. Details of the technique can be found in Ratick and Schwarz, (2009). Once the random samples were obtained, the WQI values were calculated for seven commonly used WQI models, including four weighted, inclusive of the national sanitation foundation (NSF), West Java (WJ), and weighted quadratic mean (WQM), the Scottish research development department (SRDD), and three unweighted with arithmetic mean (AM), root mean square (RMS), and Hanh models using the technique mentioned above. Table 5.2 provides the seven WQI models' functions and their properties that were used in this research for computing WQI scores. Details of the model components are described in detail in Uddin et al., (2021) and Uddin et al., (2022a). In supplementary material 2 (available at https://doi.org/10.1016/j.psep.2022.11.073), details of the WQI model outcomes are given.

5.4.2.4 Interpretation of WQI model output

To date, a number of classification schemes have been proposed for assessing water quality for various purposes in the literature. Recently, several studies have revealed that the final score of the WQI model interpretation/evaluation is critical because, currently, entire WQI models use various evaluation schemes for assessing water quality. Consequently, the evaluation results of water quality varied for the unique range of scores. Therefore, the WQI model final score does not reflect the actual information of water quality. As a result, it is difficult to evaluate water quality using index scores. In our recent study, we proposed a new classification scheme for the assessment of coastal water quality based on the attributes of coastal water. It consists of four unique qualitative classes, including “good”, “fair”, “marginal”, and “poor”. A detailed classification scheme and their definitions are given in table 5.3. The present study applied this classification to determining water quality classes.

Table 5.3 Proposed classification for assessing coastal water quality by Uddin et al., (2022b).

Classifications scheme	Range of WQI score	Descriptions
Good	80 - 100	Unpolluted waterbodies are those that meet the guidelines' values. Water quality is maintained and is suitable for all uses.
Fair	50 - 79	Waterbodies that a few indicators meet the guidelines values; water quality is usually protected with a minor degree of impairment.
Marginal	30 – 49	The majority of water quality indicators failed to meet the criteria; water quality is unprotected, which may be posing a risk for aquatic life.
Poor	0 - 29	Eutrophic waterbodies are those that fail to meet all of the criteria. Water quality is completely unprotected and unsuitable for many specifics uses

5.5 Predicting classifier algorithms for classification of water quality

5.5.1 Predictive classifiers model

In order to select the classifier(s), an initial assessment of the six most widely used algorithms, including XGBoost, SVM, artificial neural network (ANN), NB, KNN, and decision tree (DT), was carried out. Table 4 provides the initial assessment results for six classifiers. It can be seen from the table below that most classifiers achieved higher prediction accuracy during both the training and testing periods, with the exception of the ANN and the DT, whereas the XGBoost obtained the highest prediction accuracy compared to other models (Table 5.4). Therefore, the present study utilized the top four ranked algorithms for the multiclass classification of coastal and transitional water quality in Cork Harbour. Details of the algorithm rank obtained based on the model prediction performance can be found in table 5.4. The following is a brief overview of selected models that were used in this study.

(i) NB classifier

Naïve Bayes is an efficient supervised machine learning algorithms that is widely used for binary/multiclass classification (Aldhyani et al., 2020). Fundamentally, Naïve Bayes classifier developed based on the Bayes theorem (Radhakrishnan and Pillai, 2020). It is scalable, requiring a set of parameters proportional to the number of variables in a learning problem (Walley and Džeroski, 1996). Naïve Bayes makes a probability decision by comparing the likelihood of two features that are independent and of equal significance (Elmachtoub et al., 2020). In this study, the NB algorithm was utilized using the same approach that can be found in Radhakrishnan and Pillai, (2020).

(ii) KNN classifier

For binary classification, the KNN is one of the most commonly used classifier in machine learning technique (Modaresi and Araghinejad, 2014). The classification of the KNN classifier is determined by measuring N number of nearest distance of neighbors (Ahmed et al., 2019). Since the KNN classifier is a more straightforward and reliable algorithm, it can be used to quickly evaluate unknown sample class data using previous learning systems. It can be easily integrated into any machine learning system without the need for prior data distribution knowledge (Modaresi and Araghinejad, 2014). For classification, the KNN classifier first calculated the distance between all sample points, then determined new classes based on the nearest sample categories. The new sample collection is used to determine the classification by taking into account the greatest number of samples' nearest neighbors (R. C. Chen et al., 2020). The KNN assumed that the distances between groups of nearest neighbors are identical (Awan et al., 2020). Usually, the distance between samples is measured using various distance metrics such as Euclidean distance, standardized euclidean distance, Minkowski distance, chebychev distance, correlation distance, city block distance, etc. In this study, the City block distance was used that is assumed by following:

$$d_{st} = \sum_{i=1}^{n} |x_{si-}y_{ti}| \quad \dots\dots\dots\dots\dots(5.8)$$

(iii) SVM classifier

The SVM classifier is another popular algorithm for the purposes of predicting binary/multi-class classification and regression in machine learning studies (Ahmed et al., 2019). It was first introduced by Boser and Guyon in 1992 (Modaresi and Araghinejad, 2014). Although it’s basic architecture was proposed by Vapnik in 1995. The general idea underlying SVM is to construct a hyperplane that allows input data to be divided into different classes in a high-dimensional space (Mohammed et al., 2018). Since it uses a high-dimensional space to detect a hyperplane using a kernel function, the SVM generates the least error in the binary classification (R. C. Chen et al., 2020; Khullar and Singh, 2021). The right classification is given by the optimal hyperplane of SVM, which is optimized based on the minimum distance between all predictors (Haghiabi et al., 2018). The maximum predictor nearest to the hyperplane is used to calculate the best decision boundary (Khullar and Singh, 2021). The SVM classifier was implemented in this study using the same algorithm that was given in detail in Singh et al., (2011).

(iv) XGBoost classifier

Boosting is the most widely used algorithm of ensemble learning method that associates combining many weak classifier models (Bourel and Segura, 2018; Tanha et al., 2020). In ML studies, this technique has recently been extensively used to identify the potential models automatically in order to classification and regression (K. Chen et al., 2020). Moreover, this algorithm is a popular technique in a variety of machine learning problems, including feature selection, confidence estimation, missing features, incremental learning, error correction, and class-balanced data, among others (Polikar, 2012). Details algorithm of the XGBoost can be found in Tanha et al., (2020). To date, several boosting approaches have been developed including AdaBoost.MH, LogitBoost, GradientBoost, XGBoost, LightGBM, CatBoost, SMOTEBoost, RUSBoost, etc. The XGBoost is updated and optimized form of the gradientboost algorithm, which is first introduced and successfully implied by Chen in 2016 (Tanha et al., 2020). For performing water quality class prediction, the XGBoost algorithm was implemented in this research because this approach is effective, and versatile in real-world application (Bourel and Segura, 2018). The procedure of the XGBoost was applied in this study using the Uddin et al., (2022b) approaches.

5.5.2 Input preparation and data pre-process for classifier

Prior to commencing the application of classifiers algorithms, it is important to standardize predictors (water quality indicators) variables in order to optimize the model training errors. In this research, data standardized using the approach of Uddin et al., 2022b. Supplementary material 2 provides the standardize water quality indicators. For the purposes of obtaining better performance of classifiers, the present study was generated 10,000 random samples using Monte Carlo simulation technique according to the methodology of Uddin et al., 2022d. After obtaining WQI values for each WQI model, water quality classes were determined using the classification scheme in Table 5.3. Details of the WQI values for various models can be found in Table 5.S1 (Appendix 5). Once water quality classes were obtained, input dataset prepared for the prediction models, whereas it composes including seven predictors variables and four response attributes including “good”, “fair”, “marginal” and “poor”. Details input data can be found in the supplementary materials 2. When the input was prepared, four predictive models were developed for predicting water quality classes incorporating various WQI models.

Table 5.4 Model performance of different classifiers obtained from the trial and error approaches for selecting robust algorithm(s).

Classifier algorithms	Rank (based on the model accuracy)	Accuracy (%)	
		Training	Testing
XGBoost	1	98.0	100
KNN	2	93.1	94.0
SVM	3	89.8	92.0
NB	4	90.1	91.0
DT	5	81.1	85.3
ANN	6	87.93	88.2

5.5.3 Models hyper-parameterization

A number of parameters in the underlying algorithm influences the predictive model hyper-parameterization. Model performance and highest prediction accuracy of classifier(s) depends on best set of optimal parameters, that is called tuning parameters or hyperparameter (Qian et al., 2015; Thanh Noi & Kappas, 2017). Several techniques used for tuning the optimal parameters like random search (Bergstra et al., 2012; Florea & Andonie, 2020), Bayesian optimization (Victoria & Maragatham, 2021; Wang et al., 2018), genetic algorithm (Angelova & Pencheva, 2011; Yuan & Gallagher, 2005), Hybrid tuning technique (Serqueira et al., 2020; Szabo & Genge, 2020). Recently, a few studies have utilized the automated tuning technique for identifying the best parameters in order to obtain the higher accuracy of predicting models (Hamadi et al., 2013; Huang et al., 2020). Since the development of the automated tuning approaches, the application of this technique has increased because the typical tuning techniques may lead to set the wrong parameters, time consuming and computational coast is higher (Hamadi et al., 2013). For the purposes of the hyperparameterization, we used the classification learner app (CLA) with MATLAB R2021b in this research. The CLA is a compatible environment that allows users to optimize model hyperparameters using auto-tuning techniques. The dataset is divided into two groups: training (80%) and validation (20%). In details hyperparameters tuning process can be found in the MathWorks, (1993). Table 5.5 provides the best-fitting predictive models and hyper-parameters for the four classifiers. Details of the settings parameters and procedures for four classifiers are described below:

For achieving the best performance of the XGBoost classifier, it's required to optimize a few crucial parameters (Islam Khan et al., 2022; Uddin et al., 2022a). A number of parameters, including the maximum depth of the tree, the learning rate, and the number of learners, are the key tuning parameters in XGBoost, which determine the model complexity for predicting more accurately (Kavzoglu & Teke, 2022). Commonly, a larger depth of the tree is recommended for achieving higher classification accuracy (Zhang et al., 2021). Recently, several studies have reported that too many nodes in a tree may also lead to an over-fitting problem in a classifier (Latha & Jeeva, 2019; Wu et al., 2020). Moreover, the learning rate is another crucial parameter that controls the step size at each iteration of an optimization algorithm as it advances toward a minimum of the loss function (Latha & Jeeva, 2019; Wu et al., 2020). In order to determine the best set of parameters, we tested the value of "maximum depth" from 1 to 50, the learning rate ranges between 0.1 to 1, and the number of learners was tested 1000 for all seven training sample subsets whereas other parameters were set at the default value.

In the KNN classifier, the k plays a significant role in enhancing the prediction performance of the KNN (Akbulut et al., 2017; Thanh Noi & Kappas, 2017). To obtain a higher performance of the classifier, the present study used the automated Bayesian approach by implementing the CLA in MATLAB for the determination of the best value of k. In this research, the k values (k = 34) were obtained for all training sets, whereas other parameters were set as default.

On the other hand, the SVM classifier is another widely used algorithm for solving multiclass classification problems (Thanh Noi & Kappas, 2017). In terms of obtaining higher value of accuracy of the SVM, several identical parameters play a vital role in improving the SVM classifier's performance; the kernel function is one of them. Recently, different types of kernel have been widely utilized for predicting water quality using the SVM classifier in water research (Najafzadeh & Niazmardi, 2021). Commonly, four types of kernel functions, including linear, radial basis function (RBF), polynomial (cubic) and sigmoid kernels, are used most frequently in SVM algorithms (Kavzoglu & Colkesen, 2009; Talabani & Avci, 2019). In this study, the kernel function was selected using automatic tuning of hyperparameters using the Bayesian optimization approach (Victoria & Maragatham, 2021). For predicting multiclass water quality, the present study determined the cubic polynomial kernel function for all training sets. In addition, many studies have revealed that the cubic polynomial kernel function is more effective than others for predicting water quality (Chia et al., 2022; Hanoon et al., 2022; Leong et al., 2021). The box constraint is another crucial parameter in the SVM model that controls the maximum penalty rate, which may help to avoid the overfitting problem in the classifier (Kienzle & Schölkopf, 2005; Piccialli & Sciandrone, 2022). The present study optimized the box constraint using an automated Bayesian tuning technique, whereas the optimal value of the box constraint was set at 4.86 for all training sets in the SVM model (Table 5.5).

Table 5.5 Optimized hyper-parameters of four predicting classifiers models.

Model hypermeters	Optimized value			
	NB	KNN	SVM	XGBoost
Distribution	Kernel	-	-	-
Kernel type	Gaussian	-	cubic	-
Kernel scale	-	-	1	-
Box constraint	-	-	4.86	-
Iterations	30	30	30	30
Support	-	-	-	
Standardized	true	false	true	true
Number of neighbors	-	34	-	-
Distance metrics	-	City block	-	-
Distance weight	-	Squared inverse	-	-
Learning rate	-	-	-	0.2
Number of learners	-	-	-	334
Ensemble method	-	-	-	XGBoost
Maximum depth	-	-	-	5
Subsample	-	-	-	1
Lambda	-	-	-	1
Multiclass method	-	-	One-vs-all	-

In the case of Naive Bayes (NB), it is a widely used probabilistic classifier that is driven by Bayesian statistics (Banchhor & Srinivasu, 2020). Recently, this classifier has been widely used for classifying the water quality and predicting the states in water resources management (Ali Haghpanah jahromi & Mohammad Taheri, 2017; Neha

Radhakrishnan & Anju S Pillai, 2020; Suwadi et al., 2022; Venkata Vara Prasad et al., 2021). Mainly, the NB classifier's performance depends on two identical parameters, including data distribution and kernel function. Commonly, the Gaussian data distribution function is widely used to obtain the highest performance of the classifier (Suwadi et al., 2022; Venkata Vara Prasad et al., 2021). (In contrast to other classifiers, the NB classifier does not require parameter optimization or the setting of any tuning parameters (s). That is one of the great benefits of the NB model in terms of cutting down on the time and cost of computation (Qian et al., 2015).

5.5.4 Development process of predictive model

The details of the process are presented in figure 5.2 below. After completing hyperparameterization, four selective models run in the Python 3.9 environment using the scikit-learn module, which is a built-in module with the capability of compiling several packages for machine learning. Moreover, for the purposes of ROC curve analysis, the Yellowbrick module was utilized in this study, which is specially designed for the analysis of multiclass classification and visualization of ROC and AUC of ROC. Finally, model results were evaluated and visualized using the Matplotlib library. All the analysis has been carried out in this research using the Python programming language.

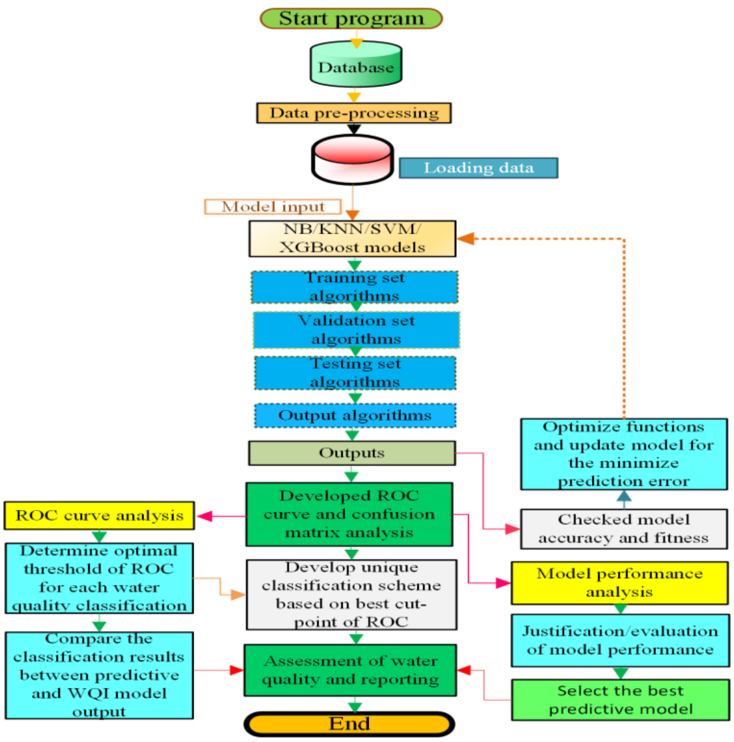


Figure 5.2. A conceptual framework of this research.

5.5.5 Evaluation criteria of predictive model

In machine learning techniques, cross validation is widely used approach to evaluate the model's performance. In this research, 10-fold cross validation was applied to measure the accuracy of the predictive model in order to allow multi-class classification. Moreover, in binary or multiclass classification, another technique is the ROC approach that is most commonly used for selecting the best predictive classifier model. In addition, the confusion matrices of the ROC curve are utilized to evaluate the diagnostic results and assess the model performance. The confusion matrices are a cross-reference tables that store the number of occurrences between cells (Figure 5.3). Figure 5.3 presents the proposed architecture of the confusion matrices of the classifier model for the solution of multi-class classification of the WQI model(s).

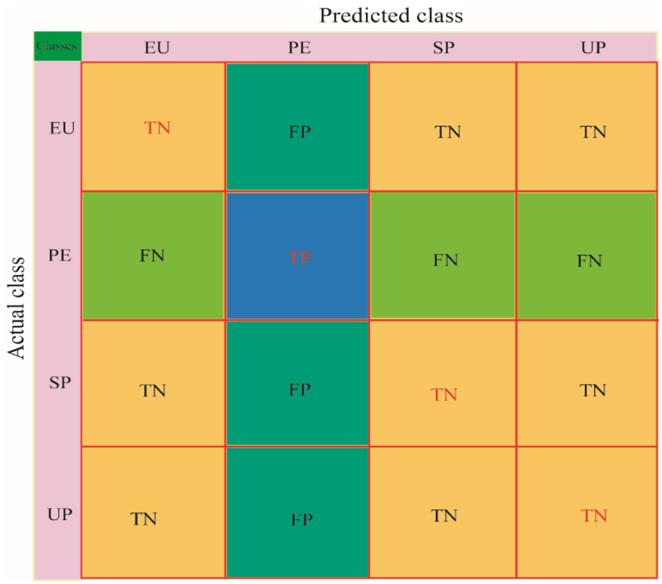


Figure 5.3. Proposed architecture of the confusion matrices of the multi-class classification predictive model of WQI model.

For evaluating the classification performance of prediction models, the confusion matrices used to evaluate the performance of model accuracy and sensitivity in a machine learning technique. Commonly, a confusion matrices composes including four components (i) true positive (TP), (ii) false negative (FN), (iii) false positive (FP) and (iv) true negative (TN). The present study, the accuracy, precision, sensitivity, F1 score and area under the curve (AUC) of receiver operating characteristics (ROC) were used. Model evaluation metrics were computed using equations (5.9) – (5.12) according to the methodology of Saberi-Movahed et al., (2022) and Mehrpooya et al., (2021).

A ROC curve associated with the average value of the sensitivity for all possible values of specificity within a predicted classifier model (Mandrekar, 2010). In this study, the ROC curve was obtained by considering the cumulative percentage of WQI probability scores (on the x axis) and the cumulative percentage of WQI values occurrence (on the y axis).

Accuracy is widely used criteria to evaluate the classification in machine learning approach (Mehrpooya et al., 2021; Saberi-Movahed et al., 2022). It is defined as follows:

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN} \dots\dots\dots\dots\dots\dots (5.9)$$

Another important measures precision refers to how close the measurements between the algorithm predictions and observations of the same classification are to each other. The precision of the model is expressed as follows:

$$Precision = \frac{TP}{TP + FP} \quad \dots\dots\dots\dots\dots\dots\dots (5.10)$$

Usually, the true positive rate refers to the model sensitivity or recall. It measures how frequently the algorithm detects the correct classification from the given data whereas the actual correct classification has occurred in dataset. In particular, false negative are the classes that have labelled as negative by the classifier model whereas the observation classes are actually positive. The sensitivity is defined as follows:

$$Sensitivity\ or\ recall = \frac{TP}{TP + FN} \quad \dots\dots\dots\dots\dots\dots\dots\dots (5.11)$$

The F1-score is another measure of a model’s accuracy on a data set. It is used to evaluate multiclass classification. It is an approach to harmonizing the precision and recall of the predictive model. The F1-score is obtained following:

$$F_1\ score = 2 \times \frac{Precision \times Sensitivity}{Precision + sensitivity} \dots\dots\dots\dots\dots (5.12)$$

where;

(i) **TP:** the actual observation indicates that water quality classes has classified accurately and the model predicted correct classification of water quality from the given data.

(ii) **TN:** the actual observation indicates that water quality classes has classified accurately but the model detected incorrect classification of water quality from the given data.

(iii) **FP:** the actual observation refers that water quality classes has not classified accurately whereas the model also detects the incorrect classification of water quality from the given data.

(iv) **FN:** the actual observation reveals that water quality classes has not classified accurately although the model predicted correct classification of water quality from the given dataset.

5.5.6 Developing the ROC curve

In general, the ROC curve computed the classification model that applies a probability, confidence interval or ranking to each prediction (Hamel, 2011). Several models, such as Nave Bayes (Fawcett, 2006), artificial neural networks (Hamel, 2011), and SVM, generate rankings as part of their algorithm (Cristianini & Shawe-Taylor, 2000). The prediction ranking is commonly employed in a ROC algorithm to achieve distinct decision thresholds in each prediction step, ranging from the highest to the minimum ranking value. Typically, prediction-rating values are used for classification to normalize decision threshold values between 0 and 1 where the default threshold is set to 0.5. In terms of model efficiency, the ROC curve was developed using the true positive and false positive rates at each threshold stage. Structurally, the traces a curve from lower left corner to upper right corner (diagonal) in the ROC curve. In order to model performance, the left part of the curve indicates the excellent performance thresholds (conservative) and the right part of the curve dealing with the poor decision thresholds (liberal) (Hamel, 2011). In this study, the ROC curves were obtained from four predictive classifier models. These are presented in figures 5.7 and 5.8 respectively for the weighted and unweighted WQI models. Commonly, a ROC curve allows examining two basic features for testing the efficiency of the model/method:

(i) To get the right classification, the ROC curve makes it possible to assess the overall performance of a predictor attribute. The significance of discrimination measures when analyzing an area under the ROC curve's (AUC);

(ii) It is to make it possible to compare efficiency between predictors in order to correct classification in terms of given classification schemes; and

It offers to identify the optimal threshold value of the predictor variable that refers to the optimal cut-point of ROC associated with true positive rate (TPR) and the lowest false positive rate (FPR).

5.5.7 Justification of predicted classification

The ROC curve technique used to evaluate the performance of predictive classifier model. Also, it is one of the most often used technique in machine learning approaches since it provides a variety of assessments in terms of model sensitivity and specificity (Morrison et al., 2003).

ROC analysis has been used in several recent studies to validate predictive models an d assess the discrimination capabilities of a continuous variable as a classifier (Cheryl A. Brown and Nelson, 2010; Yin, 2017). This technique widely used by the biomedical field in the mid-nineteenth century to evaluate the reliability of diagnostic tests (Mandrekar, 2010). In 2003, Morrison et al. (2003) applied this technique to assess the beach water quality and its ability to identify water as suitable or unsuitable for swimming purposes. Cheryl A. Brown and Nelson, (2010) provides in-depth analysis of this technique in order to assess water quality. In his analysis, Cheryl A. Brown and Nelson, (2010) identify the optimal thresholds in the ROC curve associated with the excess water quality in the ocean. The present study has utilized this technique to evaluate the classification performance of WQI model. Details technique can be found in Brown and Nelson, (2015) and Morrison et al., (2003). For the purpose of this analysis, three steps were followed in this study:

(i) A common comparison matrix was computed in order to assess the overall discrimination capacity of multiple random variables for classification into four groups. Figure 5.4 provides the confusion matrix for four predictive classifiers.

(ii) Once the comparison matrix was obtained, it was used for the direct comparison of the abilities of different variables for the determination of how many classes were classified correctly (e.g., water quality as "good," "fair," "marginal" or "poor").

(iii) Finally, the optimal cut-off point of ROC was used to determine the best WQI model, which is associated with the optimum sensitivity and specificity trade-off of the model classification.

5.5.8 Evaluation of classification performance of WQI model

The AUC of the ROC curve is an identical indicator for evaluating the model performance using AUC value; it expresses the overall measure of test performance and allows to define the level of prediction accuracy of predicted classes (Morrison et al., 2003; Tesoriero et al., 2017). It also provides the likelihood of model classification (Hamel, 2011). In the present study, we utilized the AUC value for evaluating the predicting performance of classifiers. In order to determine the correct classification, the prediction was then compared to the actual classes of water quality. The AUC value ranges from 0 (no discrimination capability) to 1 (outstanding discrimination) (Walter, 2005). Five important interpretations could be useful to evaluate the classifier's performance. According to Hosmer and Lemeshow (2004), the following interpretations:

(i) Outstanding discrimination (AUC $\geq$ 0.9): the classifier model is capable to classify all classes correctly.

(ii) Excellent discrimination capability (AUC =0.8 - 0.9): there is a high chance that the classifier is classified correctly.

(iii) Acceptable discrimination (AUC 0.70 - 0.79): classifier performance is acceptable with a few misclassification

(iv) Poor discrimination (AUC 0.5 – 0.7): classifier is classified features with higher wrong classification; and

(v) The model has no discrimination capability (AUC $\leq$ 0.5): the classifier is not able to distinguish among classes.

5.6 Results and discussion

5.6.1 Statistical summary of WQI models input (indicators) and output (WQI scores)

5.6.1.1 A statistical summary of WQI models input (indicators)

Figure 5.4 presents the Z statistics of water quality indicators in Cork Harbour during study period. Most water quality indicators were found within the limit of coastal water quality guidelines, except for DOX, MRP, DIN, TON and TRAN. (Table 5.S1). As shown in figure 5.4, normal data distribution was found for the BOD_5, MRP, and pH, whereas most indicators showed positive skew data distribution pattern except for the TRAN and TEMP (Figure 5.4). Most water quality indicators Z scores were found to be between -2 and +2 with the exception of MRP. The results of Z statistics revealed that most indicators had a significant impact on water quality in Cork Harbour except BOD_5, CHL and pH. Except these indicators, all indicators had presence the data outliers through the study period.

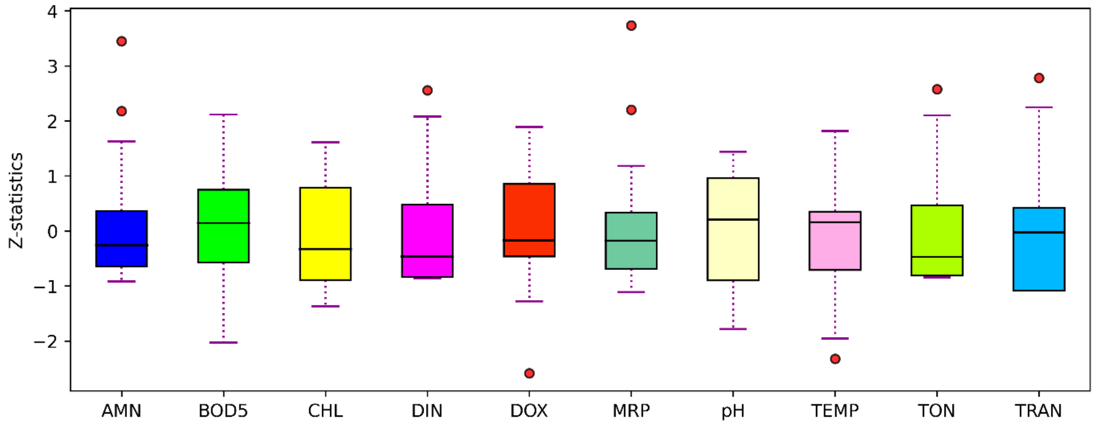


Figure 5.4. Z statistics of water quality indicators.

5.6.1.2 A statistical summary of WQI models output (WQI scores)

Figure 5.5 shows a statistical summary of different WQI scores in Cork Harbour through the study period. Appendix 5 has more information on the outcomes of different WQI models and their implications for the status of the water quality. Compared to the weighted WQI models, a significant difference was found among models, whereas higher index variation was calculated for the WJ and SRDD models, respectively. Except for the Hanh index, no noticeable differences were observed between the models when compared to the unweighted models. However, a comparatively large index score variation was found in the weighted SRDD and WJ models in Cork Harbour over the study period. The results of the WQI scores were in line with the authors' earlier studies (Uddin et al., 2022a; 2022b; 2022f).

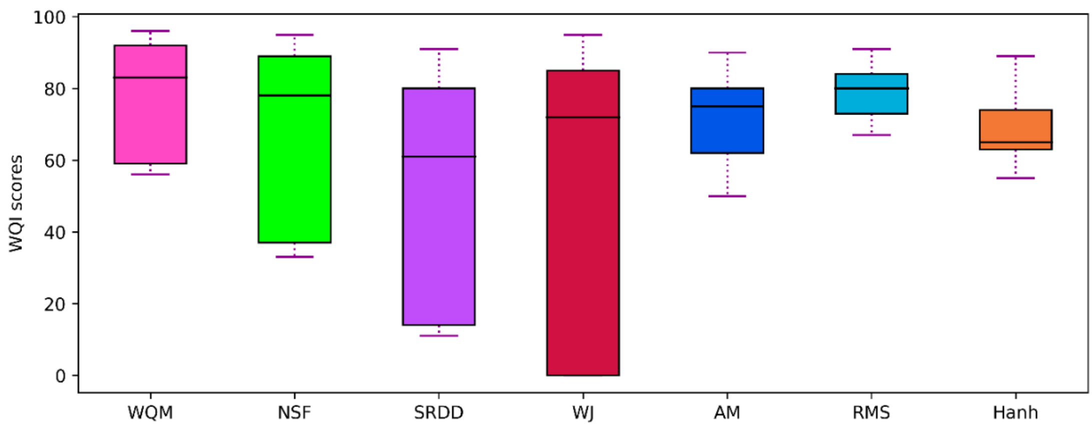


Figure 5.5. Statistical overview of various WQI model outcomes.

5.6.2 Selecting important predictors for the classifier model(s)

In order to determine the effect of water quality indicators on classification, the present study performed a relative importance analysis using the XGBoost algorithm. In this research, we found the outperforming impact of TRAN, CHL, AMN, and MRP on water quality in Cork Harbour. Figure 5.6(a) shows the indicators of importance and their relative ranks.

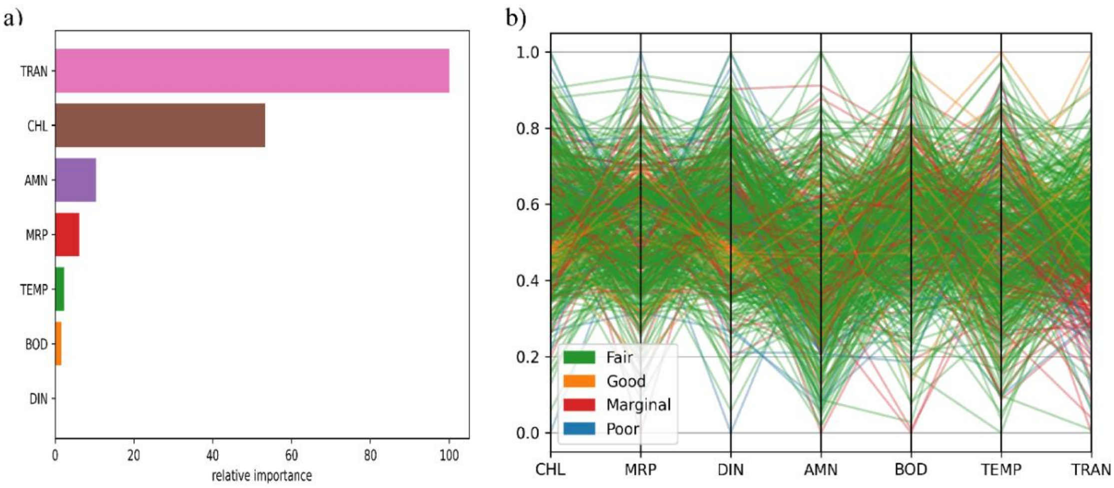


Figure 5.6. Attributes of water quality indicators: (a) relative importance and (b) parallel coordinates for seven important water quality indicators.

Moreover, in the present study, we utilized the parallel coordinates technique for the determination of relationships between water quality indicators and the tracing of the effectiveness association between them in various water quality classes. It was visualized in figure 5.6(b). It can be seen from Figure 5.6b that the TRAN and CHL highly dominated on marginal water quality, whereas DIN showed a higher impact on the poor water quality in Cork Harbour.

5.6.3 Results of confusion matrix

The aim of the present study was to compare the performance of the four machine learning classifiers in order to identify the best algorithms in terms of correct classification. The results of the classifiers were evaluated using five validation metrics (accuracy, precision, sensitivity, specificity, and F1 score) for the imbalanced dataset, the confusion matrices is one of them. Figure 5.7 shows the confusion matrix for the four predictive classifiers models. In this analysis, 10,000 observations belonging to four classifications, including “good”, “fair”, “marginal,” and “poor”, were used to predict the classification.

(i) Confusion matrix results of NB classifier

As shown in figure 5.7(a), good water quality is classified 99.2% correctly, whereas 0.8% is classified incorrectly. In contrast, the fair water quality class is correctly classified at 92.4% and wrongly classified at 7.6%, respectively. Whereas the marginal water quality is correctly classified at 89.6% and wrongly classified at 10.4%. Similarly, for poor water quality, 52.0% of observations are correctly classified, whereas 48.0% are incorrectly classified (Figure 5.7a).

(ii) Confusion matrix results of KNN classifier

The results of KNN show that four water quality classes are 100% correctly classified. There was no prediction error in the classification (Figure 5.7b). That means the KNN model had an overfitting problem, which may be due to the imbalanced dataset (Japkowicz, 2000).

(iii) Confusion matrix results of SVM classifier

In the SVM classifier, an average of 95% of the observations are classified correctly for all water quality classes except for poor water quality (Figure 5.7c). Only 78.5% of the observations were correctly classified into the poor class, whereas the remaining observations were classified wrongly.

(iv) Confusion matrix results of XGBoost classifier

The XGBoost is classified water quality 99.5% correctly for all water quality classes in Cork Harbour (Fig.5.7d).

Based on the confusion matrices results, in order to predict the correct classification of water quality, the XGBoost showed outperformance when compared to the confusion matrixes of four predictive classifiers.

Figure 5.7. Results of confusion matrices obtained from the tested four prediction models for the multi-class classification of water quality in Cork Harbour.

5.6.4 Selection of the best predictive classifier

For the purposes of the performance analysis of classifiers, the present study compared the four classification predictive models using their accuracy, precision, sensitivity, or recall, and F1 scores. Figure 5.8 shows the performance results of various predictive models. In this research, predictive accuracy was found to be 91%, 94%, 92%, and 100% for the NB, KNN, SVM, and XGBoost models, respectively. Compared to models, the excellent performance was found to be the XGBoost algorithm. The XGBoost model obtained the highest precision, sensitivity, and F1 scores, whereas the SVM model provided the lowest accuracy, precision, sensitivity and F1 scores (Figure 5.8). The results of the performance metrics indicate that the XGBoost algorithm is effective for predicting the correct classification of water quality by incorporating the WQI model. The results of the predictive classifiers performance are line with those of earlier studies (Aldhyani et al., 2020; Islam Khan et al., 2022; Khoi et al., 2022; Malek et al., 2022; Nasir et al., 2022).

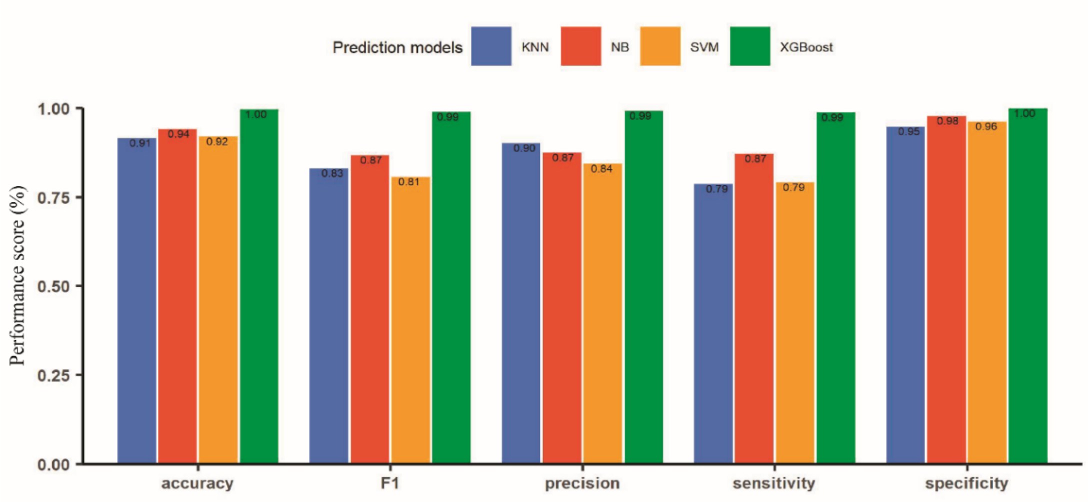


Figure 5.8. Results of evaluation criteria for various classifiers.

5.6.5 Performance analysis using ROC curve

The ROC curve is widely used to evaluate the classification abilities of the classifier predictive model (Hamel, 2011; Savira and Suharsono, 2013). Figure 5.9 and Figure 5.10 present the ROC curves for the various WQI models. They were obtained from the ROC curve technique using proposed multi-class classification schemes of coastal water quality as provided in table 5.3 above. As seen in figure 5.9 and figure 5.10, excellent performance was found for the XGBoost and KNN classifiers for the prediction of water quality using weighted and unweighted WQI models. Whereas the SVM and NB classifiers showed the worst performance for the prediction of water quality using WQI models (Fig. 5.9; Fig. 5.10). Compared to the all-predictive classifiers, the XGBoost model showed perfect performance for both weighted and unweighted WQI models. The results of ROC curves revealed that the XGBoost predictive classifier model could be effective and reliable to predict water quality class using WQI (Islam Khan et al., 2022; Khoi et al., 2022; Malek et al., 2022; Nasir et al., 2022).

Moreover, the AUC of the ROC curve is commonly used to measure the accuracy of the predictive model (Gonçalves et al., 2014; Savira and Suharsono, 2013). In this study, the AUC value was utilized to evaluate the overall performance of the predictive algorithm in order to classify water quality as good, fair, marginal, and poor. In this study, the AUC of ROC curves was calculated from the ROC curves of four predictive algorithms. According to Hosmer and Lemeshow (2004) classification based on the AUC value, the XGBoost model obtained the outstanding model discrimination for all weighted and unweighted WQI models. For all WQI models, the AUC of ROC was found to be 1, whereas the lowest values were computed for the SVM model.

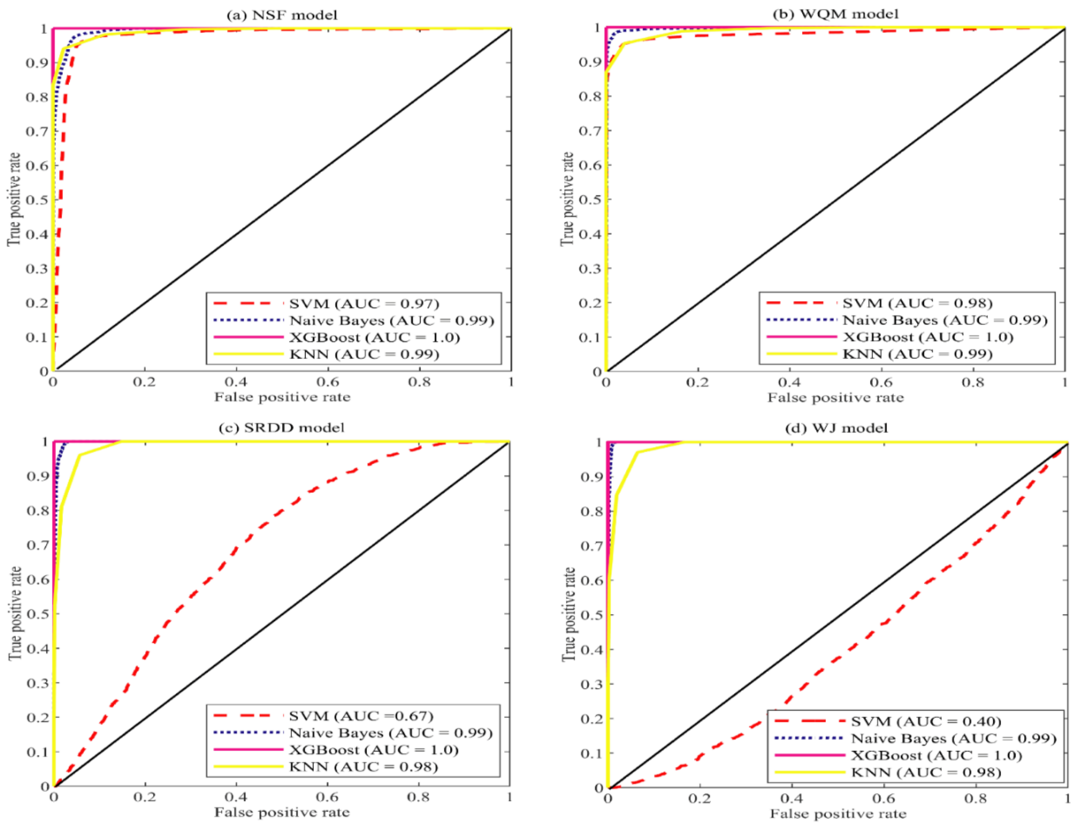


Figure 5.9. Compare the ROC curves results among algorithms for various weighted WQI models.

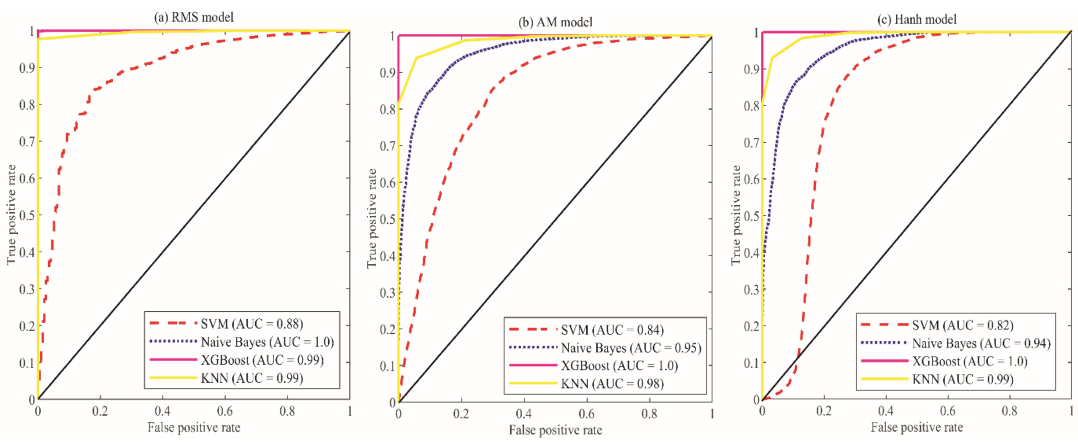


Figure 5.10. Compare the ROC curves results among algorithms for various unweighted WQI models.

5.6.6 Evaluation of classification scheme

The entire WQI index model final output composes several qualitative classes like as excellent, good, bad, very bad etc. A range of WQI models used various classification scheme to assess water quality. As a result, different methods provide a number of interpretations for same water properties that contributes a considerable uncertainty to the correct classification of water quality. In that case, the present study proposed a universal classification scheme for coastal water quality that is given in Table 5.3. In order to evaluate the classification of water quality, the present study utilized the ROC curve analysis technique. Recently, several studies applied this method to rank the water quality based on AUC of ROC curve (Asadollah et al., 2021; Garabaghi, 2021; Islam Khan et al., 2021). This method is particularly useful in finding the best cut-point value of ROC curve in terms of correct classification (Cheryl A. Brown and Nelson, 2010). For the purpose of water quality classification using WQI, the ROC curves were developed using four water quality classes, including good, fair, marginal, and poor. Figure 5.10 presents the ROC curves and AUC of the ROC curve for each water quality class. There was a significant statistical difference among the classifier models (at $p < 0.05$). As can be seen from the figure below, the XGBoost classifier correctly classifies all four water quality classes, whereas the remaining model shows excellent discrimination capability to distinguish between the four classes in accordance with Hosmer and Lemeshow (2004). The outstanding discrimination ability was found for the XGBoost model, whereas the AUC was obtained at 1.0 for each water quality class (Figure 5.11d).

Figure 5.12 shows the prediction accuracy, precision, sensitivity, specificity, and F1 score of various classifiers for predicting the water classes. As can be seen from the figure 5.11, the XGBoost classifier provided the highest accuracy for four water quality classes. The results of classifier evaluation metrics indicate that the XGBoost is the perfect classifier for predicting water quality using the WQI model.

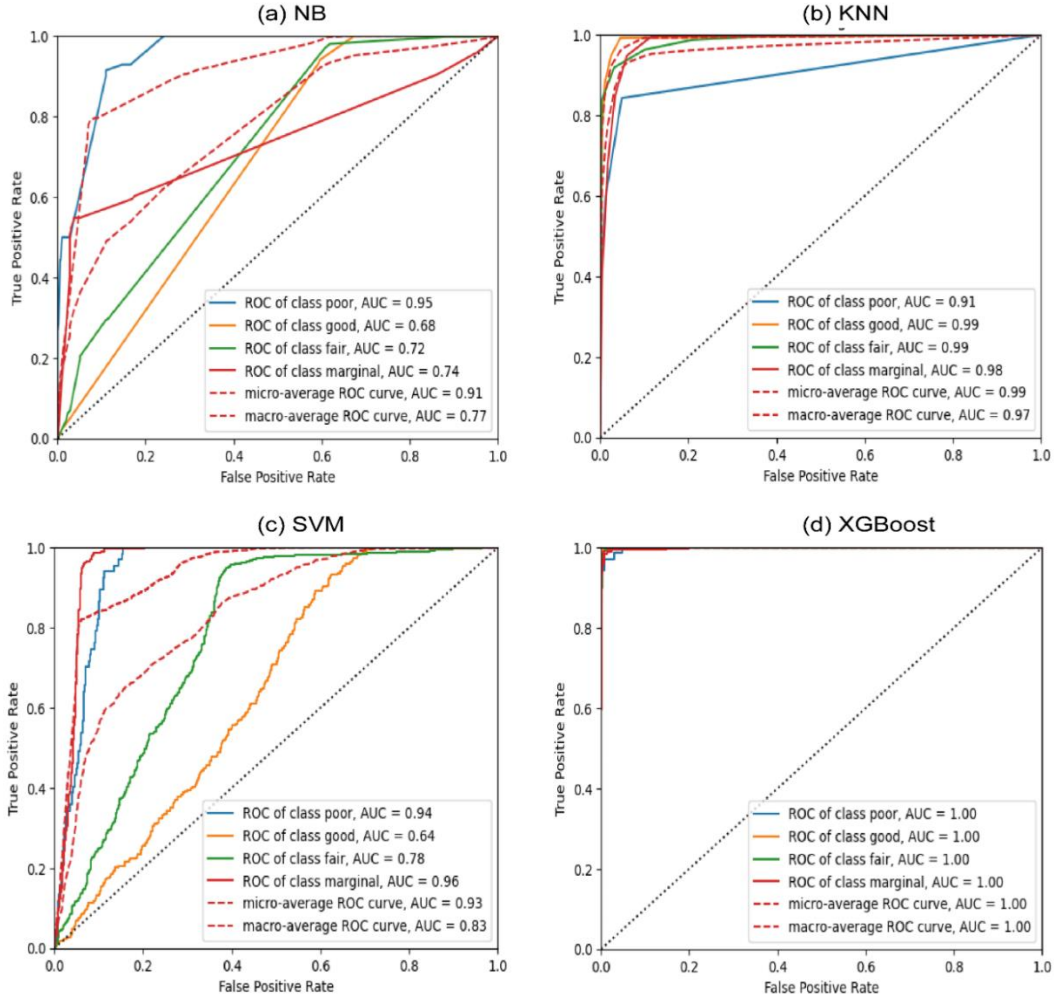


Figure 5.11. ROC curves of four classifier predictive models for the multi-class classification of water quality using WQI.

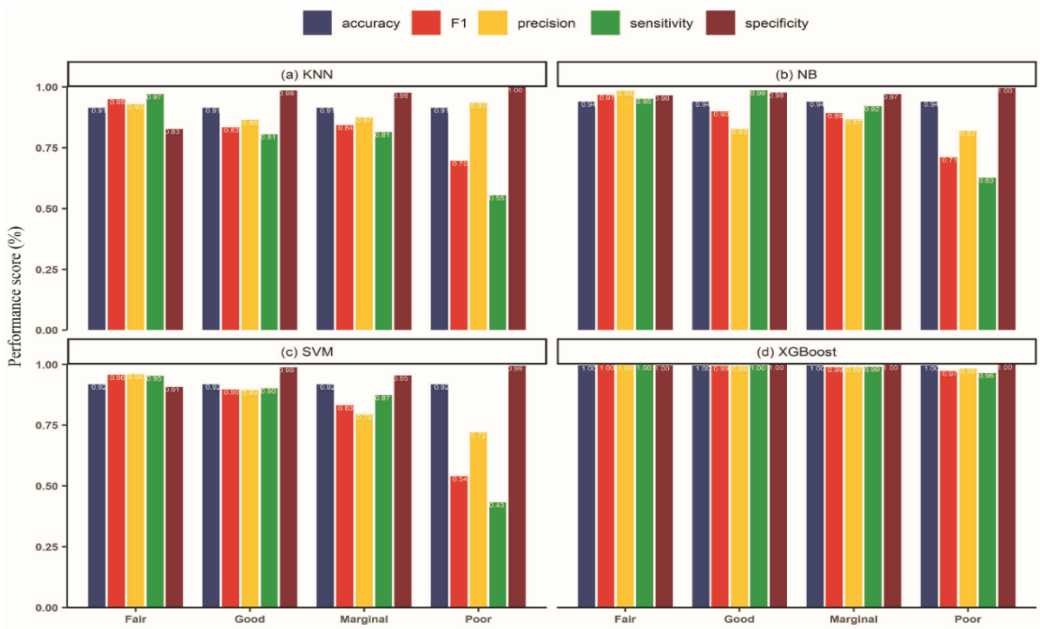


Figure 5.12. Prediction performance of various algorithms for predicting water quality classification using the WQI model.

Figure 5.12 present the prediction performance of four selected algorithms. Findings reveal that XGBoost is over performing other methods based on all five indicators. In particular, for the "good" to "marginal" classes it shows outstanding performance, while for the "poor" class it also shows nearly 96% performance score by F1, precision and sensitivity.

5.6.7 Class prediction error of classifier

Figure 5.13 presents the results of class prediction error for four classifiers. The highest class prediction error was found for the NB and SVM prediction models, whereas relatively less error was found in the KNN model. Compared to four classifiers, 99.9% of water quality classes were classified correctly by the XGBoost model. The XGBoost classified "poor" and "good" water quality nearly 100% correctly, while less than 2% prediction error was detected for the "fair" and "marginal" classes' water quality (Figure 5.13d). The results of the prediction error of classifiers consistent with those of earlier studies (Khoi et al., 2022; Malek et al., 2022; Nasir et al., 2022).

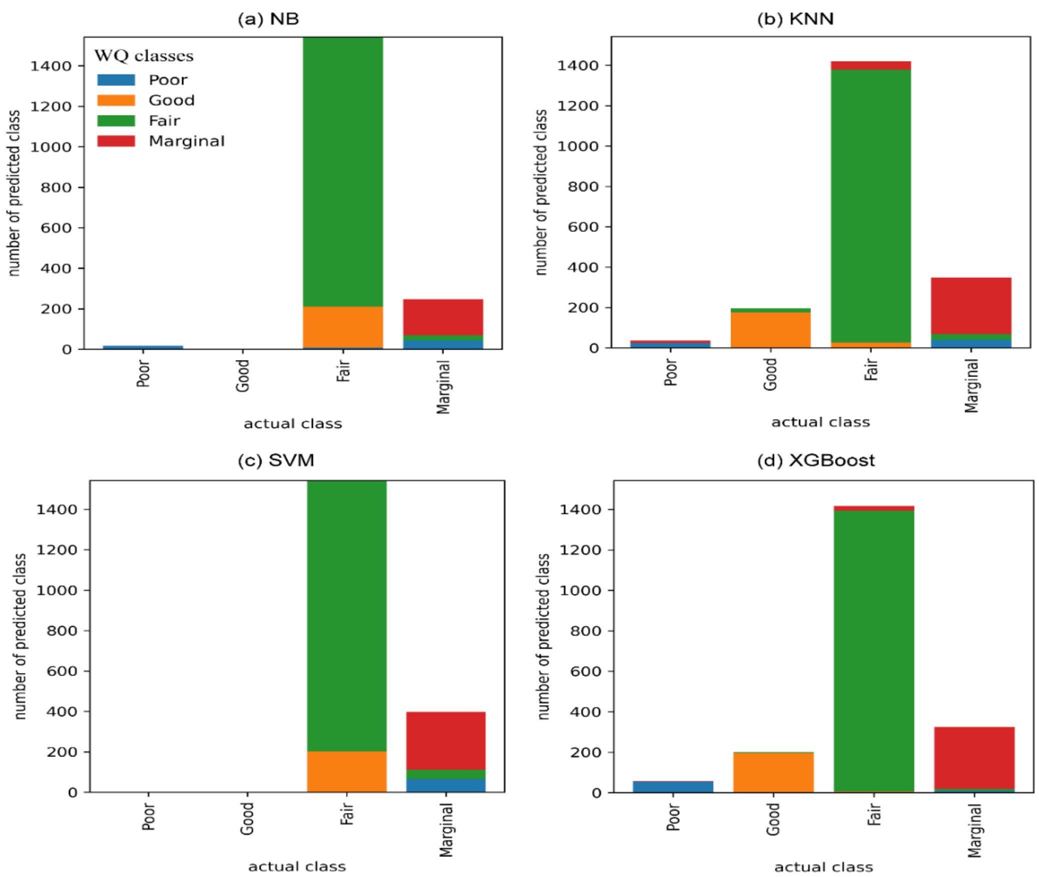


Figure 5.13. Comparing the prediction errors of water quality classification between predicted and actual classes of the WQI model.

5.6.7.1 Optimization of class prediction error

The present study used the *discrimination threshold* technique to minimize the class prediction error of the water quality index model. Commonly, it is the probability or score of the ROC curve that obtained from the tuning of the normal threshold values. This technique is widely used in machine learning studies to optimize the classification error in order to correct classification by classifier algorithm(s) (Zou et al., 2016). Figure 14 shows the discrimination threshold for the four predictive models. whereas on the x-axis presents the discrimination threshold level that is indicated by the FPR/FNR of classification; and the y-axis shows the percent of precision, recall, and F1 score of the predictive classifier(s) in terms of correct classification of water quality (Hossain et al., 2020; Zou et al., 2016). As shown in Figure 5.14 below, the discrimination threshold can be found at 0.25, 0.67, 0.32, and 0.0 for the NB, KNN, SVM, and XGBoost classifiers, respectively. At a 0.0 discrimination threshold, compared to the four classifiers, the highest scores in precision, recall, and F1 were found for the XGBoost model (Figure 5.14d). The XGBoost model classified water quality 100% correctly after tuning the normal threshold of the ROC curve. Whereas the remaining classifiers' precision, recall, and F1 scores were found between 0.80 and 0.95 (Figure 5.14d). The results of the discrimination threshold also indicate that the XGBoost classifier predictive model is effective for the classification of water quality correctly using the WQI model.

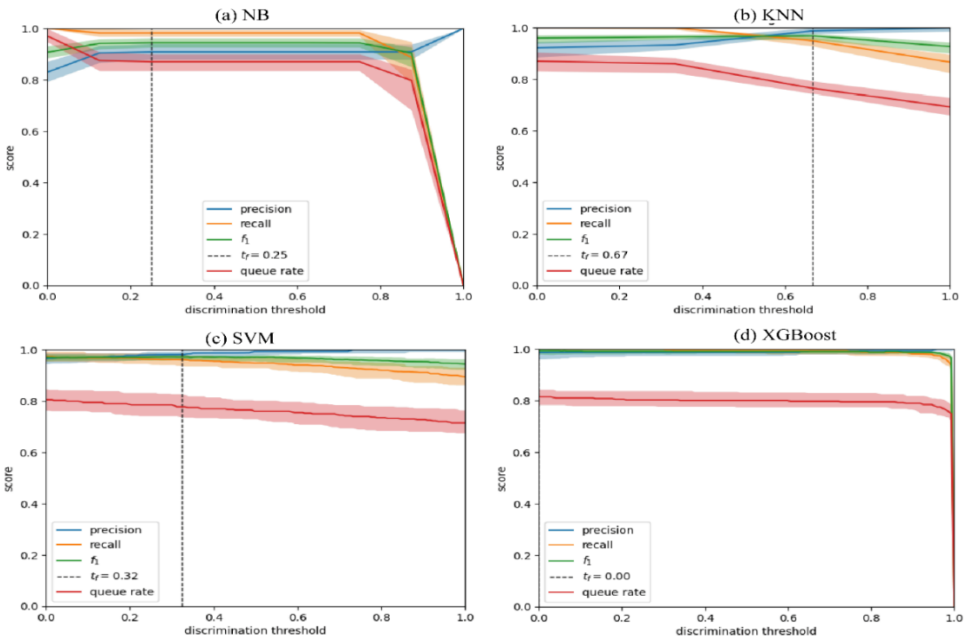


Figure 5.14. Discrimination threshold plots for four predictive classifier models.

As can be seen in figure 5.15 below, after tuning the normal threshold of ROC curve for the XGBoost model, the critical threshold values was associated at 0% false positive rate (FPR) and 100% true positive rate (TPR) of ROC curve for all ("good", "fair", "marginal" and "poor") water classes. The perfect classification performance was found for all classes. The excellent discrimination of the ROC curve indicates the optimum cut-point that is associated with the highest TPR (correctly classified) and the lowest FPR (wrongly classified) in the ROC curve (Hosmer and Lemeshow, 2004). In Figure 5.15 below, in the top-left corner, the black point indicates the optimum threshold of ROC.

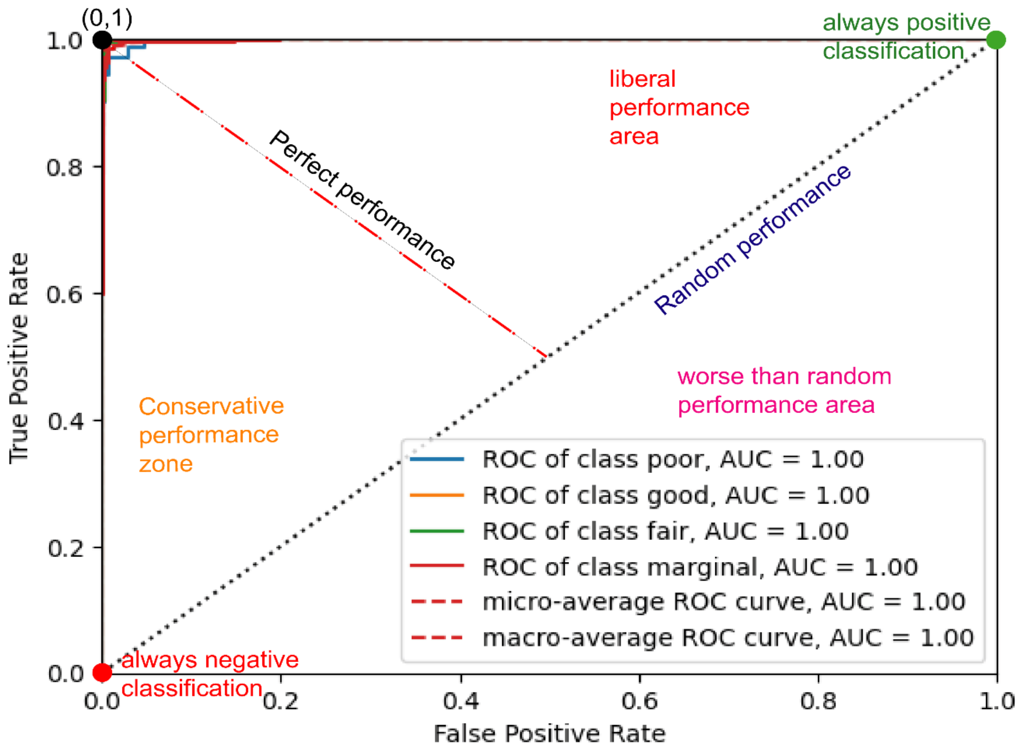


Figure 5.15. Region of ROC curve and optimal thresholds of water quality classes for water quality index model [figure outlined, and concept developed according to Hamel, 2011].

However, the critical threshold value of the ROC curve is an important measure for identifying the correct classification when a continuous variable is regarded as a discrete variable (classification). Therefore, the results of the critical threshold value of the ROC curve could help to improve the accuracy of water quality classification using the WQI model. Moreover, this approach might be useful for obtaining an accurate qualitative assessment of coastal water quality in order to reduce the uncertainty in the WQI model.

5.7 Evaluation of WQI model performance

Recently, several studies have applied the ROC curve technique to the selection of the best model or fitted dataset by comparing AUC-ROC values (Macskassy et al., 2005; Hamel, 2011; Walter, 2005). Moreover, the optimal threshold of the ROC curve allows determining the best performance point that is associated with model sensitivity and 1-specificity (Hong, 2009). Commonly, the optimal threshold indicates the highest TPR and the lowest FPR in the ROC curve where the sensitivity and specificity are most closely related to the value of the area under the ROC curve. It means the absolute difference between the sensitivity and specificity values is the smallest at the optimal point of ROC. (Gonçalves et al., 2014; Hamel, 2011; Unal, 2017).

Several studies utilized this technique to select the best model based on its classification performance (Hand, 2009; Zou et al., 2016). Commonly, the smallest cut-point value indicates the highest accuracy, and the largest value refers to the lowest accuracy of the classification. In this research, the best WQI model was selected using these approaches. The ROC curve with a pointwise 95% confidence interval was obtained from four weighted and three unweighted WQI models, respectively, using the best predictive classifier, the XGBoost model.

Figure 5.16 shows the pointwise 95% confidence intervals that are associated with the vertical averaging values of the ROC curves for fixed false-positive rates and averages the corresponding true-positive rates at each point. In figure 16, the red circle indicates the critical threshold value for each WQI model. As can be seen from the figure below, outstanding performance showed by the WQM and the NSF models with the lowest critical threshold values (Fig. 5.16a). Whereas, the AUC of ROC curves was measured at 0.98 and 0.96, respectively, for the WQM and NSF models. Relatively, excellent and acceptable discrimination capabilities were found for the SRDD and WJ models with higher critical threshold values, respectively (Fig. 5.16a). Compared to unweighted models, outstanding performance was observed for the RMS model with lower critical threshold values, whereas excellent performance was found for the AM and Hanh WQI models (Fig. 5.16b). The results of the pointwise 95% confidence intervals and critical threshold values indicate that the WQM and the NSF models could be effective for evaluating coastal water quality in order to correct classification, whereas the unweighted RMS model showed similar results.

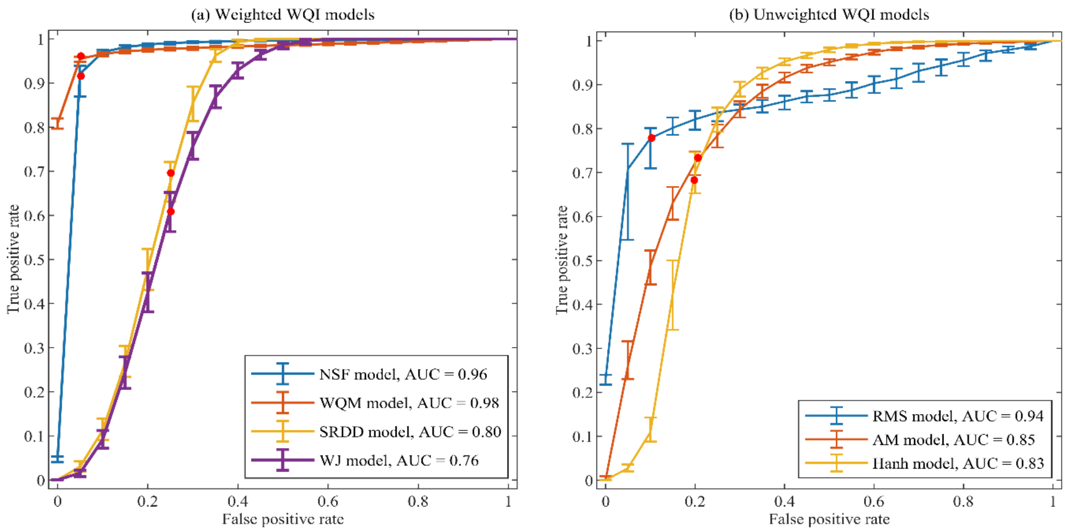


Figure 5.16. ROC with point predictions of water quality classification using XGBoost of various WQI models with a 95% confidence interval at each observation. The red circle indicates the critical threshold values of ROC.

5.7.1 Evaluation of water quality class in Cork Harbour using the XGBoost model

The ultimate goal of this study was to classify coastal water quality using the WQI model in terms of correct classification. Table 5.S2 (Appendix 5) provides the details of calculated WQI values and water quality classes for monitoring sites in Cork Harbour. In this study, the lowest error and higher predictive accuracy were found for the weighted WQM and unweighted RMS models. The results of predictive models recommended for the WQM and RMS index models could be classified effectively using the XGBoost model. In this section, Cork Harbour water quality from 29 monitoring sites was assessed using the WQM-WQI and RMS-WQI respectively, and then water quality classes were predicted using XGBoost. Figure 17 and Figure 18 shows the comparison results of water quality classes between WQI (actual class) and XGBoost models (predictive class) in Cork Harbour. The WQM model assessed "good" water quality at 27.6% (8) of the monitoring sites, whereas "fair" water quality was found for 72.4 % (21) of the monitoring sites in the Harbour (Fig. 5.17a). On the other hand, the RMS model assessed "good" water quality at 52% (15) of the monitoring sites, and "fair" water quality was assessed at 42% (14) of the monitoring sites in the harbour (Figure 5.18a). Whereas, the XGBoost model predicted 100% correct classification of water quality in the Harbour for both WQI models (Figure 5.17b; Figure 5.18b). The comparison results indicate that the weighted WQM and unweighted RMS models could be effective for assessing coastal water quality in order to correct classification.

(a) Actual water quality classes (b) Predictive water quality classes

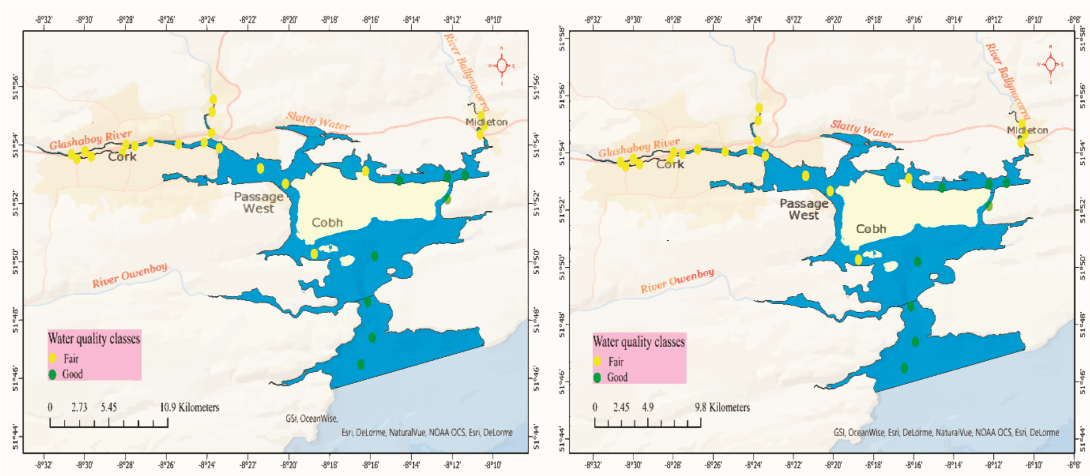


Figure 5.17. Comparison between actual and predicted water quality classifications of WQM-WQI using the XGBoost predictive model.

(a) Actual water quality classes (b) Predicted water quality classes

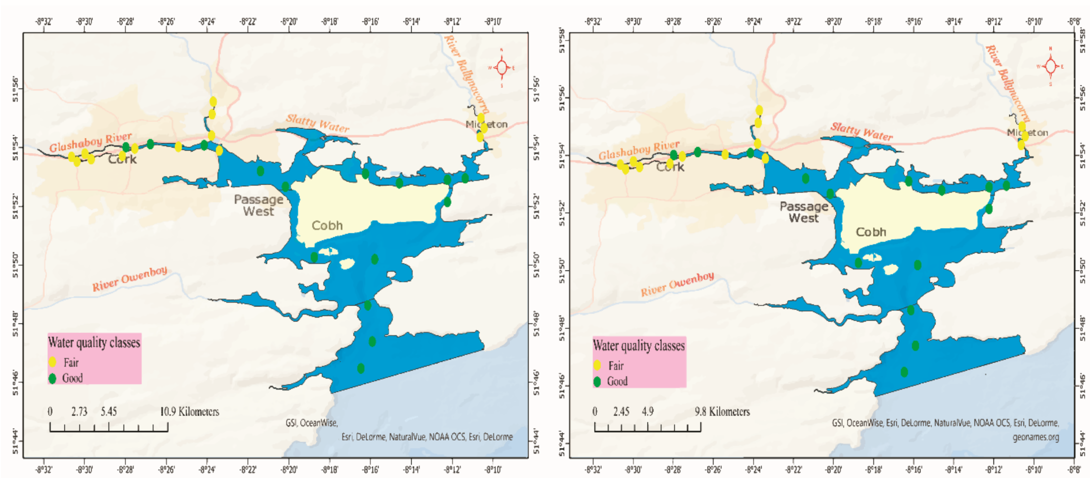


Figure 5.18. Comparison between actual and predicted water quality classifications of RMS-WQI using the XGBoost predictive model.

5.8 Conclusion

The main aims of this study were to develop a framework for assessing performance of WQI model in order to correct classification of coastal water quality. Four machine-learning classifier algorithms were utilized to identify the best algorithm for predicting water quality class. The main summary of this study are as follows:

(i) Seven WQI models including four widely used and three newly proposed were assessed in this study

(ii) XGBoost algorithm and KNN were showed the outperformed in order to correct classification of water quality

(iii) XGBoost classified most water quality classes 100% correctly except “poor” classes.

(iv) In terms of WQI model(s) performance, the weighted WQM-WQI and unweighted RMS-WQI models could be effective for assessing coastal water quality status correctly.

(v) Both models were classified water quality into two classes including “Good” and “fair” water quality in Cork Harbour over the study period.

However, as best of our knowledge, this study provides the first comprehensive approach to evaluate the performance of WQI model(s) adopting new classification scheme for multi-class classification of coastal water quality. Moreover, the results of this study could be effective in obtaining the proper classification of water quality, which might be useful to improve the WQI model accuracy, transparency, and reliability in account of the correct classification of coastal water quality. The significant limitation of this research was that it did not consider the temporal variability of water quality indicators in Cork Harbour. Further studies should be carried out to assess WQI model(s) performance using temporal resolution of indicators, with other predictive classifier algorithm(s) included. However, in spite of its limitations, the findings of this study could useful for reducing the risk of model uncertainty due to inappropriate classification, which would provide insightful information to researchers, policymakers, and water research personnel.

5.9 Declaration of competing interest

The authors state that they did not experience competing financial interests or personal relationships that could have been influenced by the work reported in this paper.

5.10 Acknowledgement

The authors gratefully acknowledge the editor’s and anonymous reviewers’ contribution to the improvement of this paper. This research was funded by the Hardiman Research Scholarship of the University of Galway, which funded the first author as part of his PhD program. The authors would like to acknowledge support from MaREI, the SFI Research Centre for Energy, Climate, and Marine research. The authors also would like to thank the Environmental Protection Agency of Ireland for providing water quality data. The authors sincerely acknowledge Charles Sturt University for providing all necessary supports to this PhD project through the excellent international co-supervision. Moreover, the authors also sincerely acknowledge the Eco HydroInformatics Research Group (EHIRG), School of Engineering, College of Science and Engineering, University of Galway, Ireland for providing computational laboratory facilities to complete this research.

5.11 References

Ahmed, U., Mumtaz, R., Anwar, H., Shah, A.A., Irfan, R., 2019. E ffi cient Water Quality Prediction Using Supervised 1–14.

Akbulut, Y., Sengur, A., Guo, Y., & Smarandache, F. 2017. NS-k-NN: Neutrosophic set-based k-nearest neighbors classifier. Symmetry, 9(9). https://doi.org/10.3390/sym9090179

Aldhyani, T.H.H., Al-Yaari, M., Alkahtani, H., Maashi, M., 2020. Water Quality Prediction Using Artificial Intelligence Algorithms. Appl. Bionics Biomech. 2020. https://doi.org/10.1155/2020/6659314

Allwein, E.L., 2000. Reducing Multiclass to Binary : A Unifying Approach for Margin Classifiers. J. Mach. Learn. Res. 1, 113–141.

Ali Haghpanah jahromi, & Mohammad Taheri. 2017. A non-parametric mixture of Gaussian naive Bayesclassifiers based on local independent features.

Asadollah, S.B.H.S., Sharafati, A., Motta, D., Yaseen, Z.M., 2021. River water quality index prediction and uncertainty analysis: A comparative study of machine learning models. J. Environ. Chem. Eng. 9, 104599. https://doi.org/10.1016/j.jece.2020.104599

Angelova, M., & Pencheva, T. 2011. Tuning genetic algorithm parameters to improve convergence time. International Journal of Chemical Engineering. https://doi.org/10.1155/2011/646917

Awan, F.M., Saleem, Y., Minerva, R., Crespi, N., 2020. A comparative analysis of machine/deep learning models for parking space availability prediction. Sensors (Switzerland) 20. https://doi.org/10.3390/s20010322

Babbar, R., Babbar, S., 2017. Predicting river water quality index using data mining techniques. Environ. Earth Sci. 76, 1–15. https://doi.org/10.1007/s12665-017-6845-9

Bergstra, J., Ca, J. B., & Ca, Y. B. 2012. Random Search for Hyper-Parameter Optimization Yoshua Bengio. In Journal of Machine Learning Research (Vol. 13). http://scikit-learn.sourceforge.net.

Bourel, M., Segura, A.M., 2018. Multiclass classification methods in ecology. Ecol. Indic. 85, 1012–1021. https://doi.org/10.1016/j.ecolind.2017.11.031

Brown, C.A., Nelson, W.G., 2015. A method to identify estuarine water quality exceedances associated with ocean conditions. Environ. Monit. Assess. 187. https://doi.org/10.1007/s10661-015-4347-3

Chia, S. L., Chia, M. Y., Koo, C. H., & Huang, Y. F. 2022. Integration of advanced optimization algorithms into least-square support vector machine (LSSVM) for water quality index prediction. Water Supply, 22(2), 1951–1963. https://doi.org/10.2166/ws.2021.303

Chamasemani, F.F., 2011. Multi-class Support Vector Machine (SVM) classifiers – An Application in Hypothyroid detection and Classification 353–358. https://doi.org/10.1109/BIC-TA.2011.51

Chen, K., Chen, H., Zhou, C., Huang, Y., Qi, X., Shen, R., Liu, F., Zuo, M., Zou, X., Wang, J., Zhang, Y., Chen, D., Chen, X., Deng, Y., Ren, H., 2020. Comparative analysis of surface water quality prediction performance and identification of key water parameters using different machine learning models based on big data. Water Res. 171, 115454. https://doi.org/10.1016/j.watres.2019.115454

Chen, R.C., Dewi, C., Huang, S.W., Caraka, R.E., 2020. Selecting critical features for data classification based on machine learning methods. J. Big Data 7. https://doi.org/10.1186/s40537-020-00327-4

Cheryl A. Brown, Nelson, W.G., 2010. Approaches to Identify Exceedances of Water Quality

Thresholds Associated with Ocean Conditions. Newport, USA.
Danades, A., Pratama, D., Anggraini, D., Anggriani, D., 2017. Comparison of accuracy level K-Nearest Neighbor algorithm and support vector machine algorithm in classification water quality status. Proc. 2016 6th Int. Conf. Syst. Eng. Technol. ICSET 2016 137–141. https://doi.org/10.1109/FIT.2016.7857553
Dezfooli, D., Hosseini-Moghari, S.M., Ebrahimi, K., Araghinejad, S., 2018. Classification of water quality status based on minimum quality parameters: application of machine learning techniques. Model. Earth Syst. Environ. 4, 311–324. https://doi.org/10.1007/s40808-017-0406-9
Elmachtoub, A.N., Liang, J.C.N., McNellis, R., 2020. Decision Trees for Decision-Making under the Predict-then-Optimize Framework. arXiv.
Fawcett, T., 2006. An introduction to ROC analysis. Pattern Recognit. Lett. 27, 861–874. https://doi.org/10.1016/j.patrec.2005.10.010
Florea, A.-C., & Andonie, R. 2020. Weighted Random Search for Hyperparameter Optimization. https://doi.org/10.15837/ijccc.2019.2.3514
Garabaghi, F.H., 2021. Performance Evaluation of Machine Learning Models with Ensemble Learning approach in Classi cation of Water Quality Indices Based on Different Subset of Features.
Gikas, G.D., Sylaios, G.K., Tsihrintzis, V.A., Konstantinou, I.K., Albanis, T., Boskidis, I., 2020. Comparative evaluation of river chemical status based on WFD methodology and CCME water quality index. Sci. Total Environ. 745, 140849. https://doi.org/10.1016/j.scitotenv.2020.140849
Gonçalves, L., Subtil, A., Rosário Oliveira, M., De Zea Bermudez, P., 2014. ROC curve estimation: An overview. Revstat Stat. J. 12, 1–20.
Gupta, S., Gupta, S.K., 2021. A critical review on water quality index tool: Genesis, evolution and future directions. Ecol. Inform. 63, 101299. https://doi.org/10.1016/j.ecoinf.2021.101299
Haghiabi, A.H., Nasrolahi, A.H., Parsaie, A., 2018. Water quality prediction using machine learning methods. Water Qual. Res. J. Canada 53, 3–13. https://doi.org/10.2166/wqrj.2018.025
Hamel, L., 2011a. Model Assessment with ROC Curves. Encycl. Data Warehous. Mining, Second Ed. 1316–1323. https://doi.org/10.4018/9781605660103.ch204
Hamel, L., 2011b. Model Assessment with ROC Curves. Encycl. Data Warehous. Mining, Second Ed. 1316–1323. https://doi.org/10.4018/978-1-60566-010-3.ch204
Hamadi, Y., Monfroy, E., & Saubion, F. 2013. Autonomous search. In Autonomous Search (Vol. 9783642214349). Springer-Verlag Berlin Heidelberg. https://doi.org/10.1007/978-3-642-21434-9
Hanoon, M. S., Ammar, A. M., Ahmed, A. N., Razzaq, A., Birima, A. H., Kumar, P., Sherif, M., Sefelnasr, A., & El-Shafie, A. 2022. Application of Soft Computing in Predicting Groundwater Quality Parameters. Frontiers in Environmental Science, 10. https://doi.org/10.3389/fenvs.2022.828251
Huang, C., Li, Y., & Yao, X. 2020. A Survey of Automatic Parameter Tuning Methods for Metaheuristics. In IEEE Transactions on Evolutionary Computation (Vol. 24, Issue 2, pp. 201–216). Institute of Electrical and Electronics Engineers Inc. https://doi.org/10.1109/TEVC.2019.2921598
Islam Khan, M.S., Islam, N., Uddin, J., Islam, S., Nasir, M.K., 2021. Water quality prediction and classification based on principal component regression and gradient boosting classifier approach. J. King Saud Univ. - Comput. Inf. Sci. https://doi.org/10.1016/j.jksuci.2021.06.003
Japkowicz, N., 2000. Learning from imbalanced data sets: a comparison of various strategies. AAAI Work. Learn. from Imbalanced Data Sets 0–5.
Juwana, I., Muttil, N., Perera, B.J.C., 2016. Uncertainty and sensitivity analysis of West Java Water Sustainability Index - A case study on Citarum catchment in Indonesia. Ecol. Indic. 61, 170–178. https://doi.org/10.1016/j.ecolind.2015.08.034
Kaur, A., Khurana, M., Kaur, P., Kaur, M., 2021. Classification and Analysis of Water Quality Using Machine Learning Algorithms, Lecture Notes in Electrical Engineering. Springer Singapore. https://doi.org/10.1007/978-981-33-4866-0_48
Kavzoglu, T., & Teke, A. 2022. Advanced hyperparameter optimization for improved spatial prediction of shallow landslides using extreme gradient boosting (XGBoost). Bulletin of Engineering Geology and the Environment, 81(5). https://doi.org/10.1007/s10064-022-02708-w
Khullar, S., Singh, N., 2021. Machine learning techniques in river water quality modelling: A research travelogue. Water Sci. Technol. Water Supply 21. https://doi.org/10.2166/ws.2020.277
Kurt, I., Ture, M., Kurum, A.T., 2008. Comparing performances of logistic regression, classification and regression tree, and neural networks for predicting coronary artery disease. Expert Syst. Appl. 34, 366–374. https://doi.org/10.1016/j.eswa.2006.09.004
Latha, C. B. C., & Jeeva, S. C. 2019. Improving the accuracy of prediction of heart disease risk based

on ensemble classification techniques. Informatics in Medicine Unlocked, 16. https://doi.org/10.1016/j.imu.2019.100203
Li, W., Yang, M., Liang, Z., Zhu, Y., Mao, W., Shi, J., Chen, Y., 2013. Assessment for surface water quality in Lake Taihu Tiaoxi River Basin China based on support vector machine. Stoch. Environ. Res. Risk Assess. 27, 1861–1870. https://doi.org/10.1007/s00477-013-0720-3
Leong, W. C., Bahadori, A., Zhang, J., & Ahmad, Z. 2021. Prediction of water quality index (WQI) using support vector machine (SVM) and least square-support vector machine (LS-SVM). International Journal of River Basin Management, 19(2), 149–156. https://doi.org/10.1080/15715124.2019.1628030
Malek, N.H.A., Yaacob, W.F.W., Nasir, S.A.M., Shaadan, N., 2022. Prediction of Water Quality Classification of the Kelantan River Basin, Malaysia, Using Machine Learning Techniques. Water (Switzerland) 14. https://doi.org/10.3390/w14071067
Mandrekar, J.N., 2010. Receiver operating characteristic curve in diagnostic test assessment. J. Thorac. Oncol. 5, 1315–1316. https://doi.org/10.1097/JTO.0b013e3181ec173d
Mehrpooya, A., Saberi-Movahed, Farid, Azizizadeh, N., Rezaei-Ravari, M., Saberi-Movahed, Farshad, Eftekhari, M., Tavassoly, I., 2021. High Dimensionality Reduction by Matrix Factorization for Systems Pharmacology. https://doi.org/10.1101/2021.05.30.446301Modaresi, F., Araghinejad, S., 2014. A comparative assessment of support vector machines, probabilistic neural networks, and K-nearest neighbor algorithms for water quality classification. Water Resour. Manag. 28, 4095–4111. https://doi.org/10.1007/s11269-014-0730-z
Mohammed, H., Longva, A., Seidu, R., 2018. Predictive analysis of microbial water quality using machine-learning algorithms. Environ. Res. Eng. Manag. 74, 7–20. https://doi.org/10.5755/j01.erem.74.1.20083
Morrison, A.M., Coughlin, K., Shine, J.P., Coull, B.A., Rex, A.C., 2003. Receiver Operating Characteristic Curve Analysis of Beach Water Quality Indicator Variables. Appl. Environ. Microbiol. 69, 6405–6411. https://doi.org/10.1128/AEM.69.11.6405-6411.2003
Muhammad, S.Y., Makhtar, M., Rozaimee, A., Aziz, A.A., Jamal, A.A., 2015. Classification model for water quality using machine learning techniques. Int. J. Softw. Eng. its Appl. 9, 45–52. https://doi.org/10.14257/ijseia.2015.9.6.05
Najafzadeh, M., Ghaemi, A., 2019. Prediction of the five-day biochemical oxygen demand and chemical oxygen demand in natural streams using machine learning methods. Environ Monit Assess 191. https://doi.org/10.1007/s10661-019-7446-8
Najafzadeh, M., Ghaemi, A., Emamgholizadeh, S., 2019. Prediction of water quality parameters using evolutionary computing-based formulations. International Journal of Environmental Science and Technology 16, 6377–6396. https://doi.org/10.1007/s13762-018-2049-4
Najafzadeh, M., Homaei, F., Farhadi, H., 2021. Reliability assessment of water quality index based on guidelines of national sanitation foundation in natural streams: integration of remote sensing and data-driven models. Artif Intell Rev 54, 4619–4651. https://doi.org/10.1007/s10462-021-10007-1
Najafzadeh, M., Niazmardi, S., 2021. A Novel Multiple-Kernel Support Vector Regression Algorithm for Estimation of Water Quality Parameters. Natural Resources Research 30, 3761–3775. https://doi.org/10.1007/s11053-021-09895-5
Neha Radhakrishnan, & Anju S Pillai. 2020. Comparison of Water Quality Classification Models using Machine Learning.
Parween, S., Siddique, N.A., Mahammad Diganta, M.T., Olbert, A.I., Uddin, Md.G., 2022. Assessment of urban river water quality using modified NSF water quality index model at Siliguri city, West Bengal, India. Environmental and Sustainability Indicators 16, 100202. https://doi.org/10.1016/j.indic.2022.100202
Polikar, R., 2012. Ensemble Machine Learning, in: Ensemble Machine Learning. https://doi.org/10.1007/978-1-4419-9326-7
Qian, Y., Zhou, W., Yan, J., Li, W., & Han, L. 2015. Comparing machine learning classifiers for object-based land cover classification using very high resolution imagery. Remote Sensing, 7(1), 153–168. https://doi.org/10.3390/rs70100153
Prakash, R., Tharun, V.P., Renuga Devi, S., 2018. A Comparative Study of Various Classification Techniques to Determine Water Quality. Proc. Int. Conf. Inven. Commun. Comput. Technol. ICICCT 2018 1501–1506. https://doi.org/10.1109/ICICCT.2018.8473168
Radhakrishnan, N., Pillai, A.S., 2020. Comparison of water quality classification Models using machine learning. Proc. 5th Int. Conf. Commun. Electron. Syst. ICCES 2020 1183–1188. https://doi.org/10.1109/ICCES48766.2020.09137903
Saberi-Movahed, Farshad, Mohammadifard, Mahyar, Mehrpooya, A., Rezaei-Ravari, M., Berahmand,

K., Rostami, M., Karami, S., Najafzadeh, M., Hajinezhad, D., Jamshidi, M., Abedi, F., Mohammadifard, Mahtab, Farbod, E., Safavi, F., Dorvash, M., Mottaghi-Dastjerdi, N., Vahedi, S., Eftekhari, M., Saberi-Movahed, Farid, Alinejad-Rokny, H., Band, S.S., Tavassoly, I., 2022. Decoding clinical biomarker space of COVID-19: Exploring matrix factorization-based feature selection methods. Comput Biol Med 146. https://doi.org/10.1016/j.compbiomed.2022.105426

Savira, F., Suharsono, Y., 2013. A classification model for water quality analysis using decision tree. J. Chem. Inf. Model. 01, 1689–1699.

Serqueira, M., González, P., & Bezerra, E. 2020. A Population-based Hybrid Approach to Hyperparameter Optimization for Neural Networks. http://arxiv.org/abs/2011.11062

Shakhari, S., Banerjee, I., 2019. A multi-class classification system for continuous water quality monitoring. Heliyon 5, e01822. https://doi.org/10.1016/j.heliyon.2019.e01822

Singh, K.P., Basant, N., Gupta, S., 2011. Support vector machines in water quality management. Anal. Chim. Acta 703, 152–162. https://doi.org/10.1016/j.aca.2011.07.027

Steele, T.D., 1987. Stratégies de la surveillance de la qualité des eaux. Hydrol. Sci. J. 32, 133–141. https://doi.org/10.1080/02626668709491178

Strobl, R.O., Robillard, P.D., 2008. Network design for water quality monitoring of surface freshwaters: A review. J. Environ. Manage. 87, 639–648. https://doi.org/10.1016/j.jenvman.2007.03.001

Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2018. Development of a water quality index for rivers in West Java Province, Indonesia. Ecol. Indic. 85, 966–982. https://doi.org/10.1016/j.ecolind.2017.11.049

Suwadi, N. A., Derbali, M., Sani, N. S., Lam, M. C., Arshad, H., Khan, I., & Kim, K. il. 2022. An Optimized Approach for Predicting Water Quality Features Based on Machine Learning. Wireless Communications and Mobile Computing, 2022. https://doi.org/10.1155/2022/3397972

Szabo, P., & Genge, B. 2020. Hybrid hyper-parameter optimization for collaborative filtering. Proceedings - 2020 22nd International Symposium on Symbolic and Numeric Algorithms for Scientific Computing, SYNASC 2020, 210–217. https://doi.org/10.1109/SYNASC51798.2020.00042

Tanha, J., Abdi, Y., Samadi, N., Razzaghi, N., Asadpour, M., 2020. Boosting methods for multi-class imbalanced data classification: an experimental review. J. Big Data 7. https://doi.org/10.1186/s40537-020-00349-y

Tesoriero, A.J., Gronberg, J.A., Juckem, P.F., Miller, M.P., Austin, B.P., 2017. Predicting redox-sensitive contaminant concentrations in groundwater using random forest classification. Water Resour. Res. https://doi.org/10.1002/2016WR020197

The MathWorks, I., 1993. Statistics and Machine Learning Toolbox™ User's Guide R2021b, User's Guide.

Thanh Noi, P., & Kappas, M. (2017). Comparison of Random Forest, k-Nearest Neighbor, and Support Vector Machine Classifiers for Land Cover Classification Using Sentinel-2 Imagery. Sensors (Basel, Switzerland), 18(1). https://doi.org/10.3390/s18010018

Tiyasha, Tung, T.M., Yaseen, Z.M., 2021. Deep Learning for Prediction of Water Quality Index Classification: Tropical Catchment Environmental Assessment. Nat. Resour. Res. 30, 4235–4254. https://doi.org/10.1007/s11053-021-09922-5

Toner, P., Bowman, J., Clabby, K., Lucey, J., Mc, McGarrigle, M., Concannon, C., Clenaghan, C., Cunningham, P., J., D., O'Boyle, S., MacCárthaigh, M., Craig, M., Quinn, R., 2005. Water Quality in Ireland 2001-2003.

Uddin, M.G., Moniruzzaman, M., Khan, M., 2017. Evaluation of Groundwater Quality Using CCME Water Quality Index in the Rooppur Nuclear Power Plant Area, Ishwardi, Pabna, Bangladesh. Am. J. Environ. Prot. https://doi.org/10.12691/env-5-2-2

Uddin, M.G., Nash, S., Olbert, A.I., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol. Indic. 122, 107218. https://doi.org/10.1016/j.ecolind.2020.107218

Uddin, Md Galal, Nash, S., Rahman, A., Olbert, A.I., 2022a. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment. Water Res. 219, 118532. https://doi.org/10.1016/j.watres.2022.118532

Uddin, M.G., Nash, S., Mahammad Diganta, M.T., Rahman, A., Olbert, A.I., 2022b. Robust machine learning algorithms for predicting coastal water quality index. J. Environ. Manage. 321, 115923. https://doi.org/10.1016/j.jenvman.2022.115923

Uddin, Galal, Nash, S., Olbert, A.I., 2022c. Optimization of Parameters in a Water Quality Index Model using Principal Component Analysis, in: Proceedings of the 39th IAHR World Congress. Proceedings of the 39th IAHR World Congress.

Uddin, Md. Galal, Nash, S., Rahman, A., Olbert, A.I., 2022d. A novel approach for estimating and

predicting uncertainty in water quality index model using machine learning approaches.
Uddin, M.G., Nash, S., Diganta, M.T.M., Rahman, A., Olbert, A.I., 2022e. A comparison of geocomputational models for validating geospatial distribution of water quality index. In: Priyanka, H., Rahman, A., Basant agarwal, Binita Tiwari (Eds.), Computational Statistical Methodologies and Modeling for Artificial Intelligence. CRC Press, Taylor & Francis Publisher, USA.
Uddin, G., Nash, S., Rahman, A., Olbert, A.I., 2022f. Assessing optimization techniques for improving water quality model. Submitted for publication.
Uddin, M.G., Stephen Nash, Olbert, A.I., 2020. Application of Water Quality Index Models to an Irish Estuary, in: Civil and Environmental Research. pp. 576–581.
Venkata Vara Prasad, D., Senthil Kumar, P., Venkataramana, L. Y., Prasannamedha, G., Harshana, S., Jahnavi Srividya, S., Harrinei, K., & Indraganti, S. 2021. Automating water quality analysis using ML and auto ML techniques. Environmental Research, 202. https://doi.org/10.1016/j.envres.2021.111720
Victoria, A. H., & Maragatham, G. 2021. Automatic tuning of hyperparameters using Bayesian optimization. Evolving Systems, 12(1), 217–223. https://doi.org/10.1007/s12530-020-09345-2
Walley, W.J., Džeroski, S., 1996. Biological Monitoring: a Comparison between Bayesian, Neural and Machine Learning Methods of Water Quality Classification. Environ. Softw. Syst. 229–240. https://doi.org/10.1007/978-0-387-34951-0_20
Wang, J., Xu, J., & Wang, X. (2018). Combination of Hyperband and Bayesian Optimization for Hyperparameter Optimization in Deep Learning. http://arxiv.org/abs/1801.01596
Wu, J., Chen, S. P., & Liu, X. Y. (2020). Efficient hyperparameter optimization through model-based reinforcement learning. Neurocomputing, 409, 381–393. https://doi.org/10.1016/j.neucom.2020.06.064
Yin, J., 2017. Using the ROC Curve to Measure Association and Evaluate Prediction Accuracy for a Binary Outcome. Biometrics Biostat. Int. J. 5, 1–10. https://doi.org/10.15406/bbij.2017.05.00134
Yuan, B., & Gallagher, M. (2005). A hybrid approach to parameter tuning in genetic algorithms. 2005 IEEE Congress on Evolutionary Computation, IEEE CEC 2005. Proceedings, 2, 1096–1103. https://doi.org/10.1109/cec.2005.1554813
Zhang, W., Wu, C., Zhong, H., Li, Y., & Wang, L. (2021). Prediction of undrained shear strength using extreme gradient boosting and random forest based on Bayesian optimization. Geoscience Frontiers, 12(1), 469–477. https://doi.org/10.1016/j.gsf.2020.03.007

6. Assessing optimization techniques for improving water quality model

This chapter was published in the **"Journal of Cleaner Production"** on December 19, 2022. Details can be found at the following web resource: https://doi.org/10.1016/j.jclepro.2022.135671

6.1 Chapter highlights

- Indicator selection technique is one of the crucial components of the WQI model.
- Existing WQI models widely use various techniques for selecting important indicators in developing model.
- Due to the inappropriate selection technique, a significant amount of input uncertainty is associated with the irrelevant indicators.
- In order to identify the best method(s), eighteen ML algorithms were analyzed and assessed for selecting crucial water quality indicators in developing a WQI model in terms of reducing input uncertainty.
- Various FS techniques could have a significant effect on model performance.
- Input sizes of water quality indicators have a substantial impact on the model.
- RF, EXT, and MI techniques are effective for selecting crucial indicators.
- The DNN algorithm outperformed others for predicting coastal water quality.
- BOD_5, DIN, MRP, TEMP, pH, DOX, TON, and TRAN could improve the WQI model's accuracy.
- Finally, the research has suggested that the RF algorithm could be effective for selecting crucial indicators in developing a WQI model in terms of optimizing the model input uncertainty.

6.2 Abstract

In order to keep the "good" status of coastal water quality, it is essential to monitor and assess frequently. The Water quality index (WQI) model is one of the most widely used techniques for the assessment of water quality. It consists of five components, with the indicator selection technique being one of the more crucial components.

Several studies conducted recently have shown that the use of the existing techniques results in a significant amount of uncertainty being produced in the final assessment due to the inappropriate indicator selection. The present study carried out a comprehensive assessment of various features selection (FS) techniques for selecting crucial coastal water quality indicators in order to develop an efficient WQI model. This study aims to analyze the effects of eighteen different FS techniques, including (i) nine filter methods, (ii) two wrapper methods, and (iii) seven embedded methods for the comparison of model performance of the WQI. In total, fifteen combinations (subsets) of water quality indicators were constructed, and WQI values were calculated for each combination using the improvement methodology for coastal water quality. The WQI model's performance was tested using nine machine-learning algorithms, which validated the model's performance using various metrics. The results indicated that the tree-based random forest algorithm could be effective for selecting crucial water quality indicators in terms of assessing coastal water. Deep neural network algorithm showed better performance for predicting coastal water quality more accurately incorporating the subset of the random forest.

Key words: coastal water quality; feature selection algorithms; artificial intelligence; machine-learning techniques; water quality index model

6.3 Introduction

Assuring the "good" state of water quality (surface and groundwater) is a critical issue in the world because, due to various factors, including natural, anthropogenic, or a combination of both, the quality of water is degraded gradually. Coastal water quality is a vital component of conserving the aquatic ecosystem and its nature. Recently, numerous studies have revealed that the aquatic environment is being depleted day by day due to water pollution. For the purposes of the management of water resources, the water quality-monitoring program is a widely used approach. In order to monitor and assess water quality, a range of tools and techniques have been utilized in the literature. The WQI model is one of them. It is a widely used, straightforward mathematical model that allows the conversion of a wide range of water quality indicators' information into unitless numerical expression (Uddin et al., 2017; 2022a; 2021). In recent decades, its application has been increasing rapidly in the field of water resources management and monitoring purposes. To date, more than thirty plus

WQI models have been developed by various countries/organizations/researchers in the world. Commonly, most WQI models are composed of four consecutive components, including the indicator selection process, indicator weighting process, sub-index functions, and aggregation function (Uddin et al., 2022a; Uddin et al., 2022b; 2022c). Recently, many studies have revealed that the existing WQI models produce considerable uncertainty when converting large amounts of water quality indicator data into a numerical form (Abbasi and Abbasi, 2012; Gupta and Gupta, 2021; Juwana et al., 2016a; Sutadian et al., 2016; Uddin et al., 2021; 2022a).

In developing a WQI model, crucial water quality indicators are selected using various techniques such as principal components analysis (Chakravarty and Gupta, 2021; Fadel et al., 2021; Hou et al., 2016; Islam Khan et al., 2021; Kumar et al., 2019; Ma et al., 2020; Parween et al., 2022; Tripathi and Singal, 2019; Zeinalzadeh and Rezaei, 2017; Uddin et al., 2022a; 2022d), correlation technique (Michalak and Kwasnicka, 2006), expert opinions (Medeiros et al., 2017; Sutadian et al., 2017a), analytical hierarchy process (Juwana et al., 2016b; Sutadian et al., 2017a, 2017b), Delphi technique (Horton, 1965), data availability (Sutadian et al., 2017a) etc. Recently, the existing techniques have received much more criticisms in terms of reliability and appropriateness of selecting indicators. Several recent studies have revealed that the existing indicator selection techniques contributed a significant amount of uncertainty in the final assessment due to inappropriate indicators selection (Chen et al., 2020; Jiang et al., 2018; Pan et al., 2022; Uddin et al., 2022a; 2021). Although, a few studies have reported that the indicators selection techniques produced less than 1% of uncertainty in the results (Uddin et al., 2022c). Details of the model uncertainties, their sources and impacts on the final assessment were discussed and investigated by Uddin et al., (2021; 2022a; 2022c).

For the optimization of model uncertainty in developing a WQI model, many studies have utilized the state-of-the-art of innovation technique such as artificial intelligence and machine learning algorithm approches (Bagherzadeh et al., 2021; Chen et al., 2020; Islam Khan et al., 2021; Naghibi et al., 2020; Othman et al., 2020; Uddin et al., 2022a; 2022b; 2022d). Features selection (FS) algorithm is one of the effective and reliable techniques for identifying the crucial variables or components in a given dataset in data science (Asadollah et al., 2021; K. Chen et al., 2020; Othman et al., 2020; Savitsky et al., 2011). Although, many mathematical and statistical methods have been introduced in past decades for selecting crucial variables from a dataset (Kotsiantis, 2011; Taha et al., 2022). Each FS method optimizes the key variables and evaluates the subset with certain criteria based on various functions that are responsible for identifying significant features for developing a model (Bagherzadeh et al., 2021). According to principle of the FS functions, it can be categorised into three groups: (i) wrapper method (like as supervised or unsupervised various algorithms) extract the relevant feature using model based algorithms that find the best subsets of features which improve the model prediction accuracy or optimize the model errors (Das et al., 2017; Taha et al., 2022); (ii) filter method (for example MI, Relief, correlation etc.) is a rank based FS strategy. This technique allows selecting relevant features using general properties of features (like as correlation information, variance and consistency) without employing any clustering algorithm to guide the search (Bagherzadeh et al., 2021; Cateni et al., 2014; Taha et al., 2022); and (iii) embedded technique is a combined approach of both the filter and wrapper methods (Bagherzadeh et al., 2021; Gao and Wu, 2020a; Saeys et al., 2007; Taha et al., 2022).

Recently, many studies have utilized various FS techniques, such as filter (Gao & Wu, 2020b; Khan & See, 2016; Michalak & Kwasnicka, 2006), wrapper (Bagherzadeh et al., 2021; R. C. Chen et al., 2020), and embedded (Asadollah et al., 2021; K. Chen et al., 2020; Islam Khan et al., 2021; Uddin et al., 2022b; Urbanowicz et al., 2018) for selecting the crucial indicators for evaluating water quality using the WQI model. The present study used eighteen FS algorithms, including (i) nine filter methods (Chi2 test, PCA, Pearson correlation (PCOR) analysis, mutual information (MI), relief, K Best (according to the K highest scores), F test, Laplacian (LAP), and minimum-redundancy-maximum-relevance (MRMR)), and (ii) two wrapper methods (recursive features elimination-support vector machine (RFE SVM) and recursive features elimination-random forest (RFE_RF), and (iii) seven embedded methods (extreme gradient boosting (XGBoost), random forest (RF), extra tree (ExT) algorithm, Boruta, linear regression (LR), Least Absolute Shrinkage and Selection Operator (LASSO) model, stepwise generalized linear regression model (SWGLM) to develop an efficient WQI model for assessing coastal water quality.

In terms of the model performance analysis using various combination of water quality indicators, eight widely used machine learning algorithms and one artificial intelligence techniques including the DNN, SVM, LSBoost, GPR, tree, LR, XGBoost, K- KNN, and RF were utilized in this research. Recently, several studies have utilized the advanced machine learning technique for assessing water quality using WQI model due to the computational complexity and inappropriate sub-indexing process of the model (Bui et al., 2020; Hassan et al., 2021; Leong et al., 2021; Uddin et al., 2022a; 2022d). Models performance were evaluated using widely used six common criteria, RMSE, MSE, MAE, MAPE, AIC, and BIC.

Nevertheless,, as best of the authors knowledge, recently, many studies have conducted to improve the WQI model for assessing surface water quality like as river, and lakes. In our recent study, we proposed an improved methodology for assessing coastal water quality using WQI approaches where we compared eight WQI models (five are established and remaining three are newly proposed). Uddin et al., (2022a) have revealed that the weighted quadratic mean (WQM)-WQI and root mean square (RMS)-WQI models are effective for assessing coastal water quality in terms of model reliability and consistence. Therefore, the present study utilized the WQM-WQI approaches for calculating WQI values. Detail methodology can be found in Uddin et al., (2022a).Therefore, the aim of this research was to select the best combination of water quality indicators in order to reduce model uncertainty. The main aspects of this study are as follows:

(1) to identify the crucial water quality indicators without losing/hiding actual information using various features selection algorithms to improve the WQM-WQI model efficiency for the assessment of coastal water quality;
(2) to assess the impact (sensitivity) of different FS techniques (subsets of indicators) on the WQM-WQI model;
(3) to determine more accurate machine learning algorithm for predicting WQI values incorporating the WQM-WQI model;
(4) to parameterize a robust subset of crucial water quality indicators for the improvement of the WQM-WQI model.

In addition, the findings of this research provide a comprehensive understanding of various indicator optimization techniques and their performance in terms of reducing the WQI model uncertainty. The results may also be useful in determining the best algorithm to choose the key input of the water model in water research studies that may be effective for advancing the WQI model's development.

The rest of the manuscript is structured as follows: Section 6.4 provides the details description of the study area, materials and methods, including data collection and preparation, WQI models and their components, various FS techniques; Section 6.5 presents details of the WQIs prediction models, input preparation, model hyperparamterization, model evaluation method, and other statistical tools and techniques. In Section 6.6, we discuss experimental results and discussion of various FS algorithms, prediction results of nine models, and results of different statistical tests. Section 6.8 - 6.10 presents the results of the water quality assessment using the best subsets of indicators. Section 6.11 is a conclusion and recommendation on the best algorithm for selecting water quality indicators for improving the WQI model.

6.4 Materials and methods

6.4.1 Model application domain

The present study was conducted in the largest natural Harbour Cork named Cork Harbour which is located on the southwest coast of Ireland. This region is heavily populated and industrialized and subject to extensive agricultural activities, which is the prime cause of the Harbour water quality depletion. Many large rivers flow into the Harbour, the River Lee is one of them, which flows through Cork City and approximately 75% of the freshwater is provided to the Harbour (Uddin et al., 2022a). In addition, several largest wastewater treatment plants (WWTPs) are situated in Cork Harbour that discharge a significant amount of wastewater into the Harbour. The EPA reported that the Harbour's water quality gradually degraded every day. In order to spatial assessment of the Harbour, the Harbour area was divided into three regions: (i) Upper Harbour (ii) Lower Harbour and (iii) Outer Harbour. Details of the Harbour regions are presented in Figure 6.1. Details of the monitoring sites and WWTPs can be found in Table 6.S1.

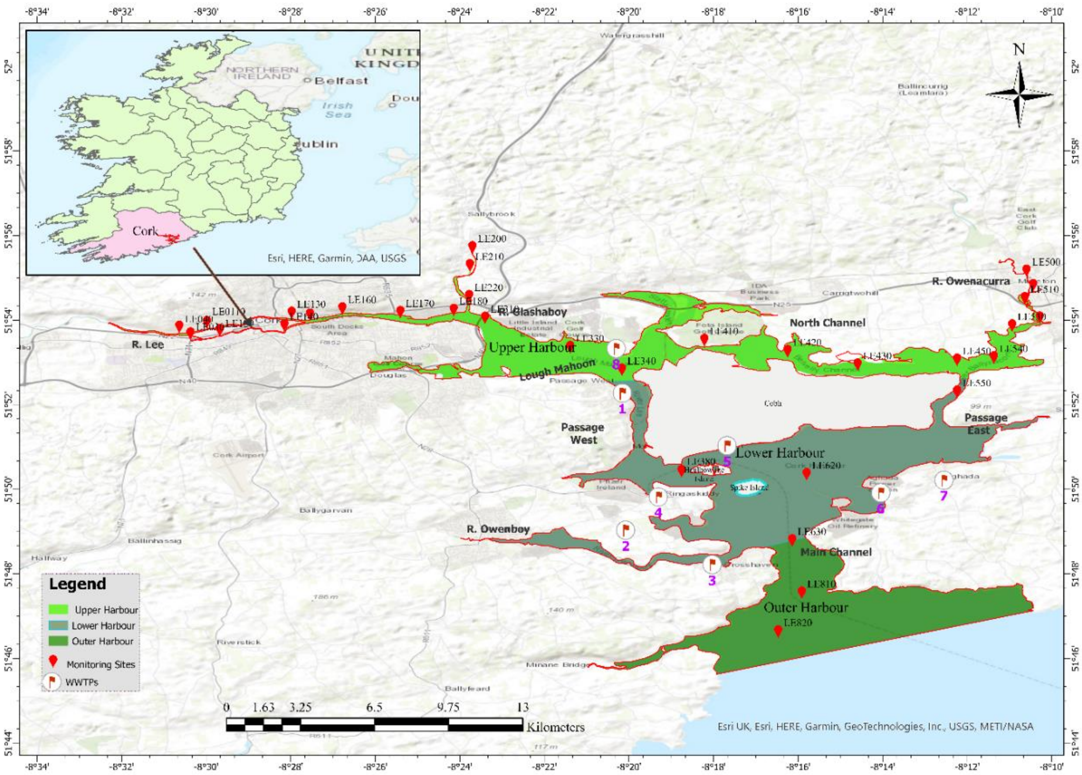


Figure 6.1. Model application domain and sampling sites locations in Cork Harbour, Ireland.

6.4.2 Data obtaining process

Water quality data for the purpose of this study was obtained from the monitoring database (https://www.catchments.ie/data/) of the Environmental Protection Agency (EPA), Ireland that is collects WQ data monthly from number of monitoring sites in several national and local water bodies. The present study used a repository of Cork Harbour; ten WQ indicators were collected from the database 2022 (January – May) including 32 monitoring sites. A comprehensive map of study domain and monitoring sites are presented in Figure 6.1. The average concentration of water quality data of eleven parameters including ammonia (AMN), biological oxygen demand (BOD), dissolved oxygen (DOX), chlorophyll a (CHL), molybdate reactive phosphorus (MRP), water pH, total oxidised nitrogen (TON), water transparency (TRAN), dissolved inorganic nitrogen (DIN) and water temperature (TEMP) were used in this research. Details of the WQ indicators, unit and their guideline values can be found Table 6.S2 and details of the WQ data are provided in Table 6.S3. By using the Uddin et al., (2022a) methodology, the guideline values for ten water quality indicators were obtained.

6.4.3 Feature selection (FS) techniques

Eighteen FS techniques including (i) Univariate filter method (unsupervised): F-Test, Chi-square (χ^2), mutual information (MI), Pearson correlation (PCOR), K_best and features transformation based principal component analysis (PCA) and multivariate based minimum redundancy maximum relevance (MRMR); (ii) filter (supervised): Relief, and Laplacian score (LAP), (iii) wrapper methods (supervised): recursive feature elimination: A support vector machine (RFE_SVM) and recursive feature elimination- random forest (RFE_RF); and (iv) embeded based (supervised): extrem gradient boosting (XGBoost), random forest (RF), linear regression (LR), Boruta, least absoulte shrinkage and selection operator (LASSO), intransic based extra tree algorithm (ExT) and step-wise generalized linear regression model (SWGLM) and (v) maximum voting approach (MAXVOT) were utilized in this research. The details of each FS method and their functions can be found in Appendix 6 as a continuation of 6.4.3.1.

6.4.4 Water quality index (WQI) model

Thus far, since the development of the WQI model, different WQI models have been developed by various countries/organizations/ researchers, all of which have a particular focus on assessing surface (rivers, lakes etc.) and groundwater quality (Uddin et al., 2021, 2022a). To the best of the author's knowledge, a limited number of indexes have given attention to coastal water quality (Uddin et al., 2022d). The authors have recently proposed an improvement methodology for assessing coastal water quality using the WQI approach. Details of the methodology can be found in Uddin et al., (2022a). In this research, WQI values were calculated for each subset of water quality indicators using the weighted quadratic mean (WQM) – WQI approach. Table 6.2 provides the details of various water quality indicators subsets. The final WQI values were obtained by using equation (6.1).

$$\text{WQM-WQI} = \sqrt{\sum_{i=1}^{n} w_i\, s_i^2} \quad \dots\dots\dots\dots\dots\dots\dots\,(6.1)$$

Where, w_i is the weight value of i^{th} indicator; s_i is the sub-index of i^{th} indicators and n is the number of water quality indicators.

6.5 WQIs prediction approaches

Recently, several studies have utilized state-of-the-art of advanced computing approaches such as machine-learning algorithm, artificial intelligence to reduce the model uncertainty. In this research, in total nine prediction models were developed using eight widely used machine-learning algorithms and one deep neural network (DNN) model including SVM, GPR, KNN, LSBoost ensemble, Tree, LR, RF and XGBoost for predicting coastal WQIs using various subsets of water quality indicators. Details of the indicator's subsets are provided in Table 6.2. The details methodological procedures of this study are presented in figure 6.2. The details of various prediction models can be found in the supplementary material as a continuation of 6.5. 1.

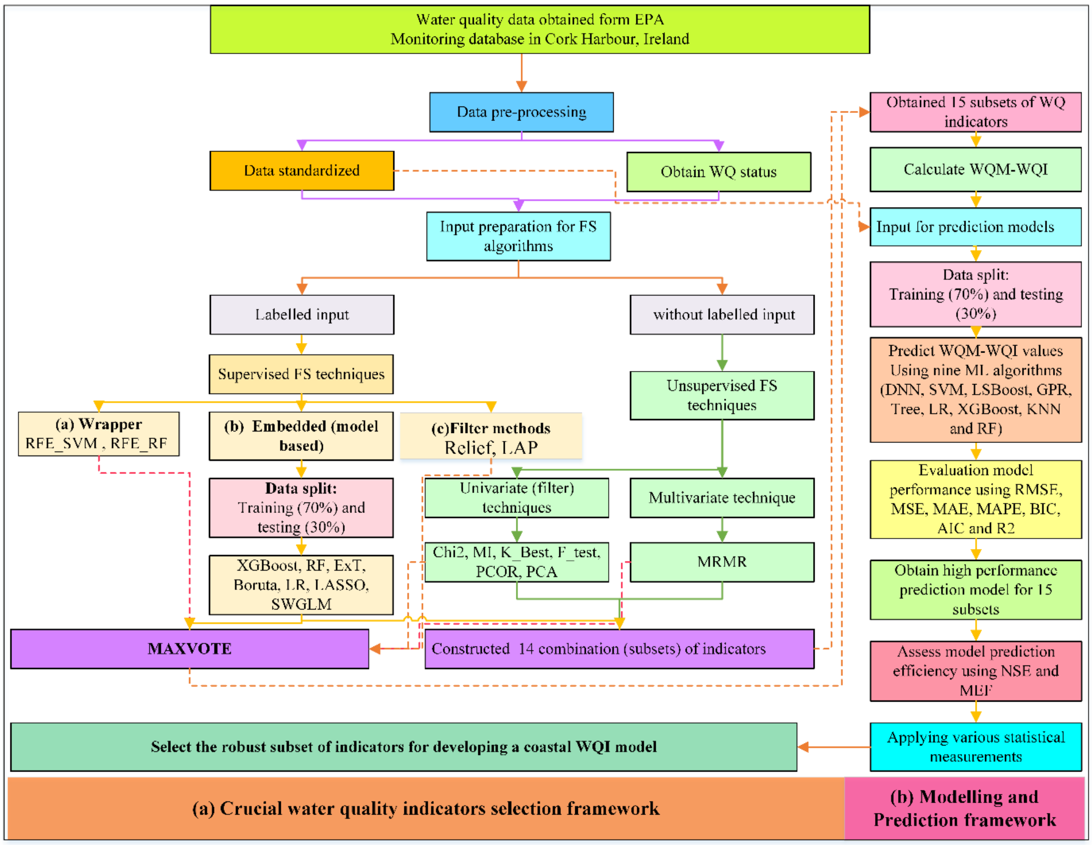


Figure 6.2. Methodological framework for selecting robust combination of water quality indicators in order to develop a coastal water quality index model.

6.5.2 Input preparation

Prior to commencing the analysis, two input datasets were constructed where one is used for supervised algorithms and other one for unsupervised methods. After collection and cleaning of indicators raw data, for the purposes of selecting relevant indicators using the supervised FS method, the input was prepared using the coastal water quality guideline. Details of the guideline values are provided in Table 6.S2. Based on guideline values WQ classified into two categories as (i) polluted and (ii) unpolluted using simple two binaries rules. If all indicators falls within permissible range it registered as unpolluted (0), on the other hand, if any indicators failed to meet the guideline values, then 1 (polluted) was assigned automatically (Uddin et al., 2022a). Details of the input for FS algorithms can be found in supplementary Table S3. It should be noted that binary labels were removed from the dataset when input was used for an unsupervised method. When obtaining water classes, the standardized z score technique was used to convert all water quality indicators to a similar scale to avoid collinearity problems (Chen Liao et al., 2008; Uddin et al., 2022d). Commonly, this techniques widely used to estimate and compare the probabilistic distribution of a score that occurs in the normal distribution among the scores of different normal distributions (Ahmed et al., 2019; Ma et al., 2020). Standardized function can be defined as follows:

$$z = \frac{(x-\bar{x})}{\sigma} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(6.2)$$

where x is measured value of the water quality indicator, $\bar{x}$ is the mean value of the indicator, and standard deviation of the indicator is σ.

6.5.3 Model hyperparameter optimization

By default, each ML algorithm composes a set of Hyperparameters that control the model's performance and prediction reliability. Commonly, two types of prediction problems, including overfitting and underfitting, are addressed in ML models that are formulated due to inappropriate hyperparameterization (Yan et al., 2019). To date now, several techniques have been developed for selecting optimal value of hyperparameters, including random search, grid search and Bayesian approach (Uddin et al., 2022c). Currently, most studies have utilized the grid search technique for hyperparameters optimization because this approach is an exhaustive optimization method that allows evaluating the model accuracy for each grid position (Elgeldawi et al., 2021; Yan et al., 2019). Compared to other approaches, the grid search method is reliable and robust to improve the model performance with incredible estimation (Villalobos-Arias et al., 2020; Yan et al., 2019). Through optimization processes, the model prediction error was measured based on the out-of-bag error (MSE) technique. Due to the incredibility of grid search technique, the present research was utilized this technique for hyperparameters optimization. The grid search results are provided in Table 6.S7 and the best-fit model (DNN) hyperparameter optimization results are presented in Table 6.4.

6.5.4 Development of prediction models

Figure 5.2(b) depicts a schematic diagram of the model development process. Prior to estimating WQM-WQIs, crucial WQ indicators were obtained from the various FS algorithms. In total, fifteen input scenarios were generated for predicting the WQM-WQI values. Table 6.2 provides the details of the input scenarios for different FS techniques. After obtaining the WQM-WQI values, a prediction model was developed to predict WQI values using normalized fifteen sub-sets of water quality indicators. In this research, the artificial intelligence based DNN and eight ML models were used to predict WQIs for various input scenarios. Details of the predictive models can be found in section 6.5. 1. For the development of the prediction model, all input scenarios data was divided into two groups: (i) 70% of the data was used for model training and (ii) 30% of the data was used for testing (validation) the model. When constructing prediction models, several common model evaluation metrics were used to assess the model's performance. The evaluation procedure is described in detail below in section 3. 5.

6.5.5 Model evaluation

In order to select the best model, various performance criteria are used in comparing different algorithms. It depends on the nature of the response variables, such as categorical or continuous. In this study, regression models were performed to predict the WQM-WQI model. The present study utilized the cross-validation (CV) approach to evaluate the predicting performance because this technique is widely used in ML technique (Uddin et al., 2022d). In this study, 10-fold CV was performed to estimate model errors at each fold of subsets. The details CV method discussed in Xiong et al., (2020). For assessing the model performance, the present research utilized root mean square error (RMSE), mean square error (MSE), mean absolute error (MAE), and mean absolute percentage error (MAPE) because most studies have used these performance (Asadollah et al., 2021; Tran et al., 2021; Uddin et al., 2022d; Xiong et al., 2020; Yan et al., 2019; Yu et al., 2020; Zaghloul and Achari, 2022). Details of these criteria can be found in Uddin et al., 2022a. All indicator values range from 0 to 1. Commonly, all criteria values are recommended as being as close to 0 as possible. The lowest values indicate the best performance of the model (Bagherzadeh et al., 2021; Uddin et al., 2022d). In addition, recently, many studies have used the Akaike Information Criterion (AIC) and the Bayesian Information Criterion (BIC) for evaluating the model performance. A few studies have applied these techniques to predict the coastal water quality (Tran et al., 2021). Details of AIC and BIC can be found in (Akaike, 1998) and Stone, (1979), respectively. In this research, these two advanced performance criteria were utilized to select the best FS algorithm for predicting WQM-WQIs. Commonly, the AIC estimates based on how well samples fit the model, while the BIC takes into account both of the how well the model fits and how complicated it is (Emmert-Streib and Dehmer, 2019; Shalizi, 2015; Tran et al., 2021). The AIC and BIC of the predictive models are calculated using the equation (6.3) and equation (6.4), respectively. The equations can be defined as follows:

$$\mathrm{AIC} = -2\log(\mathrm{L}) + 2\mathrm{k} \quad \dots\dots\dots\dots(6.3)$$

$$\mathrm{BIC} = -2\log(\mathrm{L}) + \mathrm{k}\log(\mathrm{n}) \quad \dots\dots(6.4)$$

where k is the number of water quality indicators, L is the value of model likelihood estimation and n is the number of the samples. For the estimation of likelihood estimation, the maximum likelihood estimation analysis was utilized according to the methodology of Banks and Joyner (2017). Details of the methodology can be found in Banks and Joyner (2017).

6.5.6 Model efficiency analysis

For the purposes of the hydrological model efficiency analysis, the Nash–Sutclife efficiency (NSE) index widely used. Recently, several studies have utilized the NSE index for selecting the best model in machine learning and artificial intelligence (McCuen et al., 2006). Usually, its value ranges from -∞ to 1, with a number close to 1 indicating the best model performance and a negative score indicating low model efficiency (McCuen et al., 2006; Sharif et al., 2022). The NSE index is defined as follows:

$$\mathrm{NSE} = 1\text{-}\frac{\sum_{i=1}^{n}(p_i\text{-}m_i)^2}{\sum_{i=1}^{n}(m_i\text{-}\bar{m})^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6.5)$$

where m_i is the measured and p_i is the predicted values of *i^th^* samples respectively whereas $\bar{m}$ is the mean measured value.

Moreover, the present study utilized the model efficiency factor (MEF) for identifying the best model in terms of prediction errors. A few studies have suggested this technique as the extension form of the NSE index to obtain better results of model in terms of efficiency (Sharif et al., 2022). Like the NSE index, its score ranges from 0 to 1, where the smallest value indicates the better efficiency of the model. Unlike, the MEF score of 0 refers to the bias-free model, although this is not a reliable indicator for measuring the overall performance of a model. . It can be defined as follows:

$$\mathrm{MEF} = \sqrt{1\text{-NSE}} \quad \ldots\ldots\ldots\ldots\ldots. (6.6)$$

where NSE is the Nash–Sutclife efficiency index score, which is obtained from equation (6.5).

6.5.7 Statistical significance of robust subset of indicators

To compare the performance of WQI model for various subsets of water quality indicators, the present study utilized the Z-statistic. Recently, several studies have used this technique to compare between datasets or models results for understanding the differences between estimated and predicted values (Gaur et al., 2022; Mauget, 2011; Mauget et al., 2012; Rahman and Harding, 2016). A few studies have applied this technique for estimating uncertainty in the estimation (Aslam, 2022). Commonly, Z-statistics indicate that a statistical estimation of measuring the number of standard deviations below or above the mean value, whereas the standard deviation is set to 1 and mean value refers at 0 (Andrade, 2021; Massey and Miller, 2017). The Z-statistics performed according to the approach of Rahman and Harding, (2016). It can be defined as equation 6.2 (mentioned above), with the WQI values being taken into account for the estimation of Z-statistics.

For the purposes of comparing the WQIs varition between measured and model prediction, the presented study defined the following null and alternative hypotheses to check the statistical significance of WQI values diffrences predited by the DNN model using various subsets of indicators:

Null hypothese; $H_{i0} : WQI_m = WQI_p$

Alternative hypothese; $H_{iA} : WQI_m \neq WQI_p$

where, WQI_m and WQI_p are the measured and predicted WQI values, respectively.

For testing the hypotheses, two-tailed statistical test was conducted with the critical values of -1.96 and +1.96 at 5% significant level ($p < 0.05$). If p value is less than 0.05 then the null hypotheses rejected. Detail of the hypotheses test can be found in Rahman and Harding, (2016).

6.5.8 Reliability analysis of the robust subset of indicator

Absolute standardized residual estimate analysis (ASRE) is widely used for validation of simulation results in terms of the impact of various inputs (Best et al., 2008; Rahman et al., 2013). It is a very straightforward technique to analyse the model accuracy (Rahman et al., 2013). Like as other criteria of simulation model evaluation, its values range from 0 to ∞, when the ASRE value is less than 2, it means the model performance is acceptable. When it estimates close to 0, the model performance is good and reliable, a larger value of ASRE (≥ 2) indicates the unexplained error or model results are unacceptable (McManus et al., 2020; Rahman et al., 2013). In this research, this approach was utilized to validate the model output in terms of reliability of water quality indicators and their impact on the WQM-WQI model. The ASRE can be defined as follows:

$$\text{ASRE} = \frac{\delta}{\sqrt{\text{AEMSE}}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(6.7)$$

where

$$\delta = |y_n\text{-}\hat{y}_n|$$

$$\text{AEMSE} = \frac{1}{N}\sum(y_n\text{-}\hat{y}_n)^2$$

Herein, ASRE mathematical function notations are: y_n is the measured WQI, $\hat{y}_n$ is the predicted WQI at the *n^th^* monitoring site, and N is the total number of monitoring sites, whereas AEMSE is the average empirical mean squared error of the predicted WQI values.

However, it is noted that, in order to implement feature selection algorithms, prediction models, and all statistical analyses and visualisations, the present study used the Python programming language on the Google Colab cloud-computing platform. It is a very convenient environment, and it enables users to run a variety of advanced machine learning models using the Python language.

6.6. Results and discussion

6.6.1 Water quality indicators statistical overview

A statistical summary of water quality indicators over the period of the research is given in Table 6.1. Most indicators were within the permissible limits except for the DIN, MRP, TRAN and TON (Table 6.1).

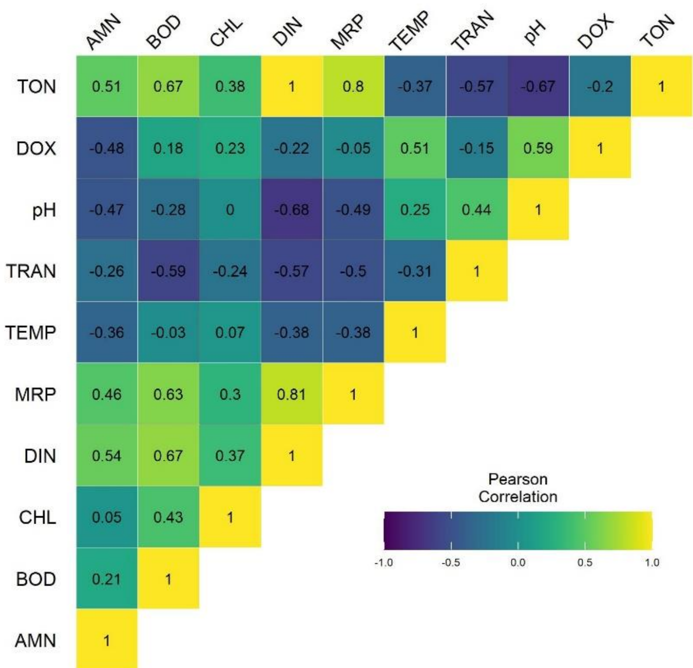


Figure 6.3. Pearson correlation results of various water quality indicators in Cork Harbour.

At the majority of monitoring sites in the upper Harbour, four water quality indicators (DIN, MRP, TRAN, and TON) exceeded the guidelines values, but the lower and outer Harbour sites met with the requirements for coastal water quality (Figure 6.S3). The authors in earlier studies also revealed similar findings (Uddin et al., 2022a, 2022b; 2022d). In addition, there was a moderate positive correlation among water quality indicators, except for the TEMP, CHL, pH and DOX, whereas the moderate negative correlation was found between TRAN, DOX, pH and other indicators (Figure 6.3). Details of the correlation are presented in figure 6.3.

6.6.2 Comparison of various FS techniques

In order to select the key indicators, all water quality indicators were ranked based on their relative significance in terms of assessing coastal water quality using various FS techniques. Details of the results of the features rank are provided in supplementary material (Figure 6.S4). Based on the rank of indicators, fourteen subsets of indicators were constructed. Table 6.2 provides the details of the indicator subsets. In terms of the number of indicators in each dataset, a significant difference was found in this study within various FS techniques. Maximum number of indicators recommended by the widely used RF and PCOR techniques. Both methods suggest that eight water quality indicators are crucial for assessing coastal water quality (Table 6.2). The second highest number of indicators (seven) were selected by the XGBoost, MI, ExT, and RFE_RF techniques. Whereas most popular technique (in existing WQI model) PCA recommended most common indicators including AMN, BOD_5, CHL, DIN, MRP, and TON as crucial. Contrary, four FS techniques (Borurta, K_Best, F_test, and relief) were recommended with a similar set of indicators, including BOD5, DIN, MRP, pH, TON, and TRAN as crucial indicators (Table 6.2). In addition, most filter methods revealed that DIN, MRP, TON, and TRAN are crucial indicators in the dataset except the χ^2 , PCOR and PCA techniques. Unlike other methods, the LASSO and SWGLM recommended completely different sets of indicators as important; those methods suggested only three indicators as being crucial, whereas the MAXVOT approach was recommended for most of the nutrient indicators for the assessment of coastal water quality, including DIN, MRP, TRAN, pH, DOX, and TON, like in the RF method (Table 6.2). There was a significant correlation among water quality indicators with the WQM-WQI values. Detail of the correlation results can be found in figure 6.S5. When compared to the WQI values, most selected indicators by various FS methods have shown a moderate to high positive correlation between WQI and most indicators, except for the TEMP and DOX; these show the weakest correlation among indicators as well as WQI values (Fig. 6.S5a; Fig. 6.S5i). The XGBoost (S3) and RF (S4) techniques suggested the most indicators as key characteristics within FS methods in this study, whereas a significant indicator variation was found in embedded FS algorithms. With the exception of TEMP and DOX, most WQ indicators and WQI within these subsets were found to have a moderate correlation (Figure 6.S5c; Figure 6.S5d). While pH and TON were common features, there was a strong correlation between indicators and WQIs (Table 6.2). However, most FS methods suggest that DIN, MRP, TRAN, pH, DOX, and TON are the key indicators for assessing coastal water quality.

6.6.3 Comparative analysis of WQM-WQI model for various scenarios of FS methods

6.6.3.1 Selected key water quality indicators subsets

One of the crucial stages of the WQI model is the indicator selection. In order to select the key indicators, the current study used eighteen FS techniques. In total fifteen subsets were constructed, where fourteen subsets (combinations) of water quality indicators were selected from the eighteen FS technique and the remaining subset was obtained using majority voting approaches. Table 6.2 provides the details of the selected key indicators. Details of the majority voting approach can be found in Table 6.S4.

Table 6.2 Different scenarios of significant water quality indicators obtained from various features selection methods.

Indicators subsets	Suggested WQ indicators	number of indicators	indicator selection methods
S1	DIN, MRP, DOX,TON,TRAN	5	RFE_SVM
S2	AMN, CHL, pH, DOX, TRAN	5	LR
S3	AMN, BOD_5, CHL, DIN, MRP, TEMP, DOX	7	XGBoost
S4	BOD5, DIN, MRP, TEMP, pH, DOX, TON, TRAN	8	RF
S5	BOD_5, DIN, MRP, TEMP, pH, TON, TRAN	7	MI/ExT
S6	DIN, pH, TON, TRAN	4	MRMR
S7	BOD_5, DIN, MRP, pH, TON, TRAN	6	Boruta/K_Best/F_test/Relief
S8	AMN, BOD_5, CHL, DIN, TEMP, pH, DOX, TRAN	8	PCOR
S9	AMN, BOD_5, DIN, MRP, pH, DOX, TRAN	7	RFE_RF
S10	AMN, BOD_5, CHL, DIN, MRP, TON	6	PCA
S11	DIN, MRP, TEMP, pH, TON, TRAN	6	LAP
S12	pH, DOX, TON, TRAN	4	Chi2
S13	pH, TON, TRAN	3	LASSO

S14	AMN, pH, TON	3	SWGLM
S15	DIN, MRP, TRAN, pH, DOX, TON	6	MAXVOT

6.6.3.2 Sub-index (SI) statistics of WQ indicators

The SI values of WQ indicators were calculated using the procedures of Uddin et al., (2022a). Recently, several studies have revealed that the SI functions contribute a significant amount of uncertainty to the final index due to the ambiguity problems. In their study, Uddin et al. (2022a) proposed three linear interpolation functions in order to calculate the SI values without ambiguity problems. Details of the SI functions can be found in Uddin et al. (2022a). Figure 6.4 provides the statistical summary of the SI values for various water quality indicators. Details of the SI results are provided in Table 6.S5. As can be seen from the figure (below), higher SI values were obtained for those indicators that are found within the permissible limits whereas the breached indicators were given relatively lower values. In this study, it was examined that the majority of SI value indicators had no ambiguity issues (Table 6.S5).

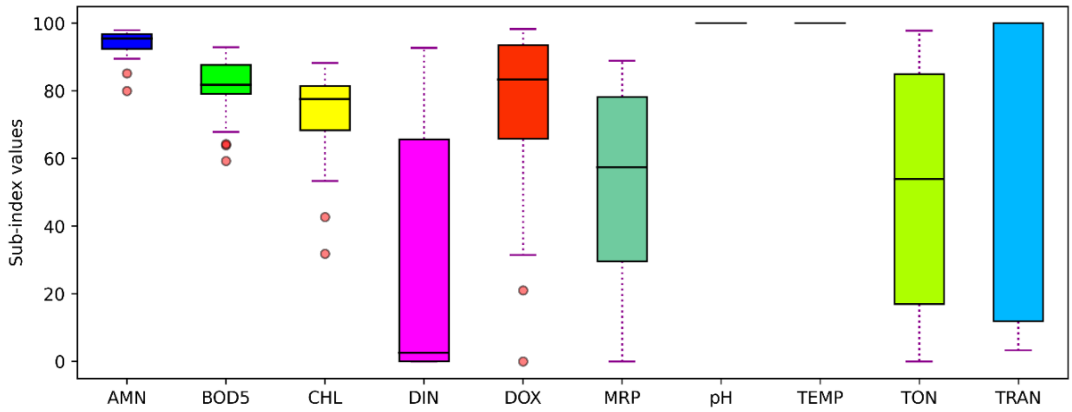


Figure 6.4. Statistical overview of the calculated SI of various water quality indicators.

6.6.3.3 Different set of indicators weight values

Prior to estimating the indicators' weight values, the present study determined the rank of the suggested indicators based on their relative importance. The present study obtained the fifteen subsets of water quality indicators using different FS techniques. After obtaining the indicator rank, weight values were estimated using the approaches of Uddin et al. (2022a). For the purposes of the WQI calculation, we estimated weight values for fifteen subsets of indicators in this research. Uddin et al.(2022a) proposed an effective method that offered a thorough methodology combining machine learning algorithms and statistical approaches to calculate indicators' weight values without the assistance of experts, allowing for the optimization of the uncertainty level in this process. This method was superior to the existing approaches (Uddin 2022c). Figure 6.S4 presents the rank order of various indications within different subsets, and Table 6.S4 provides weight values for various indicators of subsets.

6.6.3.4 Aggregation results for various scenarios

Aggregation functions allows converting SI and weight values of indicators into the single numerical expression that provides comprehensive picture of the water quality. In this research, WQIs were calculated using the approaches of Uddin et al. (2022a). Table 6.S6 contains information on the measured WQIs for various subsets of indicators. A statistical summary of WQIs for various input sizes of indicators are presented in figure 6.5 using Whisker boxplot technique. The Figure (below) shows that there was a substantial difference in WQIs between subsets of the indicators Compared to FS methods, higher measured WQIs scores were found for the S2 subset; they varied from 68 to 98, with an average of 88. Relatively, the lowest WQIs scores were calculated for the S1 subset while it ranged between 8 and 91, with an average score of 61 (Figure 6.5). Three categories of water quality—"good," "fair," and "marginal"—were found based on index values. Most subsets of indicators suggested that the water quality was classified into "good" and "fair" quality in Cork Harbour during the study period (Figure 6.5). The results of various subsets of indicators revealed that the WQIs varied due to the nature of indicators. The index results also revealed that there was no impact of model input size on WQI values. For example, the subsets S13 and S14 contained only three water quality indicators, but the index scores ranged from 58 to 99 and 66 to 99, respectively (Figure 6.5; Table 6.S6).

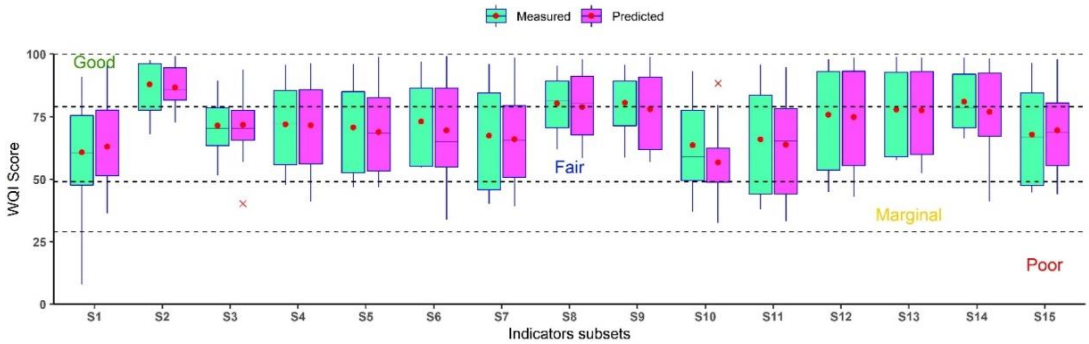


Figure 6.5. Statistical summary of WQIs for various subsets of water quality indicators in Cork Harbour.

On the other hand, the present study also found comparable statistical measures for subsets S3 (7), S4 (8), S5 (7), S8 (8), and S9 (7); herein, close brackets indicate the number of indicators for each subset (Figure 6.5; Table 6.S6). Several research have recently asserted that the quantity of indicators can affect the WQI results (Bui et al., 2020; Uddin et al., 2021). In contrast to earlier studies, in this research, there was no evidence that the WQIs model was affected by the input sizes of the indicators.

6.7 Analysis of prediction results for different subsets of indicators

6.7.1 Model optimization results

Prior to training, the training data set is divided into training-validation sets using the 10-fold cross validation approach. When data sets were constructed, the training set was used for the model fitting, whereas the validation set was employed for the optimization of the hyperparameters based on 10-fold cross validation results using the grid search technique. Table 6.S7 provides the optimal hyperparameters for the nine prediction models, including those in Table 6.3. The outperformed model hyperparameters are given in Table 6.3 below.

Table 6.3 Optimized hyper-parameters values of DNN model for various scenarios.

Model parameters	Optimum values	Definition
Learning rate	0.5	Model learning rate
Number neurons	6	Number of neuron each hidden layer
Hidden layers	5	Number of hidden layers
Activation function	ReLU	Function for neuron activation
Regularization	Dropout	Regularization techniques for control the model overfitting
Dropout	0.5	% of neuron dropped out at each iteration
Momentum (μ)	0.2	Weight values of previous update from each iteration
Weight and bias initiation	normal	Determination of initial weight
Optimizer	Adam	Defined output probability of prediction results
Loss function	Mean squared error	Used for the minimization of prediction loss
Epochs	1000	Number of training iteration
Batch size	20	Sample size of training period for each iteration
Weight decay	2	Used for preventing model overfitting problem
Type	Regression	Developed model for regression

6.7.2 Prediction results and model performance analysis

After tuning the model, nine ML algorithms were trained using various subsets of indicators. Details of the subsets can be defined in Table 6.2. Each trained model was tested after it had been developed to assess its performance. For model validation purposes, various metrics (RMSE, MSE, MAE, MAPE, AIC, and BIC) were calculated for both the training and testing datasets. Details of the metrics results of various algorithms can be found in Table 6.S8 (a – h). Based on the model error during training and testing, the best prediction model selected for predicting WQI values using each subset of indicators, where the target was measured WQI values for the relevant subset.

Table 6.4 10-fold cross validation results of DNN model for different scenarios.

Scenarios	Training						Testing					
	RMSE	MAE	MSE	MAPE	AIC	BIC	RMSE	MAE	MSE	MAPE	AIC	BIC
S1	0.77	0.63	0.60	1.37	-4.84	2.50	1.22	3.49	1.49	2.41	50	57.33
S2	1.69	13.3	2.86	3.39	92.90	100.2	0.41	0.04	0.17	0.19	90.5	-83.2
S3	1.28	5.12	1.65	2.29	62.26	69.60	0.44	0.08	0.19	0.27	69.3	-61.9
S4	**0.66**	**0.33**	**0.44**	**0.68**	**-19.6**	**-7.85**	**0.42**	**0.04**	**0.18**	**0.24**	**-83**	**-71.7**
S5	**0.56**	**0.19**	**0.32**	**0.43**	**-39.7**	**-29.4**	**0.62**	**0.31**	**0.38**	**0.63**	**-20**	**-10.1**
S6	0.91	1.98	0.83	1.06	29.92	35.79	0.69	0.42	0.48	0.78	-19	-13.9
S7	1.30	4.85	1.69	2.69	62.53	71.32	0.79	0.69	0.63	0.91	0.13	8.92
S8	0.44	0.10	0.19	0.24	-57.7	-46.0	0.48	0.11	0.23	0.28	-37	-25.4
S9	**0.41**	**0.06**	**0.17**	**0.20**	**-78.2**	**-67.9**	**0.16**	**0.00**	**0.03**	**0.03**	**-196**	**-186**
S10	1.26	5.44	1.59	2.44	66.20	75.00	0.63	0.38	0.40	0.63	-19	-9.83
S11	0.64	0.24	0.41	0.79	-33.7	-24.9	1.04	1.54	1.08	1.71	25.8	34.61
S12	1.25	3.89	1.56	2.13	51.47	57.33	1.26	4.43	1.60	2.66	55.6	61.48
S13	1.37	5.34	1.88	2.76	59.61	64.00	0.43	0.05	0.18	0.24	-88	-83.6
S14	1.25	3.29	1.56	2.06	44.12	48.56	0.73	0.48	0.53	0.62	-17	-13.2
S15	1.00	1.68	1.00	1.66	28.60	37.40	0.84	1.13	0.70	0.85	15.9	24.71

Table 6.4 provides the 10-fold cross validation results for the best predictive model. The best predictive model was determined by comparing the prediction performance metrics among nine algorithms. As mentioned earlier, details of the performance metrics can be found in Table 6.S8 and Table 6.4. Once the best prediction model was obtained, WQI values were predicted for each subset of indicators using the best algorithm. Figure 6.5 shows a statistical summary of measured and predicted WQI values for each subset. Figure 6.6 also reveals the relationship between the measured and predicted WQI values for various subsets. Details of the prediction results at each monitoring sites in Cork Harbour for each subset of indicators can be found in Table 6.S9.

Based on the performance metrics, relatively, the smallest prediction errors (RMSE, MSE, MAE, MAPE, AIC and BIC) found for the subsets S4, S5 and S9 during both training and testing periods (Table 6.4). Compared to the model validation (testing) period, model performance improved for those subsets apart from the S5, whereas model performance significantly dropped due to the model under-fitting problem (Figure 6.6). The performance of the DNN model is influenced by a number of variables, such as unstandardized data, the size of the training dataset, high bias, number of hidden layers, low variance of the model, etc. (Choudhary et al., 2022; Sarker, 2021; Uzair & Jamil, 2020) . Recent studies have shown that the number of hidden layers has a negative impact on predicting performance, which has a very negative impact on the network's efficiency (Uzair & Jamil, 2020). A few studies have reported that the DNN model underfitting problem may occur due to the small training dataset (Choudhary et al., 2022). In this research, underfitting problem may have occurred due to the small training dataset or both the small training dataset and the number of hidden layers (Uddin et al., 2022d).

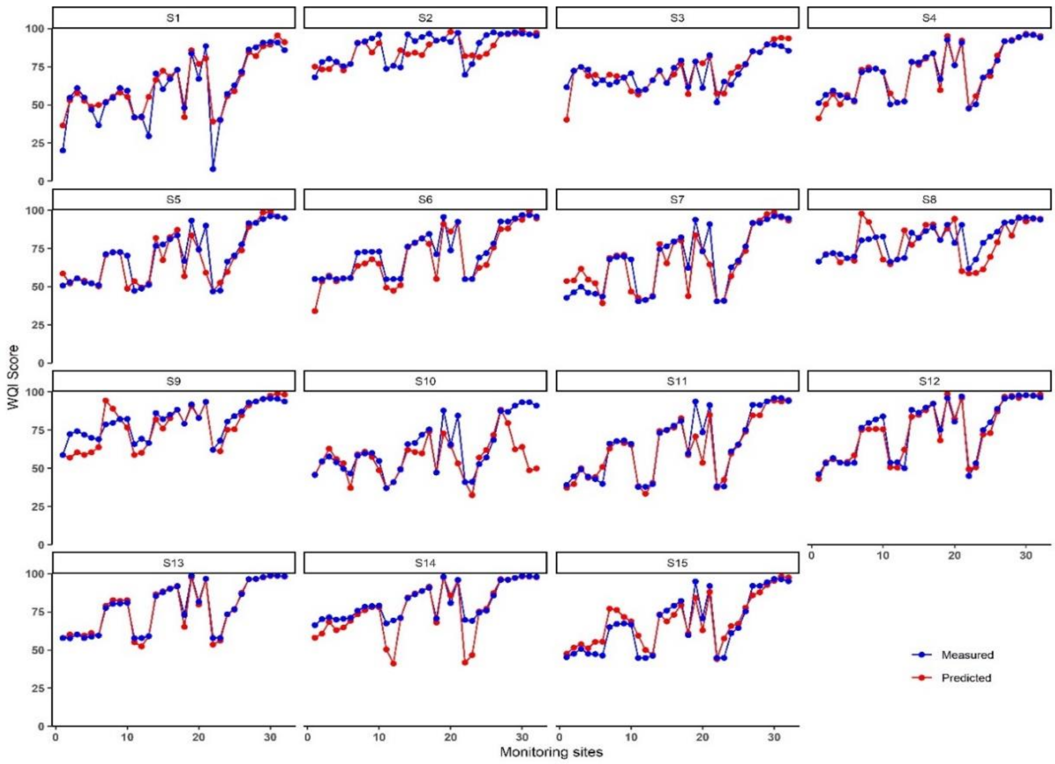


Figure 6.6. Point-base comparison between measured and predicted WQM-WQI values for different subsets of water quality indicators using DNN algorithm.

In addition, the present study found also good performance for the subset S3 for which indicators were extracted using the XGBoost technique (Table 6.2). These similar results also reported in several earlier studies (K. Chen et al., 2020; Islam Khan et al., 2021; Naghibi et al., 2020; Uddin 2022b). Due to the over-fitting issue, model performance on this subset was greatly improved over the validation (testing) period (Table 6.4).

Compare to the prediction models in terms of input sizes, the best model was built with big input sizes including subset S3(7), S4(8), S5(7), S8(8), and S9(7) where close brackets indicate the input size of indicators. The smaller input sizes for instances subsets S13 and S14, both built with just three indicators, showed, relatively, the lowest prediction performance (Table 6.4). The results of the performance metrics revealed that the input sizes of indicators could be affected the DNN model's performance. Similar finding was also reported in literatures (Bailly et al., 2022; Pasini, 2015). In addition, the prediction results also reveal that various FS techniques could have a significant effect on model performance.

6.7.2.1 Sensitivity results of various subsets

For the purposes of sensitivity analysis of various FS techniques, several studies have used correlation coefficient technique to determine the relationship between model inputs and output (S. Chen et al., 2020; Hamby, 1994; Uddin et. al., 2022a). In this research, the coefficient of determination (R^2) was utilized in the approach of Uddin et al., (2022a) to assess the sensitivity level of various water quality indicators in the WQI models. Commonly, it ranges from 1 to 0, where higher values indicates the strong relationship between model input and output (Uddin et al., 2022a; 2022d). Figure 6.7 presents the R^2 for various subsets of indicators.

Unlike other evaluation metrics, higher values indicate the highest sensitivity. According to R^2 values, the highest sensitivity was found for the S4 (R^2 = 0.96), the S11 (R^2 = 0.92), the S12 (R^2 = 0.96), S13 (R^2 = 0.98) and S15 (R^2 = 0.0.91) subsets. Most subset of indicators shown better sensitivity except for subsets S8 (R^2 = 0.26), S9 (R^2 = 0.83), and S10 (R^2 = 0.43) in this research (Figure 6.7).

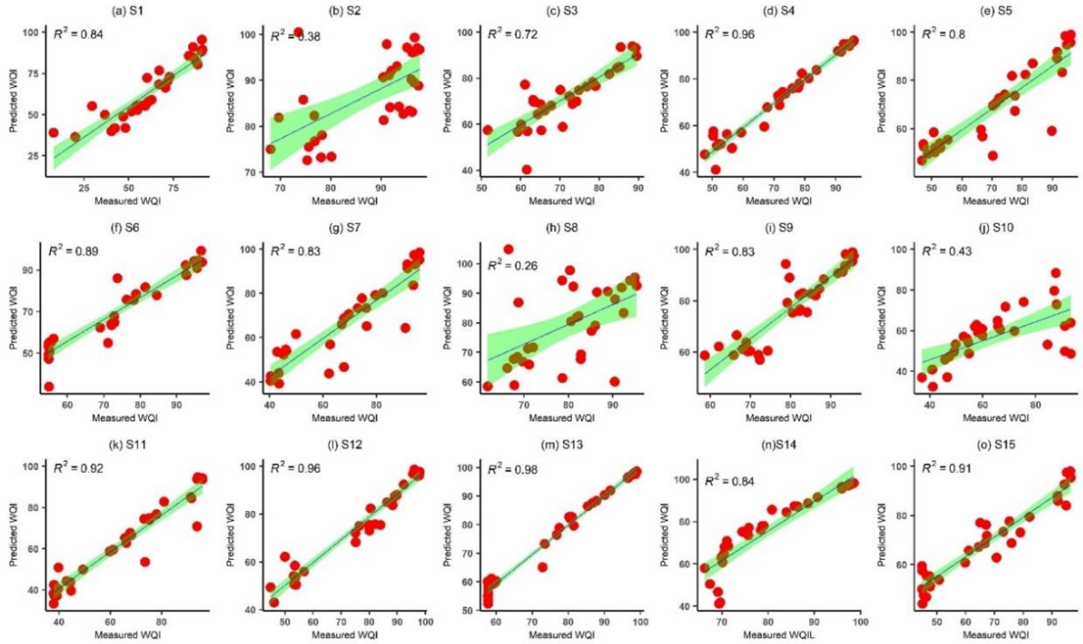


Figure 6.7. Relationship between measured and predicted WQI scores based on the different subsets of indicators.

6.7.2.2 Model efficiency analysis

In this study, the NSE and MEF computed to evaluate the model efficiency. Figure 8 shows the results of NSE and MEF for various subsets of water quality indicators. Based on the results, larger NSE and smaller MEF values were calculated for the subset S13 (Figure 6.8), although other statistical metrics are not supported for this subset.

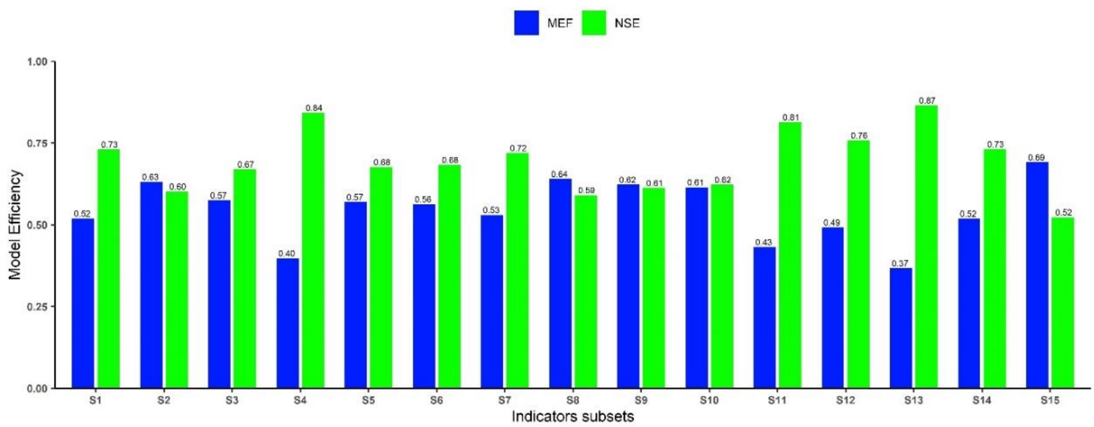


Figure 6.8. Results of DNN model efficiency for different subsets of water quality indicators.

Most metrics were found to be larger through the training (RMSE = 1.37, MSE = 5.34, MAE = 1.88, MAPE = 2.76, AIC = 59.61, and BIC = 64), whereas model performance was improved significantly due to the underfitting problem during testing (RMSE =

0.43, MSE = 0.05, MAE = 0.18, AIC = -88, and BIC = -83.6) periods (Table 6.4). Like subset S13, the larger NSE (0.84) and the smaller MEF (0.40) were also calculated for subset S4 (Figure 6.8). Compared to other metrics, all the statistical evidence shows that the subset S4 is the best for predicting the WQI values than other subsets (Table 6.4; Table 6.6).

6.8 Identification of robust subset indicators for the development of WQI model

6.8.1 Results of statistical significance of FS techniques

In this research, Z-statistics were used to identify the most reliable subset of water quality indicators for developing an efficient WQI model. Table 6.5 provides the results of the statistical hypothesis test for the various subsets of indicators in order to analyse the data differences between subsets in terms of prediction errors. Based on the results of the hypothesis test, there was a statistically significant difference between the measured and predicted WQI values for different subsets of indicators at $p < 0.05$, which meant that the null hypothesis was wrong (Table 6.5).

Table 6.5 Summary of the Z-statistics for selecting robust indicators subset for estimating the WQM-WQIs with 95% confidence level at $p < 0.05$.

Subsets	Z-Statistics	p-value
S1	-0.472	0.637
S2	0.362	0.717
S3	**-0.087**	**0.93**
S4	**0.085**	**0.932**
S5	0.423	0.668
S6	0.857	0.391
S7	0.274	0.784
S8	0.2	0.838
S9	0.818	0.413
S10	1.804	0.071
S11	0.426	0.67
S12	0.204	0.838
S13	**0.068**	**0.945**
S14	1.119	0.263
S15	-0.382	0.702

Bold indicate the least amount of data difference

It can be seen from the data in Table 6.5 avobe that the z statistics also indicate that there were no significant data differences between measured and predicted WQI values in the subset S4, whereas higher data differences between measured and predicted

WQI values were found for the S6, S9, S10, and S14 (Table 6.5). Comparatively, the lowest data difference was found in 93% of the samples for subsets S3, S4 and S13 (Table 6.5).

In addition, Figure 6.9 presents the summary of the Z-statistics by Box and whisker plot that provides the variability in z-score values for different subsets of indicators. As shown in figure, most of the subset's Z-scores were found between +1 to –1 where the data outliers of prediction WQI values were found for the S3 and S10 subsets. Relatively, the lowest standard deviation from the mean predicted WQI values was found for the S4, S3 and S13, it ranged between +0.085 and -0.087 (Table 6.5).

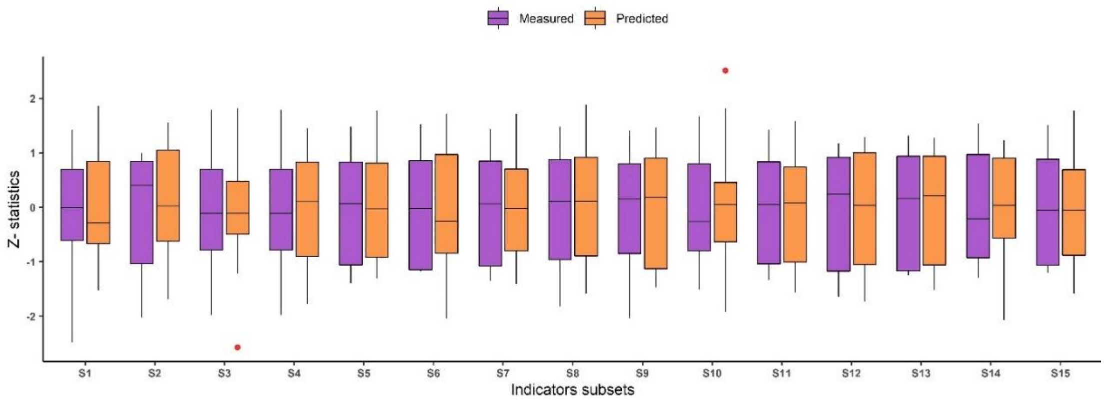


Figure 6.9. Comparison of Z-statistics between measured and predicted WQIs for various subsets of indicators. Whereas red circles indicate, the data outliers and black solid lines inside the box refer to the median values of WQIs.

However, for the purposes of determining the best subset(s), subsets were ranked (see Table 6.6) taking on the RMSE values (training and testing) from Table 6.4 as a measure of prediction error, the R^2 values from Figure 6.7 as a measure of model sensitivity, the NSE and MEF values from Figure 6.8 as a measure of model efficiency (above), the ASRE values from Figure 6.S7 (supplementary materials) as a measure of model reliability, the z statistics from Table 6.5, root mean square deviation and standard deviation from Figure 6.11 as a measure of performance of various subsets. Subsets were first scored from 1-15 separately for each metric, with 1 indicating the best performance and 15 worst. All measure' scores were then added, giving each metric equal weighting, and the subsets ranked based on the cumulative scores. A smaller cumulative score indicating good performance should be ranked first, and a larger score indicates the worst performance of the subset(s). According to the cumulative score of the various subsets, the S4 subset was ranked first, whereas the S13 was ranked second. Table 6.6 provides the details of the scoring procedures for various measures and subsets ranked above.

Table 6.6 Ranking of various subsets based on different attributes of model performance measures.

Subsets	score based on prediction performance metrics (table 4)		score based on sensitivity (Fig. 7)	score based on model efficiency (Fig. 8)		score based on reliability (Fig. S7)	score base z statistics (Table 5)	score based on root mean square deviation and standard deviation (Fig. 11)	cumulative score of various measures	Rank
	training RMSE	testing RMSE	R^2	NSE	MEF	ASRE	Z	Tylor statistics		
S1	15	6	8	6	6	4	11	8	64	7
S2	8	15	14	13	13	10	7	13	93	12
S3	7	12	12	10	10	9	3	11	74	10
S4	**6**	**5**	**2**	**2**	**2**	**5**	**2**	**2**	**26**	**1**
S5	5	3	11	9	9	15	10	10	72	9
S6	4	8	6	8	8	11	13	6	64	7
S7	3	11	10	7	7	8	6	9	61	6
S8	2	2	15	14	14	7	4	14	72	9
S9	1	1	9	12	12	12	12	7	66	8
S10	14	14	13	11	11	3	15	12	93	12
S11	13	4	4	3	3	1	9	6	43	3
S12	12	10	3	4	4	5	5	4	47	4
S13	**11**	**13**	**1**	**1**	**1**	**5**	**1**	**1**	**34**	**2**
S14	10	9	7	5	5	2	14	8	60	5
S15	9	7	5	15	15	14	8	3	76	11

Based on analysis of various statistical measures, the results indicate that the S4 subsets are effective for estimating WQI values in terms of the lowest model prediction error (Table 6.6). Details of the hypothesis test for different subsets of indicators and z-score values are provided for each monitoring site in Cork Harbour and the probability curve for measured and predicted WQI values in figure S6.1 and S6.2. Figure 6.10 shows the data differences between measured and predicted WQI values for subset S4. It can be seen from the figure below that 65% of the monitoring sites in lower Harbour Z-scores were found between ± 1, whereas relative higher data differences were found at monitoring sites in outer Harbour (Figure 6.10a). It can also be seen from the probability curve of measured [Figure 6.S6.1 (c2)] and predicted

[Figure 6.S6.1 (c3)] WQIs that the S3 subset estimates are somewhat overestimated for many monitoring sites as the probability density curve of the Z-score ranged between ±2 whereas a Platykurtic shape for the probability distribution curve was observed for the S13 subset of indicators that indicate that fewer extreme positive or negative WQI values were predicted. Compared to subsets S3, S4 and S13, a relatively normal probability distribution curve shape was found for the subset S4 (measured and predicted WQI values) (Figure 6.10b; Figure 6.10c).

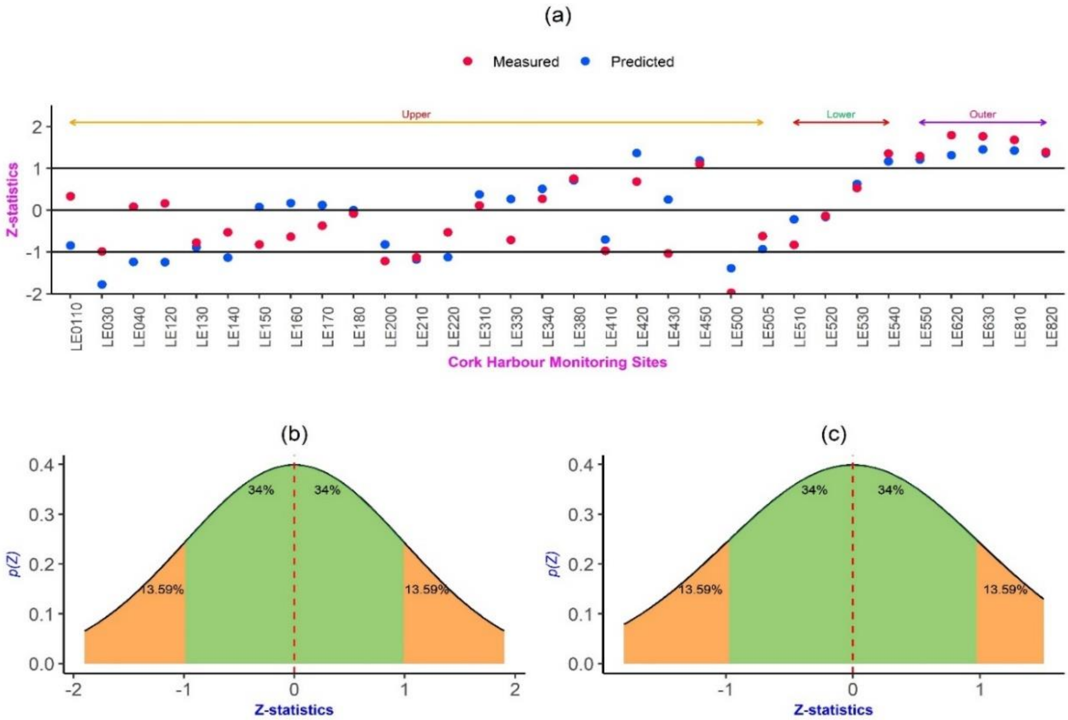


Figure 6.10. Results of the hypothesis test of WQI values for subset S4 water quality indicators: (a) Z-statistics estimation by monitoring sites; (b) Measured WQI values probability curve of Z- statistics; and (c) Predicted WQI values probability curve of Z-statistics.

However, the results of the Z-statistics indicate that the subset S4 predicted the WQI values are statistically accurate at each monitoring sites in Cork Harbour.

6.8.2 Comparison of various FS selection methods (subsets)

For the purposes of the visual comparison of the performance of various FS techniques, the present study utilized the Taylor analysis and Error Bars technique. Figure 6.11 shows the comparison results obtained from the WQM-WQI model for the various FS techniques using fifteen combinations (subsets) of water quality indicators. According to the thumb rule of the Taylor diagram, the subset S4 (RF) has a higher correlation with a lower root mean square deviation and a lower standard deviation compared with fourteen other subsets of indicators. According to the findings of Taylor statistics, the WQM-WQI model's performance was enhanced when the subset S4 indicators were used to evaluate the coastal water quality in Cork Harbour.

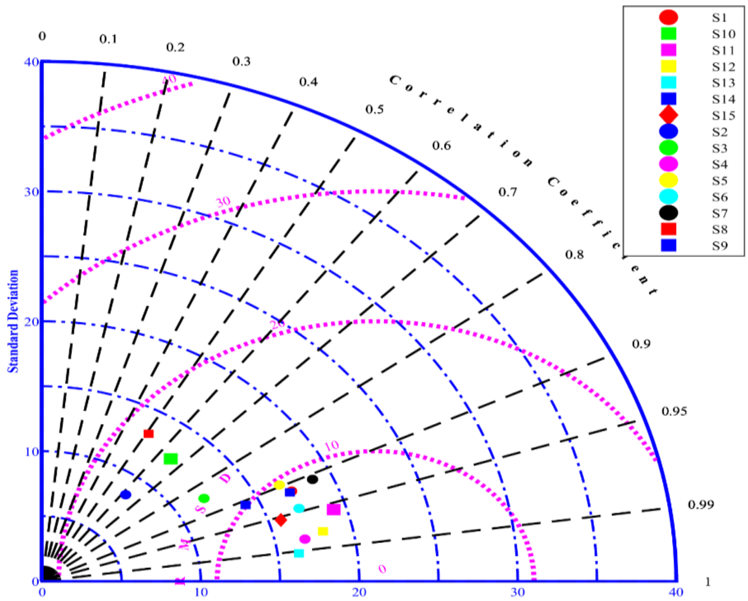


Figure 6.11. Comparison of various FS techniques performance by Taylor diagram.

In addition, the error bar results also reveals that there was no significant statistical difference at 95% confidence interval ($p<0.05$) between measured and predicted WQI values for the S4 subset in this study (Figure 6.12). The results of this study suggest that the subset S4 indicators might be helpful for the accurate assessment of coastal water quality with the substantial improvement of the WQM-WQI model's performance.

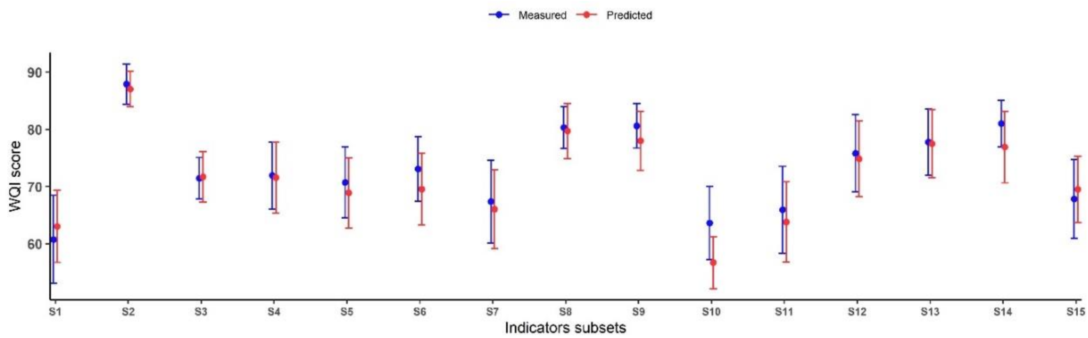


Figure 6.12. Results of 95% confidence interval (CI) of WQM-WQIs scenarios for various subsets.

6.9 Reliability results of the robust subset

In order to assess the reliability of using WQ indicators (subset S4) for the WQM-WQI model, the ASRE technique was used to validate the model results in assessing coastal water quality. The robust subset S4 contains eight indicators, including BOD5, DIN, DOX, MRP, pH, TEMP, TON, and TRAN (Table 6.2), that were obtained by the RF technique. Details of the ASRE results can be found in Figure 6.S7 for various subsets of indicators. Figure 6.13 presents the reliability of the S4 subset indicators (Figure 6.13a–Figure 6.13h) and their impact on the WQM-WQI model (Figure 6.13i). The results of ASRE indicate that the WQM-WQI model provided the most accurate and consistent results of water quality indicators in Cork Harbour. As shown in Figure 6.13, the model error was significantly higher in the monitoring sites of the upper part than in other parts of the Harbour because, most of the indicators [DIN (Fig. 13b), MRP (Fig. 6.13c), TON (Fig. 6.13g) and TRAN (Fig. 6.13h)] breached the guidelines values, whereas relatively other parts of the monitoring sites were found within the permissible range. The ASRE values confirmed that the WQM-WQI model provided the most reliable and consistent results of water quality indicators for the subset S4 in Cork Harbour. The results also indicate that the quality of Harbour water was significantly degraded at most monitoring sites in the upper Harbour, while it improved in the lower and outer parts of monitoring sites. The findings of this study are in line with those earlier studies (Uddin et al., 2022a; 2022d; 2020a). In addition, it should be highlighted that larger ASRE (ASRE $\geq$ 2) suggested that the concentration level of the indicators at those monitoring sites had high (LE030, LE200, and LE410) [that means there were unexplained errors exist in the model estimates and/or in the predicted results due to the high pressures of anthropogenic activities in the upper part of the Harbour] and these indicators had a substantial impact on the WQM-WQI model for the evaluation of coastal water quality (Fig. 6.13i). In general, the figure 6.13(i) demonstrates that most of the sites with ASRE less than two, the model produces statistically reliable results in those sites except for the LE030, LE200, and LE410.

For the assessment of the reliability of the RF technique, this study also utilized the Z-statistics using Wishker boxplot analysis according to Uddin et al., (2022a). Figure 6.14 shows the details of Z-statistics for water quality indicators in Cork harbour. For all water quality indicators of subset S4 (Figure 6.14), Z-statistics were found to be between -0.75 and 0.50. As shown in figure 6.14, most water quality indicators are normally distributed, except for AMN, BOD5, CHL and TEMP over the study period. It is noted that all water quality indicators of subset S4 had significant outliers, except for the water pH. The results of Z-statistics indicate that most identical water quality indicators have been suggested by the subset of S4 excluding pH, whereas those indicators had a significant impact on water quality in Cork Harbour. . The Z-statistics of boxplot results also revealed that the AMN and CHL had a substantial impact on water quality, but the RF technique did not suggest this indicator as the crucial one for this research.

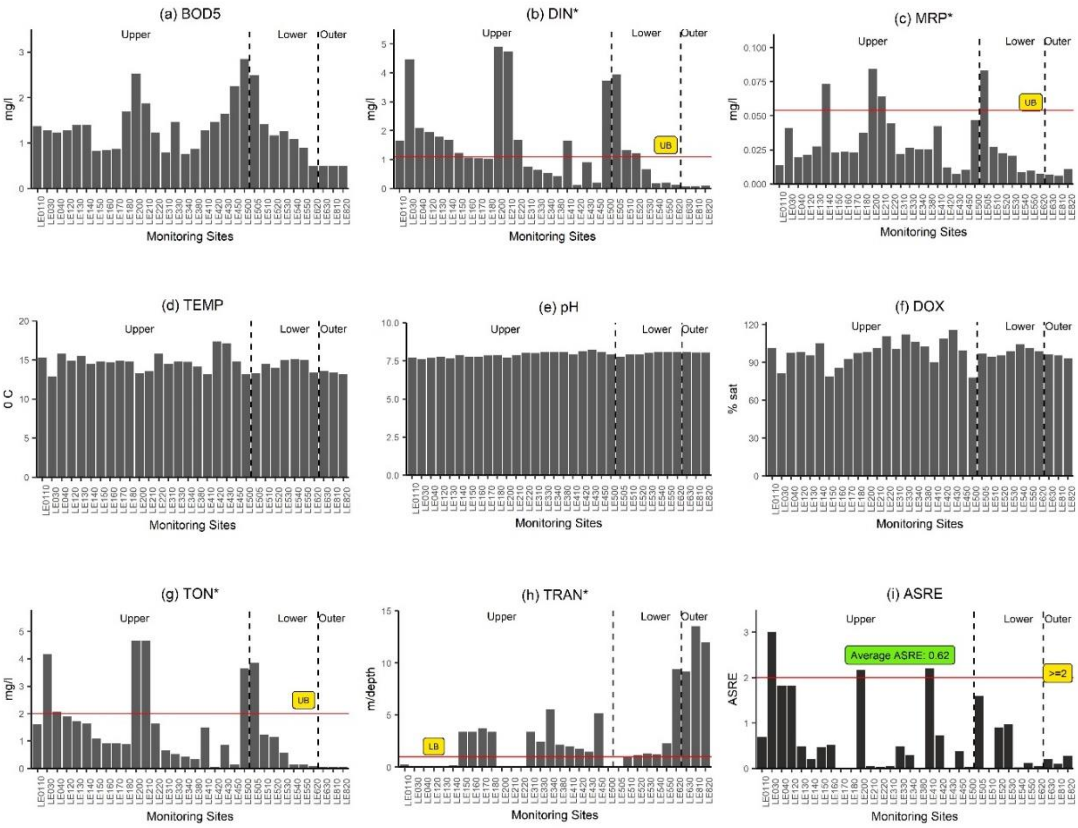


Figure 6.13.Validating WQM-WQI model results for subsets of S4 indicators using absolute standardized residual estimate (ASRE) analysis (whereas, LB = lower bound and UB = upper bound of permissible limit).

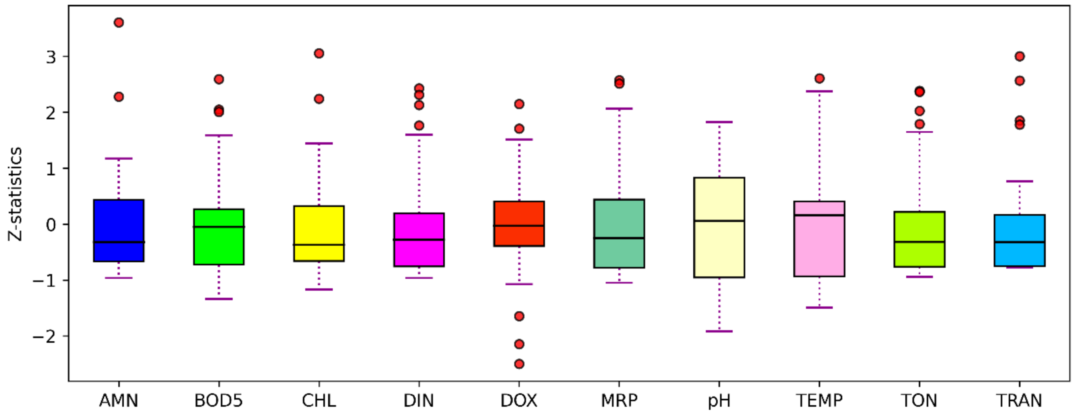


Figure 6.14. Z-statistics for robust subset (S4) of water quality indicators.

6.10 Assessment of water quality in Cork harbour

The ultimate goal of the WQI model is to assess water quality using a certain classification scheme. The present study utilized the classification scheme of Uddin et al., (2022a). Details of the classification scheme are provided in Table 6.S10. A comparative assessment of water quality using various combinations of water quality indicators is presented in Figure 6.15. Details of the assessment for each monitoring site's water quality status can be found in Table 6.S11. Most subsets of WQIs results have reported that water quality had three classes as "good", "fair", and "marginal" over the study period, except the subset of S1 (Figure 6.15). According to the monitoring sites assessment results, good (31.2%), fair (65.6%), and marginal (3.2%) classes water quality was found in Cork Harbour for the robust combination of indicators (subset S4) (Figure 16.5).

For the determination of the spatial distribution of water quality in Cork Harbour, water quality maps were produced using WQI values for the robust subset (S4) indicators. Spatial distribution maps were generated using the empirical Bayesian kriging approach by utilizing advanced ArcGIS pro 2.8.7 because, recently, several studies have revealed that this technique is effective for geospatial interpolation of water quality (Uddin et al., 2018; 2021; 2022b). Figure 6.16 shows the spatial distribution of WQI values (Figure 6.16a) and monitoring sites water quality status (Fig. 6.16b) in Cork Harbour. As shown in Figure 6.16a, higher WQI values were calculated for the lower and outer Harbour whereas relatively the lowest WQI values were found in upper part of the Harbour. The interpolated results revealed that there was a significant spatial variation of WQI values across the Cork Harbour.

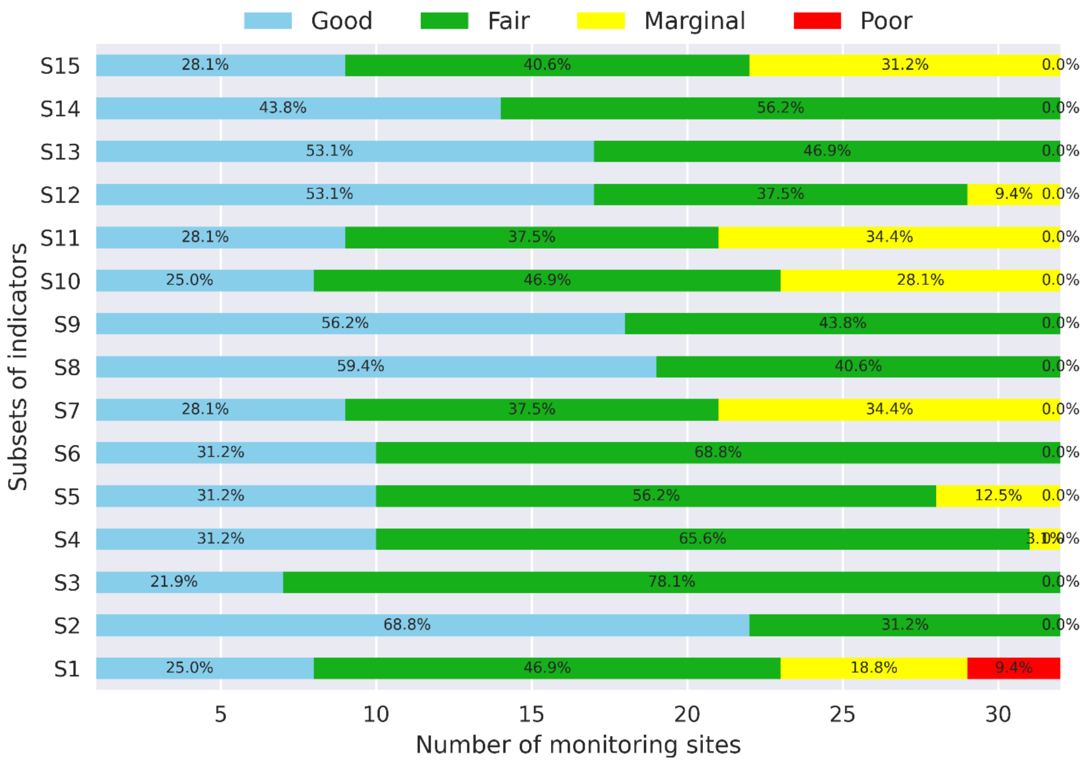


Figure 6.15. Assessment of monitoring sites water quality in Cork Harbour using different subsets of indicators.

Figure 6.16b shows qualitative assessment of monitoring sites water quality in Cork Harbour for the subset S4 indicators. The majority of the monitoring sites' water was of "good" quality. In contrast, water quality declined at monitoring sites in the upper part of the Harbour over this study period. Most monitoring sites in the lower and outer Harbour were associated with good water quality. In the river Owenacurra, a monitoring site found marginal water quality (Fig. 6.16b).

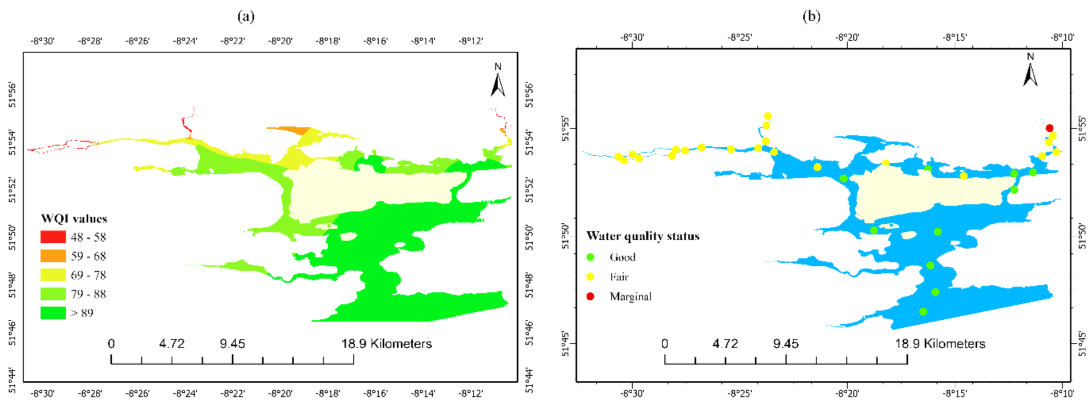


Figure 6.16. Assessment of water quality in Cork Harbour: (a) WQIs values for subset S4; and (b) monitoring sites water quality status.

The findings showed that the upper Harbour's relatively poor water quality was a result of higher anthropogenic pressures like industrial effluents, domestic waste, and agricultural activities (farming, fishing, etc.) (Hartnett and Nash, 2015; Uddin et al., 2022a; 2022d). The findings of the evaluation of the monitoring sites are consistent with the author's earlier research (Uddin et al., 2022a; 2022b, 2022d; 2020a; 2020b).

6.11 Conclusion

The present study was carried out to identify the most robust algorithm for selecting the best combination of water quality indicators to incorporate into a WQI model for evaluating coastal water quality. In total, nineteen FS algorithms were compared in order to calculate the WQI score in terms of reducing model uncertainty by optimizing crucial water quality indicators for assessing coastal water quality. The following conclusions were derived from the findings of this study as follows:

- The results of various FS techniques indicate that the embedded based tree algorithms (RF, and ExT) and filter based MI techniques are better than the commonly used filter methods (like as PCA, PCOR, etc.) for selecting the crucial water quality indicators.
- For predicting coastal water quality appropriately, the DNN algorithm outperformed compared other eight ML techniques.
- The prediction results revealed that the model performance was significantly improved for the subsets of S4 (RF), S5 (MI/ExT), and S9 (RFE_RF).
- In terms of reducing the WQM-WQI model uncertainty, Z-statistics also revealed that the tree-based RF technique might be reliable for selecting crucial water quality indicators that provided the actual water quality information to the final assessment.
- The findings of this research suggested that the water quality indicators of subset S4 (BOD5, DIN, MRP, TEMP, pH, DOX, TON, and TRAN) could be effective for the improvement of the WQM-WQI model performance in order to assess coastal water quality.

Moreover, the present study provides a comprehensive assessment of various FS algorithms in order to select important water quality indicators. This study also helps to improve the WQI model performance, which could be an effective way to reduce model uncertainty in terms of coastal water quality assessment. Further studies should be carried out to analyse the spatiotemporal sensitivity of RF algorithms for selecting crucial water quality indicators. However, the result of this study provides important information to scholars, decision-makers, and water managers for the development of the WQI model and the adoption of a suitable indicator selection method.

6.12 Declaration of competing interest

The authors state that they have no known competing financial interests or personal relationships that the work reported in this paper could have seemed to influence.

6.13 Acknowledgement

The authors gratefully acknowledge the editor's and anonymous reviewers' contributions to the improvement of this paper. This research was funded by the Hardiman Research Scholarship of the University of Galway, which funded the first author as part of his PhD program. The authors would like to acknowledge support from MaREI, the SFI Research Centre for Energy, Climate, and Marine research. The authors would like to thank the Environmental Protection Agency of Ireland for providing water quality data. The authors also sincerely acknowledge Charles Sturt University for providing all necessary supports to this PhD project through the international co-supervision. Moreover, the authors also sincerely acknowledge the Eco HydroInformatics Research Group (EHIRG), School of Engineering, College of Science and Engineering, University of Galway, Ireland for providing computational laboratory facilities to complete this research.

6.14 References

Abbasi, T., Abbasi, S.A., 2012. Water-Quality Indices, in: Water Quality Indices. Elsevier, pp. 353–356. https://doi.org/10.1016/B978-0-444-54304-2.00016-6

Ahmed, U., Mumtaz, R., Anwar, H., Shah, A.A., Irfan, R., 2019. E ffi cient Water Quality Prediction Using Supervised 1–14.

Akaike, H., 1998. Information Theory and an Extension of the Maximum Likelihood Principle 199–213. https://doi.org/10.1007/978-1-4612-1694-0_15

Andrade, C., 2021. Z Scores, Standard Scores, and Composite Test Scores Explained. Indian J. Psychol. Med. 43, 555–557. https://doi.org/10.1177/02537176211046525

Asadollah, S.B.H.S., Sharafati, A., Motta, D., Yaseen, Z.M., 2021. River water quality index prediction and uncertainty analysis: A comparative study of machine learning models. J. Environ. Chem. Eng. 9, 104599. https://doi.org/10.1016/j.jece.2020.104599

Aslam, M., 2022. Design of a new Z-test for the uncertainty of Covid-19 events under Neutrosophic statistics. BMC Med. Res. Methodol. 22, 4–9. https://doi.org/10.1186/s12874-022-01593-x

Bagherzadeh, F., Mehrani, M.-J., Basirifard, M., Roostaei, J., 2021. Comparative study on total nitrogen prediction in wastewater treatment plant and effect of various feature selection methods on machine learning algorithms performance. J. Water Process Eng. 41, 102033. https://doi.org/10.1016/j.jwpe.2021.102033

Bailly, A., Blanc, C., Francis, É., Guillotin, T., Jamal, F., Wakim, B., Roy, P., 2022. Effects of dataset

size and interactions on the prediction performance of logistic regression and deep learning models. Comput. Methods Programs Biomed. 213, 106504.
Banks, H.T., Joyner, M.L., 2017. AIC under the framework of least squares estimation. Appl Math Lett 74, 33–45. https://doi.org/10.1016/j.aml.2017.05.005
https://doi.org/10.1016/j.cmpb.2021.106504
Best, N., Richardson, S., Clarke, P., 2008. A Comparison of model-based methods for Small Area Estimation. ESRC Natl. Cent. Res. Methods 1–26.
Bui, D.T., Khosravi, K., Tiefenbacher, J., Nguyen, H., Kazakis, N., 2020. Improving prediction of water quality indices using novel hybrid machine-learning algorithms. Sci. Total Environ. 721, 137612. https://doi.org/10.1016/j.scitotenv.2020.137612
Cateni, S., Colla, V., Vannucci, M., 2014. A hybrid feature selection method for classification purposes. Proc. - UKSim-AMSS 8th Eur. Model. Symp. Comput. Model. Simulation, EMS 2014 39–44. https://doi.org/10.1109/EMS.2014.44
Chakravarty, T., Gupta, S., 2021. Assessment of water quality of a hilly river of south Assam, north east India using water quality index and multivariate statistical analysis. Environ. Challenges 5, 100392. https://doi.org/10.1016/J.ENVC.2021.100392
Chen, K., Chen, H., Zhou, C., Huang, Y., Qi, X., Shen, R., Liu, F., Zuo, M., Zou, X., Wang, J., Zhang, Y., Chen, D., Chen, X., Deng, Y., Ren, H., 2020. Comparative analysis of surface water quality prediction performance and identification of key water parameters using different machine learning models based on big data. Water Res. 171, 115454. https://doi.org/10.1016/j.watres.2019.115454
Chen Liao, Shutao Li, Zhiyuan Luo, 2008. Computational Intelligence and Security, Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics). Spinger, Guangzhou, China.
Chen, R.C., Dewi, C., Huang, S.W., Caraka, R.E., 2020. Selecting critical features for data classification based on machine learning methods. J. Big Data 7. https://doi.org/10.1186/s40537-020-00327-4
Chen, S., Ren, Y., Friedrich, D., Yu, Z., Yu, J., 2020. Sensitivity analysis to reduce duplicated features in ANN training for district heat demand prediction. Energy AI 2, 100028. https://doi.org/10.1016/j.egyai.2020.100028
Choudhary, K., DeCost, B., Chen, C., Jain, A., Tavazza, F., Cohn, R., Park, C.W., Choudhary, A., Agrawal, A., Billinge, S.J.L., Holm, E., Ong, S.P., Wolverton, C., 2022. Recent advances and applications of deep learning methods in materials science. NPJ Comput Mater. https://doi.org/10.1038/s41524-022-00734-6Das, A.K., Das, S., Ghosh, A., 2017. Ensemble feature selection using bi-objective genetic algorithm. Knowledge-Based Syst. 123, 116–127. https://doi.org/10.1016/j.knosys.2017.02.013
Elgeldawi, E., Sayed, A., Galal, A.R., Zaki, A.M., 2021. Hyperparameter tuning for machine learning algorithms used for arabic sentiment analysis. Informatics 8, 1–21. https://doi.org/10.3390/informatics8040079
Emmert-Streib, F., Dehmer, M., 2019. Evaluation of Regression Models: Model Assessment, Model Selection and Generalization Error. Mach. Learn. Knowl. Extr. 1, 521–551. https://doi.org/10.3390/make1010032
Fadel, A., Kanj, M., Slim, K., 2021. Water Quality Index variations in a Mediterranean reservoir: a multivariate statistical analysis relating it to different variables over 8 years. Environ. Earth Sci. 80, 1–13. https://doi.org/10.1007/s12665-020-09364-x
Gao, L., Wu, W., 2020a. Knowledge-Based Systems Relevance assignation feature selection method based on mutual information for machine learning. Knowledge-Based Syst. 209, 106439. https://doi.org/10.1016/j.knosys.2020.106439
Gao, L., Wu, W., 2020b. Relevance assignation feature selection method based on mutual information for machine learning. Knowledge-Based Syst. 209, 106439. https://doi.org/10.1016/J.KNOSYS.2020.106439
Gaur, N., Sarkar, A., Dutta, D., Gogoi, B.J., Dubey, R., Dwivedi, S.K., 2022. Evaluation of water quality index and geochemical characteristics of surfacewater from Tawang India. Sci. Rep. https://doi.org/10.1038/s41598-022-14760-3
Gupta, S., Gupta, S.K., 2021. A critical review on water quality index tool: Genesis, evolution and future directions. Ecol. Inform. 63, 101299. https://doi.org/10.1016/j.ecoinf.2021.101299
Hamby, D.M., 1994. a Review of Techniques for Parameter Sensitivity. Environ. Monit. Assess. 32, 135–154.
Hartnett, M., Nash, S., 2015. An integrated measurement and modeling methodology for estuarine water quality management. Water Sci. Eng. 8, 9–19. https://doi.org/10.1016/j.wse.2014.10.001
Hassan, Md. Mehedi, Hassan, Md. Mahedi, Akter, L., Rahman, M.M., Zaman, S., Hasib, K.M., Jahan,

N., Smrity, R.N., Farhana, J., Raihan, M., Mollick, S., 2021. Efficient Prediction of Water Quality Index (WQI) Using Machine Learning Algorithms. Human-Centric Intell. Syst. 1, 86. https://doi.org/10.2991/hcis.k.211203.001

Horton, R.K., 1965. An Index Number System for Rating Water Quality. J. Water Pollut. Control Fed.

Hou, W., Sun, S., Wang, M., Li, X., Zhang, N., Xin, X., Sun, L., Li, W., Jia, R., 2016. Assessing water quality of five typical reservoirs in lower reaches of Yellow River, China: Using a water quality index method. Ecol. Indic. 61. https://doi.org/10.1016/j.ecolind.2015.09.030

Islam Khan, M.S., Islam, N., Uddin, J., Islam, S., Nasir, M.K., 2021. Water quality prediction and classification based on principal component regression and gradient boosting classifier approach. J. King Saud Univ. - Comput. Inf. Sci. https://doi.org/10.1016/j.jksuci.2021.06.003

Jiang, L., Li, Y., Zhao, X., Tillotson, M.R., Wang, W., Zhang, S., Sarpong, L., Asmaa, Q., Pan, B., 2018. Parameter uncertainty and sensitivity analysis of water quality model in Lake Taihu, China. Ecol. Modell. https://doi.org/10.1016/j.ecolmodel.2018.02.014

Juwana, I., Muttil, N., Perera, B.J.C., 2016a. Uncertainty and sensitivity analysis of West Java Water Sustainability Index - A case study on Citarum catchment in Indonesia. Ecol. Indic. 61, 170–178. https://doi.org/10.1016/j.ecolind.2015.08.034

Juwana, I., Muttil, N., Perera, B.J.C., 2016b. Application of west Java water sustainability index to three water catchments in west Java, Indonesia. Ecol. Indic. 70, 401–408. https://doi.org/10.1016/j.ecolind.2016.06.017

Khan, Y., See, C.S., 2016. Predicting and analyzing water quality using Machine Learning: A comprehensive model. 2016 IEEE Long Isl. Syst. Appl. Technol. Conf. LISAT 2016. https://doi.org/10.1109/LISAT.2016.7494106

Kotsiantis, S.B., 2011. Feature selection for machine learning classification problems : a recent overview. https://doi.org/10.1007/s10462-011-9230-1

Kumar, B., Singh, U.K., Ojha, S.N., 2019. Evaluation of geochemical data of Yamuna River using WQI and multivariate statistical analyses: a case study. Int. J. River Basin Manag. 17, 143–155. https://doi.org/10.1080/15715124.2018.1437743

Leong, W.C., Bahadori, A., Zhang, J., Ahmad, Z., 2021. Prediction of water quality index (WQI) using support vector machine (SVM) and least square-support vector machine (LS-SVM). Int. J. River Basin Manag. 19, 149–156. https://doi.org/10.1080/15715124.2019.1628030

Ma, X., Wang, L., Yang, H., Li, N., Gong, C., 2020. Spatiotemporal analysis of water quality using multivariate statistical techniques and the water quality identification index for the qinhuai river basin, east china. Water (Switzerland) 12. https://doi.org/10.3390/w12102764

Ma, Z., Li, H., Ye, Z., Wen, J., Hu, Y., Liu, Y., 2020. Application of modified water quality index (WQI) in the assessment of coastal water quality in main aquaculture areas of Dalian, China. Mar. Pollut. Bull. 157. https://doi.org/10.1016/j.marpolbul.2020.111285

Massey, A., Miller, S.J., 2017. Tests of Hypotheses Using Statistics. Math. Dep. Brown Univ. Provid. RI 2912 1–32.

Mauget, S., 2011. Time series analysis based on running Mann-Whitney Z Statistics. J. Time Ser. Anal. 32, 47–53. https://doi.org/10.1111/j.1467-9892.2010.00683.x

Mauget, S.A., Cordero, E.C., Brown, P.T., 2012. Evaluating modeled intra- to multidecadal climate variability using running mann-whitney Z statistics. J. Clim. 25, 1570–1586. https://doi.org/10.1175/JCLI-D-11-00211.1

McCuen, R.H., Knight, Z., Cutter, A.G., 2006. Evaluation of the Nash–Sutcliffe Efficiency Index. J. Hydrol. Eng. 11, 597–602. https://doi.org/10.1061/(asce)1084-0699(2006)11:6(597)

McManus, S., Rahman, A., Horta, A., Coombes, J., 2020. Applied Bayesian Modeling for Assessment of Interpretation Uncertainty in Spatial Domains. Stat. Data Sci. Policy Anal. 3–13. https://doi.org/10.1007/978-981-15-1735-8_1

Medeiros, A.C., Faial, K.R.F., do Carmo Freitas Faial, K., da Silva Lopes, I.D., de Oliveira Lima, M., Guimarães, R.M., Mendonça, N.M., 2017. Quality Index of the surface water of Amazonian rivers in industrial areas in Pará Brazil. Mar. Pollut. Bull. 123, 156–164. https://doi.org/10.1016/j.marpolbul.2017.09.002

Michalak, K., Kwasnicka, H., 2006. Correlation-based feature selection strategy in neural classification. Proc. - ISDA 2006 Sixth Int. Conf. Intell. Syst. Des. Appl. 1, 741–746. https://doi.org/10.1109/ISDA.2006.128

Naghibi, S.A., Hashemi, H., Berndtsson, R., Lee, S., 2020. Application of extreme gradient boosting and parallel random forest algorithms for assessing groundwater spring potential using DEM-derived factors. J. Hydrol. 589, 125197. https://doi.org/10.1016/j.jhydrol.2020.125197

Othman, F., Alaaeldin, M.E., Seyam, M., Ahmed, A.N., Teo, F.Y., Ming Fai, C., Afan, H.A., Sherif, M., Sefelnasr, A., El-Shafie, A., 2020. Efficient river water quality index prediction considering

minimal number of inputs variables. Eng. Appl. Comput. Fluid Mech. 14, 751–763. https://doi.org/10.1080/19942060.2020.1760942
Pan, B., Han, X., Chen, Y., Wang, L., Zheng, X., 2022. Determination of key parameters in water quality monitoring of the most sediment-laden Yellow River based on water quality index. Process Saf. Environ. Prot. 164, 249–259. https://doi.org/10.1016/J.PSEP.2022.05.067
Parween, S., Siddique, N.A., Mahammad Diganta, M.T., Olbert, A.I., Uddin, Md.G., 2022. Assessment of urban river water quality using modified NSF water quality index model at Siliguri city, West Bengal, India. Environmental and Sustainability Indicators 16, 100202. https://doi.org/10.1016/j.indic.2022.100202
Pasini, A., 2015. Artificial neural networks for small dataset analysis. J. Thorac. Dis. 7, 953–960. https://doi.org/10.3978/j.issn.2072-1439.2015.04.61
Rahman, A., Harding, A., 2016. Validation and Measure of Statistical Reliability. Small Area Estim. Microsimulation Model. 221–248. https://doi.org/10.1201/9781315372143-10
Rahman, A., Harding, A., Tanton, R., Liu, S., 2013. Simulating the characteristics of populations at the small area level: New validation techniques for a spatial microsimulation model in Australia. Comput. Stat. Data Anal. 57, 149–165. https://doi.org/10.1016/J.CSDA.2012.06.018
Saeys, Y., Inza, I., Larrañaga, P., 2007. A review of feature selection techniques in bioinformatics. Bioinformatics 23, 2507–2517. https://doi.org/10.1093/bioinformatics/btm344
Sarker, I. H., 2021. Deep Learning: A Comprehensive Overview on Techniques, Taxonomy, Applications and Research Directions. In SN Computer Science (Vol. 2, Issue 6). Springer. https://doi.org/10.1007/s42979-021-00815-1
Savitsky, T., Vannucci, M., Sha, N., 2011. Variable selection for nonparametric Gaussian process priors: Models and computational strategies. Stat. Sci. 26, 130–149. https://doi.org/10.1214/11-STS354
Shalizi, C., 2015. Lecture 21 : Model Selection 1–21.
Sharif, O., Hasan, M.Z., Rahman, A., 2022. Determining an effective short term COVID-19 prediction model in ASEAN countries. Sci. Rep. 12, 1–11. https://doi.org/10.1038/s41598-022-08486-5
Stone, M., 1979. Comments on Model Selection Criteria of Akaike and Schwarz. J. R. Stat. Soc. Ser. B 41, 276–278. https://doi.org/10.1111/J.2517-6161.1979.TB01084.X
Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2017a. Development of a water quality index for rivers in West Java Province, Indonesia. Ecol. Indic. 85, 966–982. https://doi.org/https://doi.org/10.1016/j.ecolind.2017.11.049
Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2017b. Using the Analytic Hierarchy Process to identify parameter weights for developing a water quality index. Ecol. Indic. 75, 220–233. https://doi.org/10.1016/j.ecolind.2016.12.043
Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2016. Development of river water quality indices—a review. Environ. Monit. Assess. https://doi.org/10.1007/s10661-015-5050-0
Taha, A., Cosgrave, B., Mckeever, S., 2022. Using Feature Selection with Machine Learning for Generation of Insurance Insights.
Tran, D.A., Tsujimura, M., Ha, N.T., Nguyen, V.T., Binh, D. Van, Dang, T.D., Doan, Q. Van, Bui, D.T., Anh Ngoc, T., Phu, L.V., Thuc, P.T.B., Pham, T.D., 2021. Evaluating the predictive power of different machine learning algorithms for groundwater salinity prediction of multi-layer coastal aquifers in the Mekong Delta, Vietnam. Ecol. Indic. 127, 107790. https://doi.org/10.1016/j.ecolind.2021.107790
Tripathi, M., Singal, S.K., 2019. Use of Principal Component Analysis for parameter selection for development of a novel Water Quality Index: A case study of river Ganga India. Ecol. Indic. 96, 430–436. https://doi.org/10.1016/j.ecolind.2018.09.025
Uddin, M.G., Moniruzzaman, M., Khan, M., 2017. Evaluation of Groundwater Quality Using CCME Water Quality Index in the Rooppur Nuclear Power Plant Area, Ishwardi, Pabna, Bangladesh. Am. J. Environ. Prot. https://doi.org/10.12691/env-5-2-2
Uddin, M.G., Moniruzzaman, M., Quader, M.A., Hasan, M.A., 2018. Spatial variability in the distribution of trace metals in groundwater around the Rooppur nuclear power plant in Ishwardi, Bangladesh. Groundw. Sustain. Dev. 7. https://doi.org/10.1016/j.gsd.2018.06.002
Uddin, M.G., Olbert, A.I., Nash, S., 2020a. Assessment of water quality using Water Quality Index (WQI) models and advanced geostatistical technique, in: Civil Engineering Research Association of Ireland (CERAI). pp. 594–599.
Uddin, M.G., Stephen Nash, Olbert, A.I., 2020b. Application of Water Quality Index Models to an Irish Estuary, in: Civil and Environmental Research. pp. 576–581.
Uddin, G., Nash, S., Olbert, A.I., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol. Indic. 122, 107218.

https://doi.org/10.1016/j.ecolind.2020.107218
Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022a. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment. Water Res. 219, 118532. https://doi.org/10.1016/j.watres.2022.118532
Uddin, M.G., Nash, S., Diganta, M.T.M., Rahman, A., Olbert, A.I., 2022b. A comparison of geocomputational models for validating geospatial distribution of water quality index, in: Priyanka, H., Rahman, A., Basant agarwal, Binita Tiwari (Eds.), Computational Statistical Methodologies and Modeling for Artificial Intelligence. CRC Press, Taylor & Francis Publisher, USA.
Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022c. A novel approach for estimating and predicting uncertainty in water quality index model using machine learning approaches. Manuscript submitted for publication.
Uddin, M.G., Nash, S., Talas, M., Diganta, M., Rahman, A., Olbert, A.I., 2022d. Robust machine learning algorithms for predicting coastal water quality index. J. Environ. Manage. https://doi.org/https://doi.org/10.1016/j.jenvman.2022.115923
Urbanowicz, R.J., Meeker, M., Cava, W. La, Olson, R.S., Moore, J.H., 2018. Relief-based feature selection : Introduction and review. J. Biomed. Inform. 85, 189–203. https://doi.org/10.1016/j.jbi.2018.07.014
Uzair, M., Jamil, N., 2020. Effects of Hidden Layers on the Efficiency of Neural networks, in: Proceedings - 2020 23rd IEEE International Multi-Topic Conference, INMIC 2020. Institute of Electrical and Electronics Engineers Inc. https://doi.org/10.1109/INMIC50486.2020.9318195Villalobos-Arias, L., Quesada-López, C., Guevara-Coto, J., Martínez, A., Jenkins, M., 2020. Evaluating hyper-parameter tuning using random search in support vector machines for software effort estimation. PROMISE 2020 - Proc. 16th ACM Int. Conf. Predict. Model. Data Anal. Softw. Eng. Co-located with ESEC/FSE 2020 31–40. https://doi.org/10.1145/3416508.3417121
Xiong, Z., Cui, Y., Liu, Z., Zhao, Y., Hu, M., Hu, J., 2020. Evaluating explorative prediction power of machine learning algorithms for materials discovery using k-fold forward cross-validation. Comput. Mater. Sci. 171, 109203. https://doi.org/10.1016/j.commatsci.2019.109203
Yan, J., Jia, S., Lv, A., Zhu, W., 2019. Water Resources Assessment of China’s Transboundary River Basins Using a Machine Learning Approach. Water Resour. Res. 55, 632–655. https://doi.org/10.1029/2018WR023044
Yu, X., Shen, J., Du, J., 2020. A Machine-Learning-Based Model for Water Quality in Coastal Waters, Taking Dissolved Oxygen and Hypoxia in Chesapeake Bay as an Example. Water Resour. Res. 56, 1–19. https://doi.org/10.1029/2020WR027227
Zaghloul, M.S., Achari, G., 2022. Application of machine learning techniques to model a full-scale wastewater treatment plant with biological nutrient removal. J. Environ. Chem. Eng. 10, 107430. https://doi.org/10.1016/j.jece.2022.107430
Zeinalzadeh, K., Rezaei, E., 2017. Determining spatial and temporal changes of surface water quality using principal component analysis. J. Hydrol. Reg. Stud. 13, 1–10. https://doi.org/10.1016/j.ejrh.2017.07.002

7. A sophisticated model for rating water quality

This chapter was published in the Journal of **“Science of The Total Environment”** on January 18, 2023. Details can be found at the following web resource:

https://doi.org/10.1016/j.scitotenv.2023.161614

7.1 Chapter highlights

- An improved WQI model was developed that could be referred to as the **"Irish Water Quality Index Model,"** also abbreviated as **"IEWQI".**

- The proposed IEWQI model have composed five components, including -

  (1) For the optimization of model input, the random forest algorithm has been recommended for the IEWQI.
  (2) Three newly developed linear interpolation rescaling functions have been proposed for computing sub-index of the IEWQI these are effective to avoid the eclipsing problem.
  (3) In order to estimate the accurate weight values of indicators, a comprehensive approach combining the random forest technique incorporating with mathematical function of rank sum technique proposed for the IEWQI.
  (4) To compute the WQI scores more accurately, a completely new weighted quadratic mean (WQM) function has been introduced as the "aggregation function" of IEWQI that could be effective for reducing model ambiguity problem.
  (5) A brand new classification scheme including four identical water classes like “good”, “fair”, “marginal”, and “poor” has been suggested for assessing coastal water quality using IEWQI.
- Developed model was tested across four Irish waterbodies successfully for assessing coastal waters.
- Model validated using the EPA’s water quality monitoring data.
- Model sensitivity analysis using various set of water quality indicators in terms of spatial resolution.

- Based on results, the IEWQ model is a reliable method for determining the accuracy, reliability, and affordability of transitional and coastal water quality.
- Model could be efficient for optimizing model eclipsing and ambiguity problems in order to reduce model uncertainty
- Uncertainty results indicate that the model that computed WQI scores is more reliable because it produces only less than 2% uncertainty in the final assessment across four domains.
- Overall, the model performance was evaluated using a range of statistical measures like NSE, MEF etc. and ML approaches.
- Based on the findings, the performance of IEWQI applications reveals that suggested indicators might be adequate and reliable to monitor water across Irish waterbodies.

7.2 Abstract

Here, we present the Irish Water Quality Index (IEWQI) model for assessing transitional and coastal water quality in an effort to improve the method and develop a tool that can be used by environmental regulators to abate water pollution in Ireland. The developed model has been associated with the adoption of water quality standards formulated for coastal and transitional waterbodies according to the water framework directive legislation by the environmental regulator of Irish water. The model consists of five identical components, including (i) indicator selection technique is to select the crucial water quality indicator; (ii) sub-index (SI) function for rescaling various water quality indicators' information into a uniform scale; (iii) indicators' weight method for estimating the weight values based on the relative significance of real-time information on water quality; (iii) aggregation function for computing the water quality index (WQI) score; and (v) score interpretation scheme for assessing the state of water quality. The IEWQI model was developed based on Cork Harbour, Ireland. The developed IEWQI model was applied to four coastal waterbodies in Ireland, for assessing water quality using 2021 water quality data for the summer and winter seasons in order to evaluate model sensitivity in terms of spatio-temporal resolution of various waterbodies. The model efficiency and uncertainty were also analysed in this research. In terms of different spatio-temporal magnitudes of various domains, the model shows higher sensitivity in four application domains during the summer and

winter. In addition, the results of uncertainty reveal that the IEWQI model architecture may be effective for reducing model uncertainty in order to avoid model eclipsing and ambiguity problems. The findings of this study reveal that the IEWQI model could be an efficient and reliable technique for the assessment of transitional and coastal water quality more accurately in any geospatial domain.

Keyword: water quality model, sensitivity, model efficiency, uncertainty, assessment of water quality

7.3 Introduction

Water is an essential component of the environment, but environmental sustainability is dependent on "good" water quality. Surface water is one crucial resource for the management of aquatic ecosystems and their components (Parween et al., 2022; Uddin et al., 2017; 2018; 2021; 2022a). Unfortunately, gradually, the surface water quality has been degraded due to the association of various natural, like hydrological, climatic, topographical, lithological, etc., and anthropogenic events such as agricultural activities, mining, production and disposal of waste from various sources like industries, municipal activities, domestic waste, medical waste, etc. (Uddin et al., 2021; 2020a). In that case, it is very hard to keep all bodies of water in "good" water quality (Uddin et al., 2022a).

For the purpose of maintaining a "good" state of water quality in all states, a number of tools and techniques have been developed by various countries/organizations/agencies. For example, the water framework directive was formulated in 2000 to keep "good" water quality within the extent of the European countries (Zotou et al., 2018). The water framework directive is one kind of policy that guides a set of rules and regulations on how to obtain the goals of the framework. But, the framework does not refer to any specific tools or techniques for achieving "good" water quality (Carsten Von Der Ohe et al., 2007; Uddin et al., 2022a). Consequently, the EU countries have been striving for the optimization of a technique in order to assess water quality more accurately which technique could be adopted by all EU countries as a "universal" technique (Carsten Von Der Ohe et al., 2007). In terms of global aspects, similar problems have been experienced in the rest of the world. They have been trying to explore the best solution for achieving a "good" state of water quality in all waterbodies (Carsten Von Der Ohe et al., 2007; Uddin et al., 2022a; Zotou et al., 2018).

Currently, most of the countries widely used very typical monitoring approach for assessing water quality due to a few constraints of this technique. It has received much more criticisms for its technical aspects and data accuracy (Strobl and Robillard, 2008). Recently, several studies have reported that the traditional monitoring program is not affordable for both developing and developed countries due to it is required a few basics requirements, like the need for highly equipped and advanced laboratory facilities, skilled manpower, sufficient funding, etc. (Sutadian et al., 2017; Uddin et al., 2022a). Moreover, this technique is a very expensive and time-consuming approach (Jiang et al., 2020; Strobl and Robillard, 2008).

Consequently, to date, different hydrological models have been utilized for assessing surface water quality (lake, river, transitional, coastal, etc.). The water quality index (WQI) model is one of them. Horton first introduced it in 1960 for assessing the river water quality (Uddin et. al., 2021, Horton, 1965). The WQI method is a point-based rapid assessment technique that converts a series of water quality data into a single numerical expression. Since then, this technique has become a widely used technique for assessing water quality (surface, groundwater etc.) by following a few common frameworks. To date, several WQI models have been developed by various organizations/countries/researchers for assessing water quality, specially they are focused on specific domains or waterbodies like lakes, rivers, groundwater, mine water, wastewater etc. To the best of the author's knowledge, there are no existing WQI models focused on coastal water quality, but a few studies have utilized the common WQI models like the NSF index (Gupta et al. 2003, Jha et al. 2015), the CCME Index (de Rosemond et al. 2009); and modified NSF WQI (Ma et al. 2020) for assessing coastal water quality. In earlier studies and a literature review, the authors discussed the details of various WQI models' histories, architectures, components, and applications in order to develop a WQI model focused on coastal water quality. Details of the study can be found in Uddin et al., (2021).

Based on the model architecture, it typically consists of five identical components, including (i) **the indicators selection process** used to select the crucial water quality indicators in terms of their relative significance; (ii) **sub-index functions** that allow to transfer various water quality data into the unit less form without hiding any real information about indicators; (iii) **weight generation technique** mainly used for assigning the importance of indicators based on their influential capabilities of water quality; (iv) **the aggregation function** that is provided to convert sub-index and weighting values into the single numerical number that is called "WQI score", and (v) **the classification scheme** is used to interpret the WQI score in order to classify the water quality as "good", "fair", "marginal" etc. The existing WQI models have received much more criticism with regard to their reliability and accuracy. Recently, several studies have revealed that the entire models have contributed a significant amount of uncertainty to the final assessment of water quality. A number of studies have reported that each component of the model produces its own uncertainty (Uddin et al., 2021; 2022c; 2022d; 2022e).

Recently, the WQI model has received much more criticism due to the model's reliability, validity, and inconsistency of the results. Several studies have revealed that the WQI model has produced a significant amount of uncertainty from the various components of this model (Uddin et al., 2022a; 2022b). Many researchers have argued that a considerable amount of uncertainty is contributed to the WQI model by the indicators' selection process, sub-index functions, and using inappropriate aggregation functions (Sutadian et al., 2017; Uddin et al., 2021; 2022a; 2022c). Moreover, a few studies have revealed that the weighting technique also provided a considerable uncertainty to the final assessment. Considering all the findings in the literature, in recent years, the authors have carried out several studies in terms of investigating the appropriate technique for selecting crucial indicators, sub-index functions, weighting techniques, aggregation functions, classification schemes, sources of uncertainty or inappropriateness of the model outcomes in order to develop an improved model for assessing transitional and coastal waters by the following studies:

(i) Model development history, nature, architecture, applications, using tools and techniques, sources of uncertainties, ambiguity, the eclipsing problem, classification schemes, etc. has been published in Uddin et al., (2021).

(ii) Analysed the sensitivity of various established WQI models for assessing coastal water quality in terms of geospatial regulation in Uddin et al., (2020a).

(iii) Analysed various existing models performance for assessing coastal water quality in Uddin at al., (2020b).

(iv) Based on the existing problems, the authors proposed an improved methodology for developing a water quality index model with completely new sub-index functions, a new approach for estimating weight values, a new aggregation function, and a new classification scheme for coastal water in Uddin et al., (2022a).

(v) Optimization algorithm(s) for predicting the weighted quadratic mean (WQM) -WQI architecture in order to reduce model uncertainty in Uddin et al., (2022b).

(vi) In terms of model uncertainty, the authors have been carried out another study on estimating uncertainty at each step of improved WQI model and compared with existing seven established models using machine learning approach for determining the scenarios of uncertainty of various model in Uddin et al., (2022c).

(vii) In order to select the crucial indicators, the authors proposed the random forest algorithm after revising the improved model in Uddin et al., (2022d).

(viii) A number of studies have revealed that the existing WQI model provides improper classes due to its inappropriate classification schemes. The authors revised existing classification schemes and analysed model performance using a proposed classification scheme for coastal water quality incorporating four widely used machine learning classifiers in Uddin et al., (2022e).

(ix) For the purposes of determining the uncertainty production rate of the various weighting techniques, the authors compared four widely used subjective based mathematical techniques in Uddin et al., (2022g).

It should be noted that the investigation studies mentioned above were conducted in Cork Harbour, Ireland (see Fig. 1B), with a particular emphasis on the quality of the transitional and coastal waters. After conducting the aforementioned studies, the authors of this paper would like to propose a more accurate and improved WQI model for evaluating transitional and coastal water quality. This model could be referred to as the **"Irish Water Quality Index Model,"** also abbreviated as **"IEWQI".** The proposed IEWQI model consists of five components, which are as follows:

(i) For the optimization of model input, the random forest algorithm has been recommended for the IEWQI.

(ii) Three newly developed linear interpolation rescaling functions have been proposed for computing the sub-index of the IEWQI.

(iii) In order to estimate the accurate weight values of indicators, a comprehensive approach combining the random forest technique incorporating with the mathematical function of the rank sum technique proposed for the IEWQI.

(iv) To compute the WQI scores more accurately, a completely new weighted quadratic mean (WQM) function has been introduced as the "aggregation function" of the IEWQI.

(v) A brand new classification scheme including four identical water classes like “good”, “fair”, “marginal”, and “poor” has been suggested for assessing coastal water quality using IEWQI.

The present paper is structured as follows : Section 7.4 provides a short description of the model application domains, Section 7.5 -7.6 describes in detail the IEWQI model components and model validation techniques, Section 7.7 presents results and discussion of the IEWQI model, sensitivity, efficiency and model uncertainty, Section 7.8 - 7.13 presents the application results of the IEWQI model for assessing transitional and coastal water quality in four selected domains in Ireland, Section 7.14 summarizes the findings and recommendations.

7.4. Model application domains

The present study selected four application domains that cover the entire extent of the transitional and coastal waterbodies in Ireland in order to assess the sensitivity of the model in terms of spatiotemporal resolution. The following are the selected four coastal waterbodies:

(i) ***Dublin Bay*** is located on the east coast of Ireland (see Figure 7.1A). This bay is primarily used for international navigation, and it is where Dublin Port is located. In Dublin Bay, the river Liffey is one of the most significant inflow rivers so far. Relatively, Dublin Bay is well known as a commercial hub of Ireland, and the surrounding hinterland is dominated by the various economic, industrial, and agricultural activities that directly influence the bay's water quality (Wall et al., 2020). Recently, a few studies have revealed that the Dublin Bay has received around 8.875 million cubic meters square of untreated sewage and storm water between 2017 and 2020 (Environmental Protection Agency, 2020). Due to the wastewater and storm water discharged into Dublin Bay from the treatment plant, Bay water quality has degraded significantly in the last few years (DUBLIN PORT COMPANY, 2021; Environmental Protection Agency, 2020);

(ii) ***Cork Harbour*** is located on the southwest coast and the largest Harbour in Ireland (see Figure 7.1B). Several major tributary rivers which flows into the mainstream the Harbour (Hartnett & Nash, 2015; Uddin et al., 2022a);

(iii) ***Galway Bay*** is situated on the southeast coast and is one of the longest catchment areas in Ireland, whereas the largest urban centre in the catchment is the eastern part of Galway City (see Figure 7.1C). A number of rivers are included in this catchment area, like the Athenry, Louyghrea, Gort, and Oranmore. Recently, several studies have reported that the Galway Bay receives a significant amount of domestic waste each year, which has a significant impact on the water quality of the Bay (Donnelly, 2017; Environmental Protection Agency, 2020); and

(iv) ***Mulroy Bay*** - is the most convoluted of the marine inlets that and is located on the north-west coast of Ireland (see Figure 7.1D). This bay is particularly important for aquaculture, particularly salmon farming, and for scallop spat collection. Recently, a few studies have addressed the impacts of aquaculture on water quality in Mulroy Bay, but there is no significant issue at the current pressure level of farming. Although, the EPA reported that a number of pressures like domestic waste and agricultural pressures are impacting on the water quality in this Bay.

7.5 Methods and materials

7.5.1 Data descriptions

For the purposes of the present study, water quality data for selected four domains were retrieved from the monitoring database of the Irish Environmental Protection Agency (EPA). Usually, the EPA throughout the year monitors water quality frequently at approximately high and low tides across the different waterbodies like the Lake River, Harbour, Bay etc. in Ireland. For the purposes of sensitivity analysis of the IEWQI model in terms of the spatio-temporal resolution, the present study used 2021 monitored water quality data and data divided into two seasons, including (i) summer (April–September), and (ii) winter (October–February). Data for indicators was obtained from the Dublin Bay, Cork Harbour, Galway Bay, and Mulroy Bay, respectively, twenty-four, thirty-seven, twenty-two, and fourteen monitoring sites that were selected based on data availability of a full suite of indicators that required this analysis and coverage of the full extent of the application domain. Details of the monitoring sites and their geographical locations can be found in Table 6.S1 (Appendix 7). For consistency of data, only 1 m depth samples from the water surface were considered in this research. Details of the data attributes can be found at https://www.catchments.ie/data.

In total, nine water quality indicators were used in this research, whereas six common indicators included salinity (SAL), dissolved oxygen (DOX), biological oxygen demand (BOD_5), pH, water temperature (TEMP), transparency (TRAN), and three nutrient enrichment indicators included total oxidized nitrogen (TON), dissolved inorganic nitrogen (DIN), and molybdate reactive phosphorus (MRP). The depth average and seasonal average concentration of water quality indicators for each monitoring site were obtained by calculating the mean of monitored concentrations in a certain season (summer or winter). Details of the water quality indicator concentration at each monitoring site can be found in Table 7.S2. It is noted that the SAL concentration is only used to determine the guideline values (moving thresholds) for the nutrient enrichment indicators (MRP, DOX, and DIN) using the median value according to the methodology of Uddin et al., (2022a). Table 7.S10 provides the details of the moving thresholds for certain median value of SAL. A statistical summary of SAL concentration across the four domains is presented in figure 7.2 below.

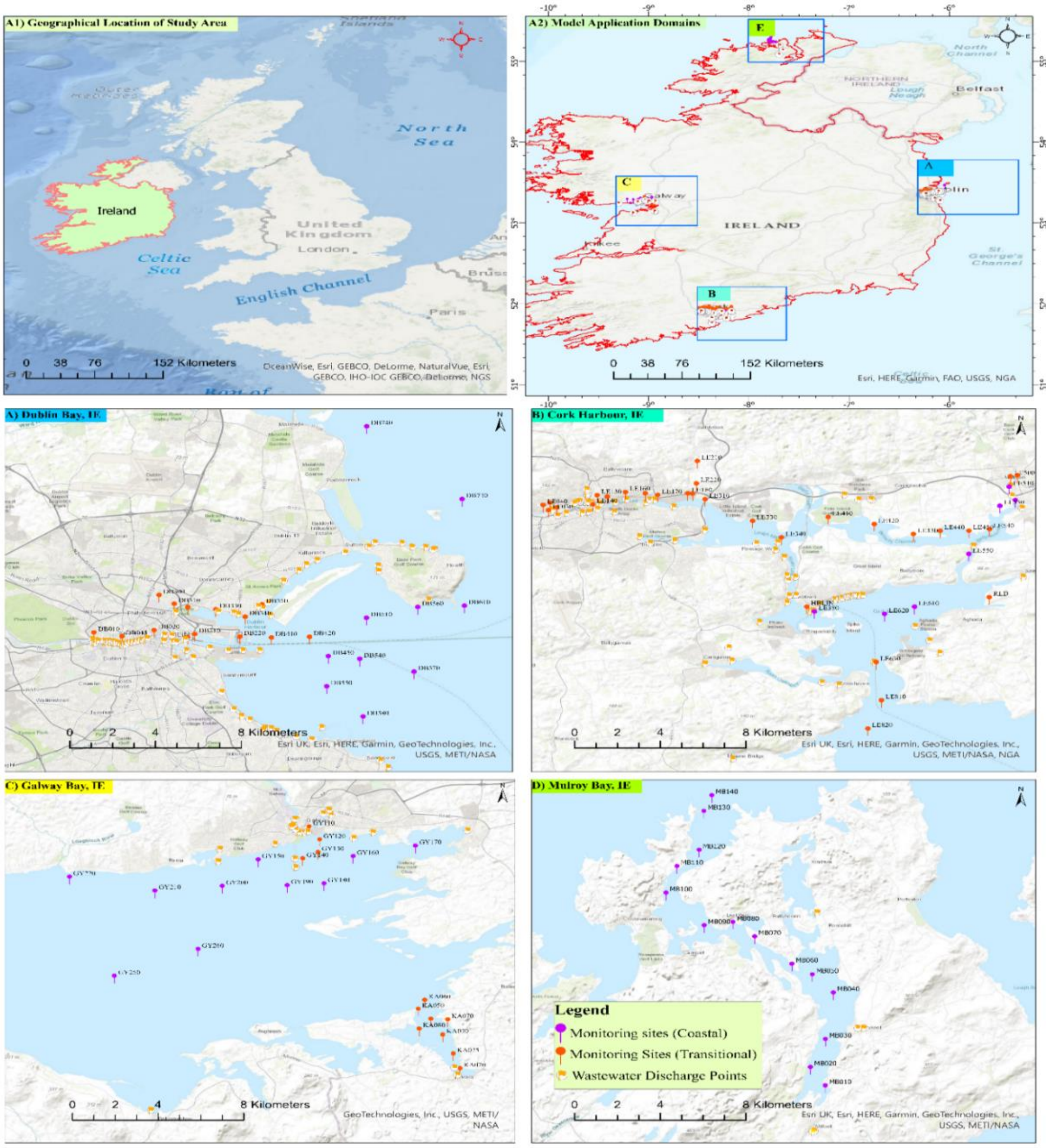


Figure 7.1. Model application domains for assessing transitional and coastal water quality across for waterbodies in Ireland.

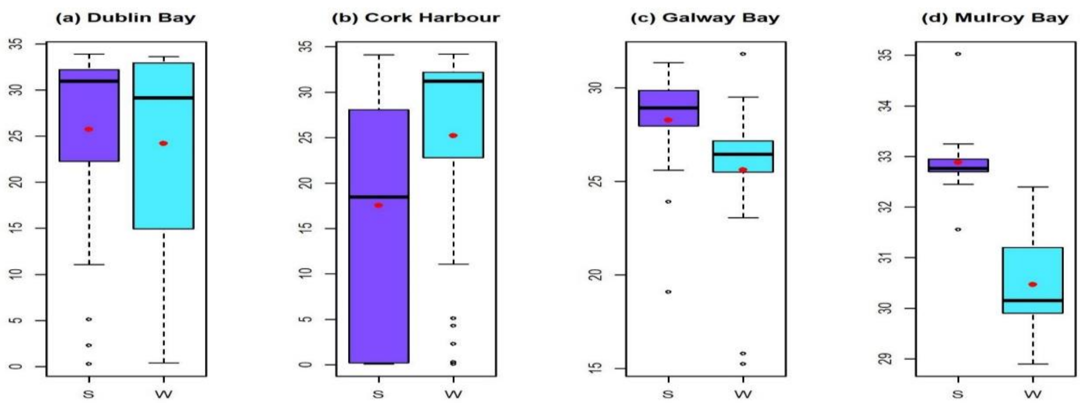


Figure 7.2. A statistical overview of SAL concentration across a range of application domains in Ireland.

7.5.2 Irish Water Quality Index (IEWQI) model

Here, we presented the details of the IEWQI model components. Like other established WQI models, the IEWQI model consists of five identical elements. There are: (i) indicators selection technique; (ii) sub-index functions; (iii) weight values obtaining technique; (iv) aggregation function; and (v) IEWQI score interpretation framework. Figure 7.3 provides the fundamental architecture of the IEWQI model. Details of each component are described below in systematic order.

7.5.2.1 Indicators selection technique

The WQI indicator selection technique is the primary component of the WQI model that is used to select the crucial indicators for the input of the WQI model (Parween et al., 2022; Uddin et al., 2022a; Uddin et al., 2022f, 2021). Currently, a number of tools and techniques, including principal component analysis (Guo et al., 2002; Parween et al., 2022; Tao et al., 2016; Uddin et al., 2022a), correlation technique(Ibrahim et al., 2021; Kumar and Chong, 2018), Delphi technique(Almeida et al., 2012; Mladenović-Ranisavljević and Žerajić, 2018; Neary et al., 2001; Smith, 1990), expert panel judgement(House, 1990, 1980), analytical hierarchical process(Sutadian et al., 2018, 2017), data availability (Sutadian et al., 2018; Thi Minh Hanh et al., 2010), based on environmental significance of indicators (Horton, 1965; Liou et al., 2004; Said et al., 2004) etc., are widely used for selecting the important water quality indicators in considering the relative importance of indicators in literature (Gupta and Gupta, 2021; Uddin et al., 2021). In an earlier review study, the authors identified a range of techniques that are widely utilized in order to extract the importance indicator in existing WQI models. The details of the findings of this critical review can be found in Uddin et al., (2021). Recently, several studies have revealed that the entire indicator selection technique contributed a significant amount of uncertainty to the final assessment due to the inappropriate indicator selection (Gupta and Gupta, 2021; Parween et al., 2022; Sutadian et al., 2016; Uddin et al., 2022a; 2022d). In order to reduce the model uncertainty through the indicator selection process, a few studies have utilized different machine learning algorithms like random forest, support vector machine, tree algorithm, gradient boosting algorithm, k-nearest neighbour, artificial neural network etc. to avoid human or expert intervention in this process (Geurts et al., 2006; Islam Khan et al., 2022, 2021; Touzani et al., 2018; Uddin et al., 2022b; 2022e, 2022c; Vergara and Estévez, 2014).

In a recent study, the authors used the gradient boosting algorithm by comparing the performance of four widely used machine-learning techniques in order to select important indicators of coastal waters (Uddin et al., 2022a). This study has suggested that the gradient boosting algorithm is effective for selecting crucial water quality indicators in terms of the relative significance of variables. Details of the findings of this research can be found in Uddin et al., (2022a). Many studies have also recommended the gradient boosting algorithm for selecting important indicators for other waterbodies like lakes, rivers, etc., in a given dataset (Huan et al., 2020; Islam Khan et al., 2022; Naghibi et al., 2020; Touzani et al., 2018; Uddin et al., 2022d, 2022f). In terms of the reliability of this technique, a few studies reveal that the gradient boosting algorithm does not reflect the actual scenarios of significant indicators that express the relative value of the indicators in terms of influencing coastal water quality (Uddin et al., 2022a; Uddin et al., 2022d). Moreover, a few studies have reported that the gradient boosting algorithm shows an over fitting problem in predicting important features (Ahmed et al., 2019; Islam Khan et al., 2021; Uddin et al., 2022b; 2022d). Consequently, recently, the authors have carried out a comprehensive assessment of eighteen feature section algorithms to select important indicators for assessing coastal water quality and have analysed the reliability of these techniques (Uddin et al., 2022d).

Uddin et al., (2022d) have revealed that the random forest algorithm is effective for selecting important water quality indicators in terms of justifying the reliability of the selected indicators that influence coastal water quality. In addition, this study also showed that compared to other techniques, random forest techniques could significantly reduce the model uncertainty (Alnahit et al., 2022; Uddin et al., 2022d). Details of the findings of this study can be found in Uddin et al., (2022d). Moreover, many water research and machine learning studies have also suggested this technique for choosing the key features in a provided dataset in order to develop an accurate prediction model, whereas the selected features can represent the overall attributes of data in a database (Alnahit et al., 2022; Hou et al., 2022; Jović et al., 2015; Malek et al., 2022a)**.** The present study was used the random forest technique for selecting the crucial water quality indicators according to the methodology of Uddin et al., (2022d).

Details of the algorithm, model optimized hyperparmeters and model performance can be found in Uddin et al., (2022d). The random forest technique is one of the most widely used state-of-the-art tree-based algorithms that applies multiple base models using subsets of the given data, whereas model decisions are made based on the average of each individual tree decision (Ali Khan et al., 2022; Malek et al., 2022b; Xu et al., 2021). Details of the algorithm architecture can be found in A Liaw and Wiener, (2002). Table 1 and Table 7.3 provides the selected eight water quality indicators obtained from the random forest technique, unites, and their standard threshold for assessing coastal water quality and rank of them, respectively.

Table 7.1 Standard thresholds (guideline) of water quality indicators for coastal water quality.

	Indicators	unit	Standard threshold (summer)		Standard threshold (winter)	
			Lower	Upper	Lower	Upper
(i) Constant thresholds for common indicators	BOD5*(ii)*	mg/l	0	7	0	7
	pH*(iii)*	-	5	9	5	9
	TEMP*(ii)*	^{0}C	-	25	-	25
	TON*(iv)*	mg/l as N	0.0	2	0.0	2
	TRAN*(v)*	m/depth	>1	-	>1	-
(ii) Moving thresholds for nutrient enrichment indicators						
(a) Dublin Bay			*thresholds for SAL median value of 31*		*thresholds for SAL median value of 29*	
	DOX*(i)*	% sat	78	122	77	123
	MRP*(i)*	mg/l as P	0.0	0.044	0.0	0.047
	DIN*(i)*	mg/l	0.0	0.51	0.0	0.633
(b) Cork Harbour			*thresholds for SAL median value of 31*		*thresholds for SAL median value of 18*	
	DOX*(i)*	% sat	78	122	71	129
	MRP*(i)*	mg/l as P	0.0	0.044	0.0	0.059
	DIN*(i)*	mg/l	0.0	0.51	0.0	1.336
(c) Galway Bay			*thresholds for SAL median value of 29*		*thresholds for SAL median value of 26*	
	DOX*(i)*	% sat	77	123	75	125
	MRP*(i)*	mg/l as P	0.0	0.047	0.0	0.050
	DIN*(i)*	mg/l	0.0	0.630	0.0	0.825
(d) Mulroy Bay			*thresholds for SAL median value of 33*		*thresholds for SAL median value of 30*	
	DOX*(i)*	% sat	79	121	77	123
	MRP*(i)*	mg/l as P	0.0	0.042	0.0	0.046
	DIN*(i)*	mg/l	0.0	0.380	0.0	0.57

1. *ATSEBI standards, determine the standard values based on median value of Salinity (see details* (Toner et al., 2005), *pp. 72 – 76).*
2. *EPA, Ireland (2001), recommended values for the surface water/freshwater/river water/aquatic life.*
3. *Estuary Monitoring Manual for pH and Alkalinity, EPA,USA*
4. *The European Communities (Quality of surface water intended for the abstraction of drinking water) regulations, 1989 (S.I. No. 294/1989).*
5. *Bathing Water Quality Regulations 2008, (S.I. No. 79/2008).*

7.5.2.2 Sub-index functions

Sub-index (SI) functions are used to transfer various water quality indicators into the uniform scale without hiding/losing any actual information about water quality (Uddin et al., 2021; 2022a). Different approaches are used for computing the SI values in the literatures by existing WQI models (Gupta and Gupta 2021; Uddin et al. 2022a; 2022d). For the purposes of obtaining the SI values, a few WQIs are used as indicators of concentration directly as SI values (Dinius, 1987; Horton, 1965; Liou et al., 2004; Said et al., 2004; Štambuk-Giljanović, 2003), some indices are used liner interpolated functions (Misaghi et al. 2017, Parween et al. 2022, Sutadian et al. 2018, Tomas et al. 2017; Uddin et al. 2021; 2022a), and several models are widely used the rating curve functions (Almeida et al. 2012, Fathi et al. 2022, Sim et al. 2015), respectively. Commonly, it ranges from 0 to 100, whereas 0 refers to "poor" and 100 indicates "excellent" water quality, respectively (Uddin et al., 2021; 2022a).

Table 7.2 Binary rules for determining the SI functions for various water quality indicators according to Uddin et al., (2022a).

Indicators	Conditions	Sub-index functions
BOD_5, MRP, DIN, TON	-	Eq. (1)
DOX	(i) if DOX > 100 (ii) if, DOX < 100 (iii) if, DOX = 100	Eq. (2) Eq. (2) SI = 100
pH	(i) If, pH ≥ 5.0 and pH < 7.5 (ii) If, pH > 8.5 and pH ≤ 9.0 (iii) If, pH ≥ 7.5 and pH ≤ 8.5	Eq. (2) Eq. (3) 100
TEMP	(i) If, TEMP ≤ 25 (ii) If, TEMP > 25	100 0.0
TRAN	(i) If. TRAN < 1.0 (ii) If. TRAN ≥ 1.0	Eq. (3) 100

Recently, several studies have revealed that the SI functions contribute a significant amount of uncertainty in the final assessment of water quality (Gupta and Gupta 2021; Sutadian et al. 2016; Uddin et al. 2021; 2022b). In an earlier study, the authors revealed that the existing SI techniques have suffered from ambiguity problems that may contribute to a considerable amount of the uncertainty in WQI results (Uddin et al., 2022a). The ambiguity refers to the inappropriate rescaling issue with the function(s), which arises when the function(s) either computes lower SI values ("poor" quality) without any input of indicators that are not exceeding the critical threshold or computes higher SI values ("excellent" quality) with the input of a few indicators that exceed the range of the critical threshold of the indicator (s). Details of the ambiguity, its nature, and measurement methodology can be found in Uddin et al., (2022a).

Recently, the authors developed and validated three entirely new linear interpolation rescaling functions to compute SI values more accurately for different water quality indicators, avoiding the ambiguity issues in the WQI model (Uddin et al., 2022a). The appropriate SI function(s) for each indicator is adopted based on a few binary rules. Details of the binary rules for determining the correct SI function(s) can be found in Table 7.2.

The present study introduced three completely new SI functions for the IEWQI model. SI values for selected indicators were computed using the equations (7.1) to (7.3) according to the improved methodology of Uddin et al.,(2022a), whereas the indicator(s) threshold range was obtained from table 1 (above).

$$SI = (SI_u - SI_l) - \frac{(SI_u \times WQ_m)}{(STD_u - STD_l)} \quad \dots\dots\dots\dots\dots\dots (7.1)$$

$$SI = \frac{(WQ_m - STD_l)}{(STD_u - STD_l)} \times SI_u \quad \dots\dots\dots\dots\dots\dots\dots.. (7.2)$$

$$SI_i = (SI_u - SI_l) - \frac{(WQ_m - STD_l)}{(STD_u - STD_l)} \quad \dots\dots\dots\dots\dots\dots\dots. (7.3)$$

Where, SI is sub-index value of indicator(s), SI_u is threshold upper value (100 for "excellent") of the respective water class, SI_l is threshold lower value (0 for "poor") of the respective water class, STD_u is threshold upper limit of the standard for regarding indicator, STD_l is threshold lower limit of the standard for regarding indicator, and WQ_m is the measured or actual concentration of water quality indicator. Details of the threshold ranges can be found in table 7.1.

7.5.2.3 Obtaining indicators weight values

The indicator weighting technique is another crucial component in the development of the WQI model. Commonly, weight generation techniques are used to estimate the weight values of water quality indicators that should reflect the relative importance of indicators in the WQI model (Uddin et al., 2022b; 2022a; 2021).

The existing WQI system uses a variety of tools and techniques, including subjective method that are driven by professionals or decision makers [like expert judgement (Singh et al., 2018; Sutadian et al., 2018), Delphi method (Dadolahi-Sohrab et al., 2012) , etc.], objective methods that associated with a number of mathematical functions that estimate indicator weight values without requiring human involvement (such as the entropy method, rank sum technique, rank order centroid technique, equal or unequal weighting methods), and hybrid methods (like the analytical hierarchy process, the most widely used technique have been utilized for estimating indicator weight values (Sutadian et al., 2017).

Recently, several studies have revealed that the existing weighting approaches have contributed to a significant amount of uncertainty in water quality assessment due to inappropriate weight estimation (Uddin et al., 2022a; 2022c; 2021). A few studies have also reported that the WQI model produced a considerable amount of uncertainty due to its subjective based weighting system(Uddin et al., 2022a; 2022b). Moreover, the authors have conducted another critical review study on the WQI models recently. This study has also addressed a list of current weighting techniques, broadly discussed their pros and cons, and examined their impacts on the WQI system in terms of producing model uncertainty. Details of the study are discussed in Uddin et al., (2021). In addition, most studies have utilized the state-of-the-art machine learning techniques for estimating the features weight values based on their relative importance in machine learning studies.

Given the current state of various weighting techniques, the authors recently proposed a novel weighting approach that allows for the incorporation of machine learning techniques and objective-based mathematical functions (Uddin et al., 2022a). This approach consist of two sub-sequential processes, (i) ranking indicators based on their relative importance using machine learning techniques; and (ii) estimating weight values of indicators using an objective based rank order centroid technique (Uddin et al., 2022a). The details of the methodology can be found in Uddin et al., (2022a). In an earlier another study, the authors also compared various objective based weighting techniques and evaluated their performance in terms of contributing uncertainty to the model. This study revealed that there were no significant differences across the ranks based on various weighting functions (Uddin et al., 2022g). For the purposes of estimating indicator weight values more accurately, the present study utilized the approach of Uddin et al., (2022a). A tree-based random forest machine learning technique is used to rank indicators of water quality in order to accurately estimate the weight values of each indicator in relation to their relative importance. The authors' recent study has revealed that the random forest algorithm is a reliable technique for ranking water quality indicators that accurately reflects the relative information of indicators. Details of this study can be found in Uddin et al., (2022d). Finally, the objectively based the rank sum mathematical function used to estimate the weight values of indicators outperformed the other methods in terms of reducing model uncertainty in the WQI model (Uddin et al., 2022g). Moreover, recently, many studies have reported that this technique is more reliable and effective than other objective methods in estimating weight values accurately(Li et al., 2009; Odu, 2019; Roszkowska, 2013; Song and Kang, 2016). It can be defined as follows:

$$\textit{Rank sum method:}\ \mathrm{w_i} = \frac{\mathrm{n+1\text{-}i}}{\sum_{\mathrm{j=1}}^{\mathrm{n}} \mathrm{j}} = \frac{2(\mathrm{n+1\text{-}i})}{\mathrm{n(n+1)}}, \mathrm{i} = 1,2,3 \dots \dots, \mathrm{n} \ \dots \dots \dots \dots (7.4)$$

where *n* is the total number of ranked indicators; *i* is the i^{th} indicator rank; *j* is the summation of rank and *w* is the weight value.

7.5.2.4 Aggregation function

Aggregation function is the final component of the WQI model. It allows converting the SI and weight values of various water quality indicators into a numerical value that is well known as the WQI index or WQI score(s). Commonly, the aggregation functions can be classified into two groups: (i) weighted functions (required estimation of indicator weight values), and (ii) unweighted functions (not require indicator weight formulation and only use the SI values). Up to date, different aggregation functions have been used in entire WQI approaches including arithmetic including additive (Horton 1965) and multiplicative (Alphayo and Sharma 2018; Asadollah et al. 2021; Gradilla-Hernández et al. 2020; Mladenović-Ranisavljević and Žerajić 2018; Parween et al. 2022; Tomas et al. 2017;Zotou et al. 2019), geometric(Liou et al. 2004; Sutadian et al. 2017; Thi Minh Hanh et al. 2010), combined approaches: combination of arithmetic and geometric (Almeida et al. 2012; Bordalo et al. 2006; Cude 2001; Dadolahi-Sohrab et al. 2012), and minimum operator functions (Smith 1990) etc. Details of the various aggregation functions, mathematical expressions and their applications can be found in Uddin et al., (2021).

Recently, several studies have revealed that the existing aggregation functions contributes a significant amount of uncertainty to the final assessment due to the inappropriate aggregation process. In an earlier study, the authors have revealed that the existing aggregation functions have been influenced by the ambiguity problem (Gupta and Gupta 2021, Uddin et al. 2022a). Ambiguity is another great concern that could have contributed to the considerable amount of uncertainty in the final assessment by hiding the real state of water quality that is contained in the model inputs (Uddin et al., 2022a). As a consequence, that led to the misclassification of water quality for environmental managers or assessors. It can be categorized into two types: overestimating and underestimating ambiguity, which are associated with the inappropriate aggregation process. Details of the ambiguity problems of the aggregation process are briefly discussed in Uddin et al., (2021; 2022a). In their recent study, the authors compared eight aggregation functions, including four weighted and four unweighted, whereas five are established functions that are widely used in the existing WQI approaches and three (one weighted and two unweighted) were newly proposed for the purposes of comparing the model performance. Details of the findings can be found in Uddin et. al. (2022a). In terms of model uncertainty, Uddin et al., (2022a) have revealed that the newly proposed weighted quadratic mean (WQM) and unweighted root mean squared (RMS) aggregation functions showed the best outperformance in assessing coastal water quality. Relatively, both functions have been found to be free from these issues (both types of ambiguity), while the majority of commonly used techniques, like the CCME, SRDD, WJ, etc., have been significantly influenced by the ambiguity problems (Uddin et al., 2022a).

Moreover, another earlier study by the authors revealed that the WQM and the RMS functions are effective for computing the WQI score in order to reduce the model uncertainty. Also, these functions are highly efficient for reducing model ambiguity and eclipsing problems significantly (Uddin et al. 2022c). According to their research, these aggregation functions produce less than 2% of uncertainty during the aggregation process, compared to nearly or more than 10% of uncertainty produced by other existing techniques. Details of the findings of uncertainty for various aggregation functions can be found in Uddin et al., (2022c). To the best of the author's knowledge, the earlier mentioned studies are the first initiatives to analyse and estimate model uncertainty at each step of the WQI process for different models. In that case, most aggregation functions do not enable the expression of the actual water quality information. Consequently, the existing functions provide a significant amount of uncertainty in the final assessment (Gupta and Gupta 2021; Uddin et al. 2021; Uddin et al. 2022a;2022b). Therefore, for the purposes of the aggregation of SI and weight value(s), the present study utilized the weight quadratic mean (WQM) aggregation function for the computation of the WQI index for the IEWQI model. It can be defined as follows:

$$\mathrm{IEWQI} = \sqrt{\sum_{i}^{n} w_i s_i^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots. \quad (7.5)$$

where s_i is the sub-index value for parameter i; w_i is weight value of respective variables and n is the number of parameters.

The IEWQI scores were computed using the FORTRAN language programing most accuratly. Details of the programing codes and functions can be found in Appendix 10.

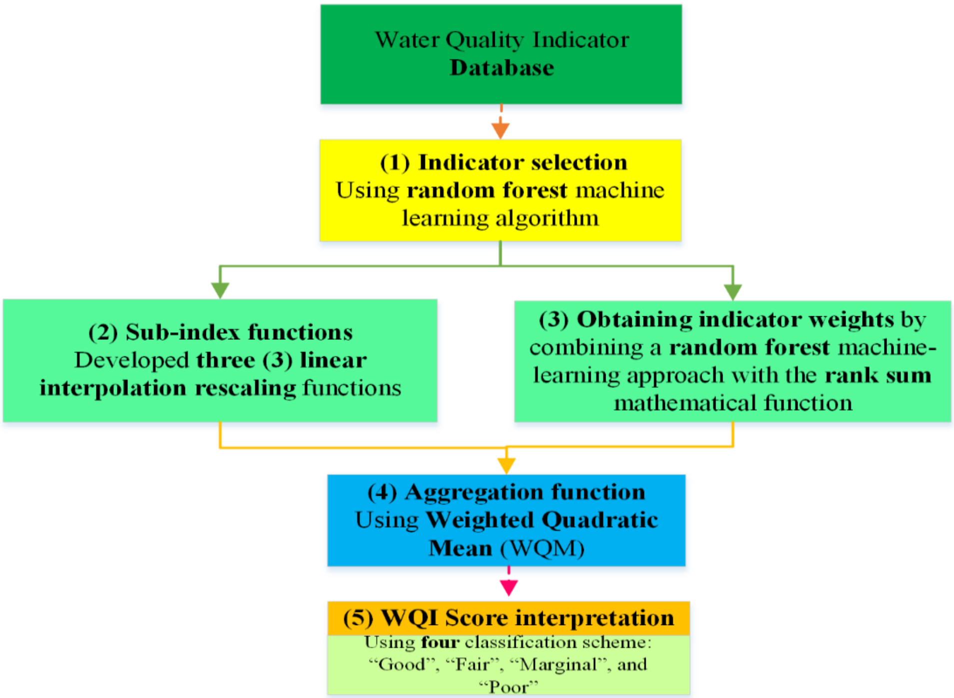


Figure 7.3. Proposed fundament architecture for the Irish water quality index model.

7.5.2.5 Evaluation of IEWQI model outcomes

The ultimate goal of the IEWQI model is to classify the water quality using a classification scheme. Commonly, the WQI model's final output is a numerical value that is called an index score, that ranges between 0 (poor quality) and 100 (good quality). For the interpretation of the WQI score, the existing WQI system used a range of classification schemes in the literature (Uddin et al., 2021). Recently, several studies have revealed that a significant amount of uncertainty has been produced due to inappropriate classification schemes. Consequently, the typical classification schemes can provide inconsistent results in the final assessment of water quality for similar groups of water quality indicators (Uddin et al., 2022a; 2022e). Moreover, recently many studies have reported that the widely used classification scheme "One Out-All Out" technique of the water framework directive has also received much more criticism due to the inaccurate classification of water quality (Latinopoulos et al., 2021; Prato et al., 2014). Therefore, in order to avoid this inaccurate assessment, the authors have proposed a universal classification scheme for assessing coastal and transitional water quality in an earlier study (Uddin et al. 2022a). Uddin et al., (2022a) have revealed that the results of water quality assessing using the universal scheme reflect the accurate scenarios of water quality. In this research, the IEWQI model output interpreted using the classification approach of Uddin et al., (2022a). Table 7.3 provides the classification schemes and their definitions for the quality of coastal water. Details of the classification procedures can be found in Uddin et al., (2022a).

Table 7.3. Classification scheme for coastal water quality of Uddin et al., (2022a).

Classes	WQI score	definition
Good	80-100	Good waterbodies that meet the standard values and thus water quality is suitable for all use.
Fair	50-79	Waterbodies that a few indicators meet the standard values and the water quality is usually protected with a minor degree of impairment.
Marginal	30-49	The majority of the water quality indicators failed to meet the criteria; water quality in unprotected, which may be posing a risk for aquatic life.
Poor	0-29	Poor waterbodies are those that failed to meet all the criteria; water quality is completely unprotected and unsuitable for many specific usages.

7.6 Model sensitivity analysis

7.6.1 Machine learning approaches

Machine learning is an advanced state-of-the-art technology that is widely used to predict or classify unknown objects based on the previous learning model (Uddin et al., 2022b). Recently, this technique has been most widely utilized for evaluating the sensitivity of water quality models in terms of the accurate assessment of water quality or classification. The present study used the multilinear regression (MLR) machine learning algorithm for evaluating the IEWQI model's sensitivity according to the approach of Uddin et al. (2022a). Details of the methodology for the MLR analysis can be found in Uddin et al., (2022a). In earlier studies, many researchers have successfully utilized this technique in order to investigate the effect of model predictors (water quality indicators) on the response (IEWQI score) in water quality research (Chaudhary and Hantush, 2017; Uddin et al., 2022a). The model sensitivity was assessed by comparing the coefficient of determination (R2) between the IEWQI scores and the MLR predicted scores using the same water quality indicators for both techniques. In this research, the MLR algorithm has been performed using the regression learner apps in MATLAB 2022a. Details of the regression learner apps and their applications can be found in Uddin et al., (2022c).

7.6.2 Model evaluation

Once the MLR prediction model was developed, the model’s performance was evaluated using the various performance metrics. The present study was used root mean square error (RMSE), mean square error (MSE), and mean absolute error (MAE) to assess the performance of the regression model because; most studies in water research have widely used these metrics to assess prediction models using machine learning and artificial intelligence techniques. The present study used root mean square error (RMSE), mean square error (MSE), and mean absolute error (MAE) to assess the performance of the regression model because, recently, most studies have widely used these metrics in evaluating prediction models using machine learning and artificial intelligence techniques(Asadollah et al., 2021; Uddin et al., 2022b; 2022a; Zaghloul and Achari, 2022). To estimate the performance criteria, the cross-validation technique is widely used in machine learning and artificial intelligence regression model. In this research, the 10-fold cross-validation technique was performed using the approaches of Uddin et al., (2022a) and (2022b). The performance criteria score typically ranges from 0 to1, with all criteria expecting a score as low as possible. The lowest score indicates the best model performance.

7.6.3 Model efficiency analysis

For the purposes of model efficiency analysis, a range of statistical and mathematical tools and techniques are used; the Nash–Sutclife efficiency (NSE) index is one of them (McCuen et al., 2006; McManus et al., 2020). Recently, several scientific studies in various domains have utilized this technique for assessing the model's performance in terms of efficiently predicting (Chaudhary and Hantush, 2017; Uddin et al., 2022d). It allows measuring and determining the magnitude of residual variation in a comparison to recorded data variance (Izhar Shah et al., 2021; Minh et al., 2022). Details of the NSE index can be found in McCuen et al., (2006). The NSE score typically ranges from -∞ to 1, with a score close to 1 indicating the best model performance and a negative score indicating poor model performance (Sharif et al., 2022; Uddin et al., 2022d). Moreover, a few studies have proposed the model efficiency factor (MEF) in order to analyse the model efficiency more reliably (Sharif et al., 2022). This technique is an extended form of the NSE index and is a more comprehensive and reliable tool than other techniques. In recent studies have utilized this method successfully in water research to identify the best prediction model in terms of the prediction errors (Uddin et al., 2022d). Like the NSE score, the MEF scores also ranged between 0 and 1, whereas 0 refers to the bias free model and 1 indicates the lowest efficiency of the model, respectively (McCuen et al., 2006; Sharif et al., 2022; Uddin et al., 2022d). These techniques were used in this study to assess the IEWQI model's efficiency in terms of reliable water assessment. Details of these techniques are discussed in Uddin et al., (2022d).

7.6.4 Uncertainty analysis

Uncertainty estimation is an important component of any mathematical or computational model. Because it provides a concrete idea of exactly how much data inconsistency the model has produced, which could be helpful for the improvement of the model architecture (Liang et al., 2016; Uddin et al., 2022c). Recently, the WQI model has received much more criticism due to the uncertainty issues. In an earlier study, the authors compared five existing WQI models with the improved methodology. This study reported that the improved methodology produced the least uncertainty compared to other traditional approaches. Details of this study can be found in Uddin et al., (2022a). Therefore, the present study used this improved technique for assessing coastal water quality in Ireland in order to estimate the uncertainty and compare it in terms of the spatio-temporal resolution of application domains. For the purposes of estimating uncertainty, the present study used the inferential error bar analysis approach by following the approach of Uddin et al., (2022a), because several studies have been carried out using this approach for estimating and modelling the data uncertainty in measuring value (Commowick and Warfield, 2010; Cumming et al., 2007; Cumming and Finch, 2005; Jolliffe, 2007). Details of the methodology are discussed in (Uddin et al., 2022a). Moreover, recently, a few water research studies have utilized this technique for modelling the expected amount of uncertainty in a measurement using the predicted interval of WQI scores. In this research, both MLR predicted IEWQI scores and the WQM aggregation scores have been used for modelling the amount of uncertainty in both WQM aggregation function and prediction scores, respectively (Krueger, 2017; Seifi et al., 2020; Uddin et al., 2022b, 2022a).

7.7 Results and discussion

7.7.1 Statistical summary of selected water quality indicators

Indicator selection is the initial step in developing the WQI model. The present study selected eight water quality indicators, including DOX, MRP, DIN, TON, BOD_5, pH, TEMP, and TRAN, using the improved methodology of Uddin et al., (2022a). Details of the indicator concentration at each monitoring site can be found in Tables 7.S2 to 7.S9 (Appendix 7). Figure 7.S1 shows Pearson correlations among selected water quality indicators. There was a significant negative correlation between nutrient enrichment indicators and other common indicators over the various domains through both the summer and winter seasons (Figure 7.S1). Figure 4 shows a statistical summary of eight water quality indicators from various application domains over the course of the study. As shown in the figure below, a significant difference existed in the concentration level of various indicators between the summer and winter seasons across different waterbodies.

As regards Dublin Bay and Cork Harbour, most indicators were found between the guide values, except the TON, TRAN, DIN, and MRP. These indicators exceeded the permissible limit during both the summer and winter seasons (Figure 7.4a; Figure 7.4b). In contrast to those domains, in Galway Bay, a slight data difference was found for water quality indicators throughout the year, whereas the majority of indicators were found within the permissible limit, with the exception of MRP for summer and

DIN and MRP for winter, respectively, whereas those indicators breached the guide values for indicators in Galway Bay (Figure 7.4c). Compared to other waterbodies, relatively, higher concentration differences were found between the summer and winter seasons in Mulroy Bay. The majority of indicators varied significantly throughout the year, but all indicators were found to be within the allowable limit during both seasons (Figure 7.4d).

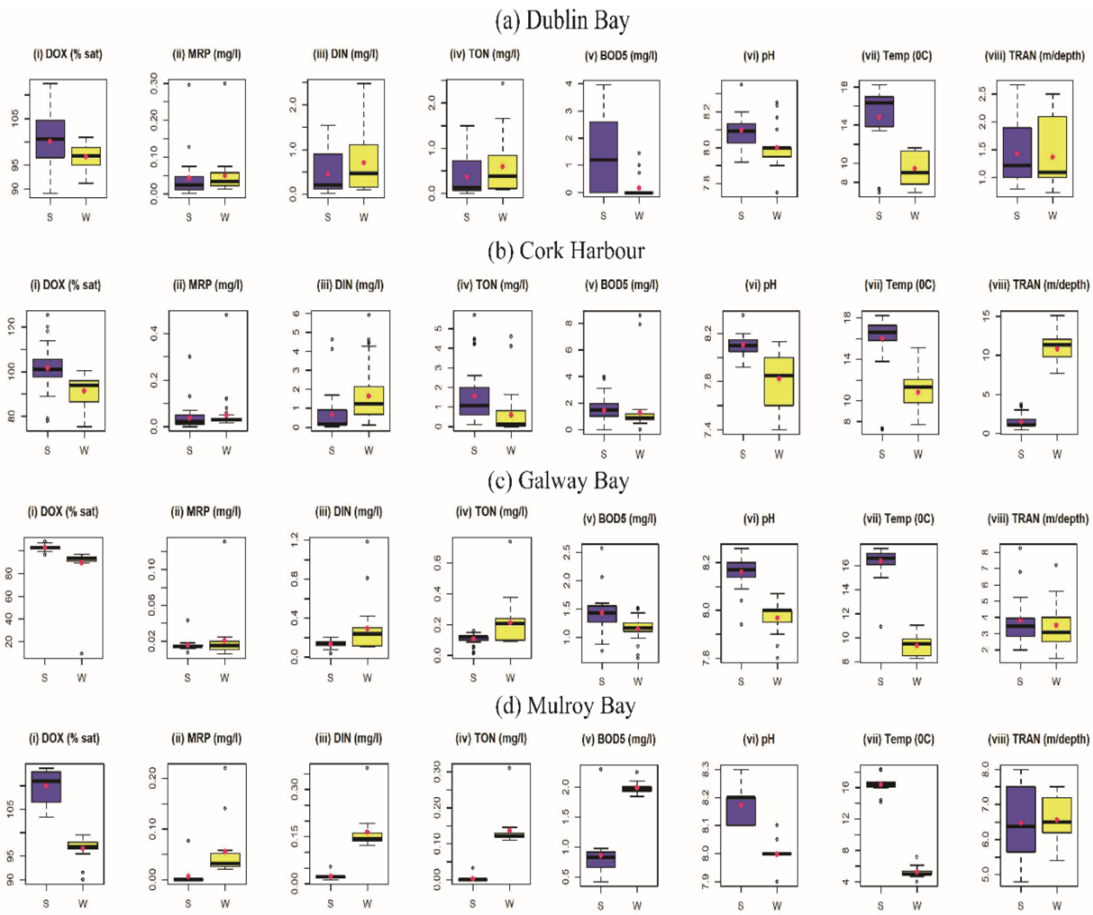


Figure 7.4. Statistical summary for selected water quality indicators over the four application domains in Ireland, whereas S and W on the x-axes refer to summer and winter, respectively.

7.7.2 Sub-index results

In order to reduce the ambiguity problem in estimating SI values, the present study used three newly developed SI functions. Higher SI values typically denote "excellent" water quality, while lower values denote "poor" water quality. These SI functions were used in this research for computing the SI values due to their reliability and validity. Because these functions are effective in avoiding the ambiguity problem in computing

SI values (Uddin et al., 2022a). Details of the SI functions and ambiguity can be found in Uddin et al., (2022a). Figure 7.5 illustrates the sensitivity of aggregation functions using an example of a water quality indicator for Dublin Bay during the summer. Each black dot represents the SI value at a particular site for a given indicator concentration. The detailed SI values for each monitoring site across various water bodies during the study period are provided in Tables 7.S11 to 7.S18 (Appendix 7).

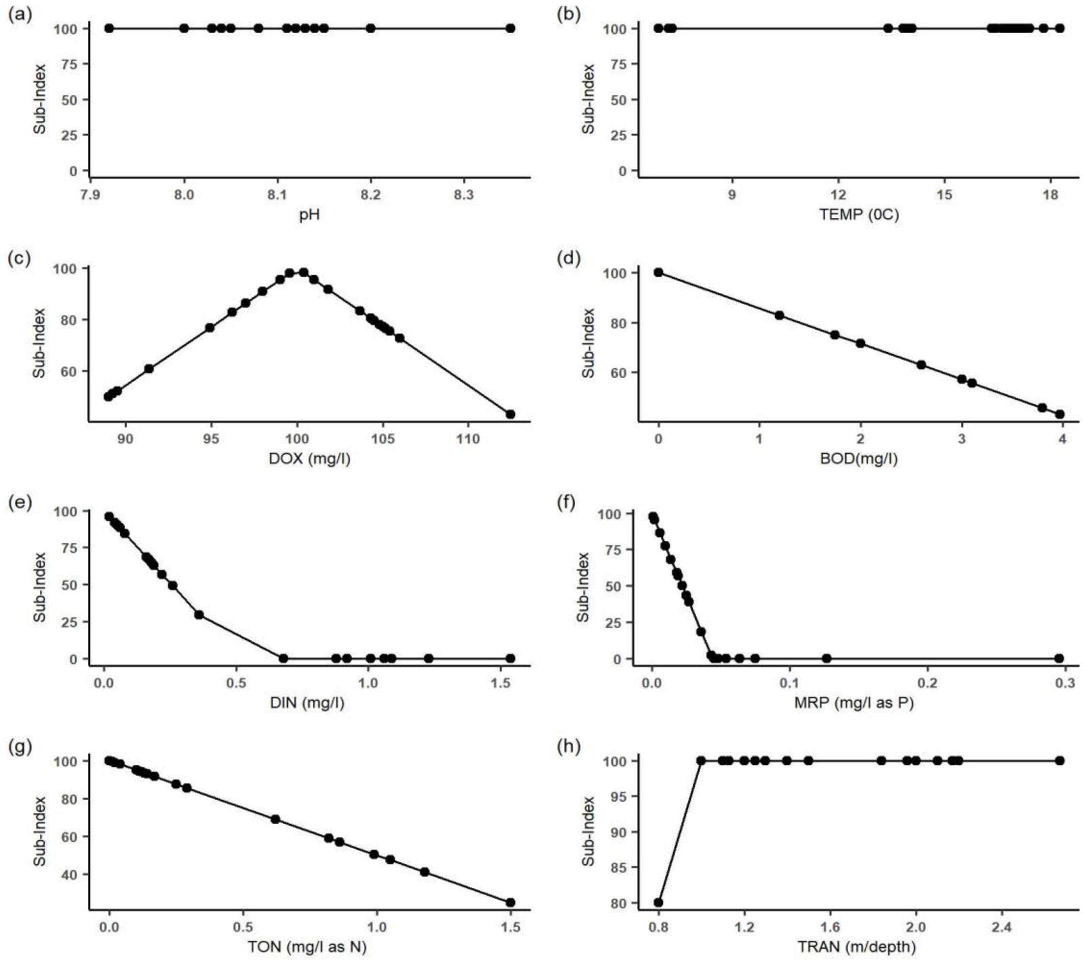


Figure 7.5**.** SI values vs. indicator concentration at each monitoring sites in Dublin Bay over the summer season. Each black dot represent the SI value for each indicator at particular monitoring site.

Figure 7.6 presents a statistical summary of SI values for various application domains through the summer and the winter periods. From the figure below, it can be seen that a significant SI values differences were found between the summer and winter seasons across the application domains. Most indicators' SI values were varied significantly through the year except for pH, TEMP, and TRAN (Figure 7.6a). Contrary to the waterbodies, BOD_5, and DOX were significantly fluctuated over the study period, but relatively higher SI values were obtained for those indicators during the winter period in Dublin Bay.

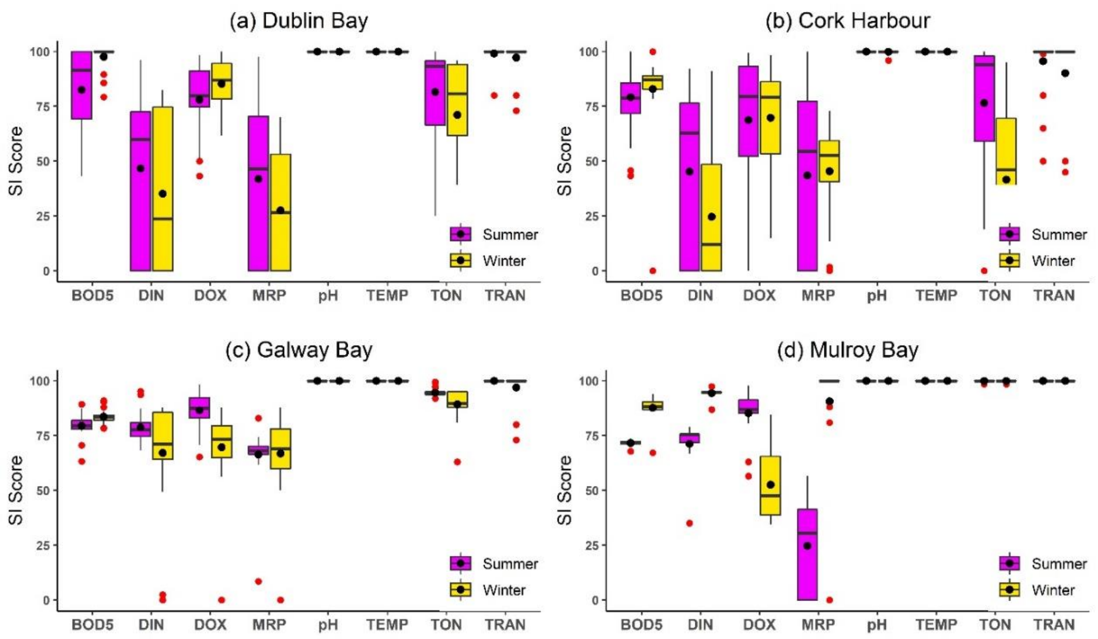


Figure 7.6. A statistical overview of the computed SI scores for selected eight water quality indicators across various waterbodies through the summer and winter season.

Unlike Dublin Bay, a significant SI values difference was found between summer and winter periods for MRP and TON, whereas higher SI values were computed for those indicators in Cork Harbour over the summer season (Figure 7.6b). Figures 7.6c and 7.6d make it clear that SI values for the majority of water quality indicators in Galway Bay and Mulroy Bay varied seasonally. In both waterbodies, the majority of indicators' SI values were calculated between 75 and 100, with the exception of MRP in Mulroy Bay. The results of the SI values of various water quality indicators reveal that the SI functions are highly sensitive to the spatio-temporal resolution of the waterbodies.

7.7.3 Indicators weight values

The present study computed the indicator weight values using the improved methodology of Uddin et al., (2022a). Table 4 provides the weight values for the eight indicators used to calculate the WQI scores. From the weight values in Table 4, nutrient indicators (TON, DIN, and MRP) achieved the highest weight values, whereas 0.222, 0.194, and 0.111, respectively, for TON, DIN, and MRP, had the most significant indicators in this research. Moreover, water TRAN and pH were also suggested as the crucial indicators in terms of the physical attributes of coastal water quality. Contrarily, the water TEMP and DOX had the lowest significance when evaluating the quality of the coastal waters. The results of the weight values indicate that nutrient elements are more significant indicators for assessing coastal water quality than other indicators.

Table 7.4 Weight values of water quality indicators for the IEWQI model.

Indicators	Rank*	Weight values
TON	1	0.222
DIN	2	0.194
TRAN	3	0.167
pH	4	0.139
MRP	5	0.111
BOD5	6	0.083
TEMP	7	0.056
DOX	8	0.028
Sum		**1.00**

Note: **Indicators rank are assigned based on the relative importance obtained from the random forest technique*

7.7.4 Results of the aggregation functions

The present study used the WQM aggregation function to transform the sub-indexes and weight values of selected indicators into the IEWQI score. The authors of a recent study have revealed that the WQM aggregation function is more effective and reliable compared to other functions in the existing system in terms of reducing model uncertainty. Details of this study can be found in Uddin et al., (2022a). The detailed results of the aggregation function at each monitoring site for four waterbodies during the summer and winter seasons can be found in Tables 7.S2 to 7.S9 (Appendix 7). Figure 7.7 shows the summary statistics of WQI scores across various domains during the summer and winter, respectively. Figure 7.8 presents the WQI scores at the monitoring site over the different waterbodies through the summer and winter seasons. From the figure (below), relatively higher WQI scores were found during the summer season, whereas scores were significantly lower during the winter season. As shown in figure 7.7, a significant difference was found in WQI scores between the summer and winter seasons for Cork Harbour. During both seasons, the data outlier's presence was found for Galway Bay and Mulroy Bay, whereas it was found only for Cork Harbour throughout the winter period. The results of the outliers indicate that the WQI scores had significant differences between both the summer and winter seasons (Islam Khan et al., 2022; Uddin et al., 2022a).

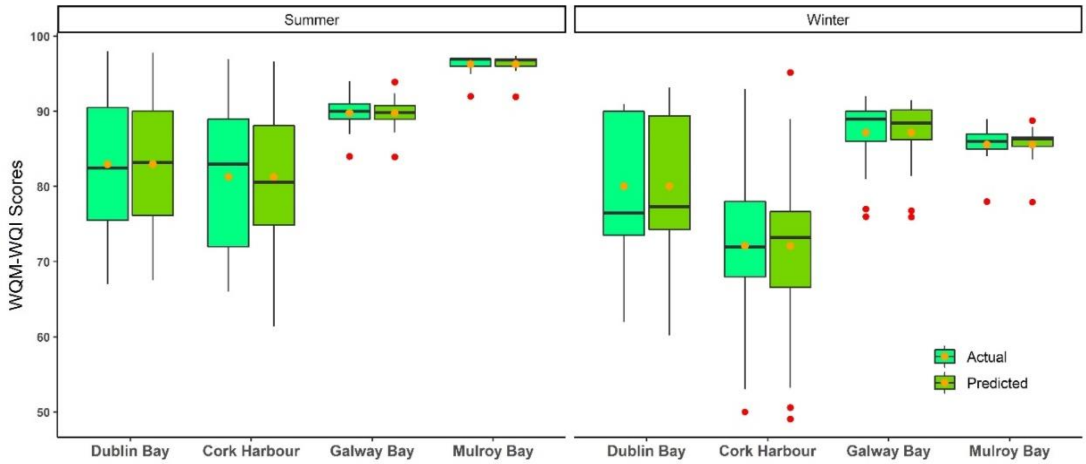


Figure 7.7. Statistical summary of IEWQI scores across the application domains in Ireland. The yellow circle indicates mean score; black line refers to the median score whereas the red circles designates the presence of data outliers.

For the determination of the relationship between IEWQI and inputs, the present study utilized the Pearson correlation analysis. Figure 7.S1 presents the Pearson correlation between various indicators and IEWQI scores. The correlation results indicate that most nutrient enrichment indicators have a strong negative correlation with the IEWQI scores, whereas water pH and TRAN shows a strong positive correlation with IEWQI scores across four application domains during both seasons (Figure 7.S1).

7.7.4.1 Sptio-temporal differences of IEWQI scores

Figures 7.9 and 7.10 present the spatiotemporal effects on aggregation function and variation of the calculated WQI score at each monitoring site across the various application domains, respectively. As shown in figure 7.8 (above), a slight difference in WQI scores was found between the summer and winter seasons for all waterbodies, with the exception of Cork Harbour. It can be seen from figures 7.8(b), 7.9(b), and 7.10(b), a significant WQI discrepancy was found between the summer and winter seasons in Cork Harbour. Relatively, lower WQI scores were estimated for the monitoring sites in the upper part of the Harbour (river Lee, north channel and outer part of the Harbour), whereas higher WQI scores were calculated at the monitoring sites in the lower Harbour, river Owenacurra, and river Glashaboy (Figure 7.9b) throughout the summer. Details of the monitoring sites' descriptions can be found in Table 7.S1 and figure 1, respectively. The results of the spatio-temporal variation of WQI's in Cork indicate that the upper Harbour is sensitive in terms of receiving various pressures like anthropogenic, domestic wastewater, agricultural wastewater, etc. (Figure 7.18b; Figure 7.19b). In addition, the EPA Ireland also identified the upper part of the Harbour as a nutrient sensitive area (EPA, 2021). The spatio-temporal results of the QM-WQI scores in Cork Harbour are in line with those of previous studies (EPA, 2021; Uddin et al., 2022a; 2022b; 2020a; 2020b).

Like in Cork Harbour, relatively lower WQI scores were computed at the monitoring sites in the upper part of Dublin Bay, whereas higher scores were calculated from the farthest monitoring sites in the Bay during both the summer and winter seasons (Figure 7.9a; Figure 7.10a); because the upper part has received a considerable amount of domestic wastewater (EPA, 2021). It is noted that the EPA Ireland also noted the upper part of the Bay as a nutrient sensitive zone in previous reports (Barr and Mcelroy, 2019; DUBLIN PORT COMPANY, 2021). In contrast to the waterbodies, there were no significant differences in WQI scores for Galway Bay and Mulroy Bay throughout the study period (Figure 7.9c; Figure 9.9d; Figure 7.10c; Figure 7.10d). However, it can be easily figured out from the figure below that relatively higher WQI scores are computed at each monitoring site for most waterbodies through the winter period. The results of the spatio-temporal variation of WQI scores indicate that significant effects of spatio-temporal resulation were had on the IEWQI model. The results of the spatio-temporal variation of WQI scores show that spatio-temporal resolution had a significant effect on the IEWQI model. As a result of the computed spatio-temporal differences in WQI scores, it is possible to conclude that the IEWQI model is highly sensitive to spatial attributes and that the model could compute the WQI score by taking the spatio-temporal resolution of waterbodies into account. Additionally, the IEWQI model could be integrated with the various anthropogenic and natural pressures present in the application domain and modelled as a result.

Figure 7.8**.** Monitoring sites based IEWQI results across the four application domains in Ireland. The horizontal lines refer the IEWQI score to classify water quality using the classification scheme (see Table 2).

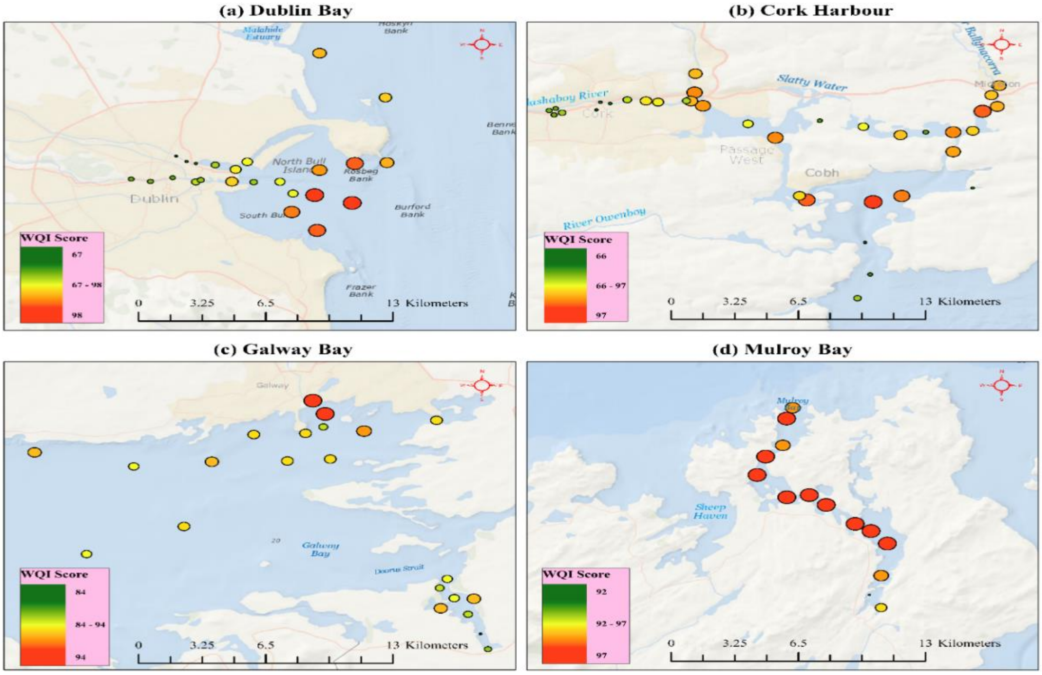


Figure 7.9. Spatio-temporal variation of the IEWQI scores are presented using the proportional symbol across various domains during the summer season.

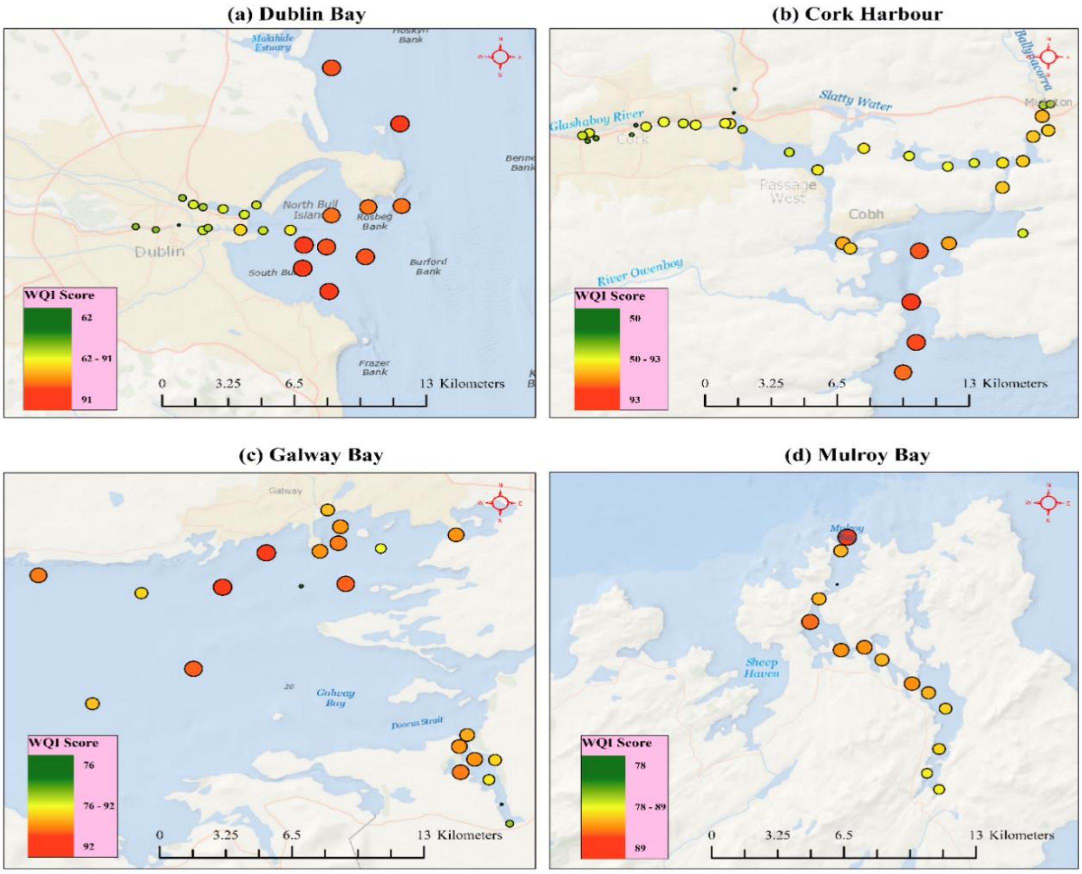


Figure 7.10. Spatio-temporal variation of the IEWQI scores are presented using the proportional symbol across various domains during the winter season.

7.8 Impact of eclipsing and ambiguity attributes on the WQM aggregation function

A number of factors play a vital role in producing the uncertainty in the WQI model; the eclipsing and ambiguity are two of them. Details of the eclipsing and ambiguity attributes and their role in the WQI model can be found in Uddin et al., (2021) and Uddin et al., (2022a). Recently, several studies have revealed that these two attributes to contribute a significant amount of uncertainty in the final assessment of water quality using the WQI model. In earlier studies of the authors, they have reported that the aggregation function is greatly influenced by these attributes. In their studies, Uddin et al., (2022a) proposed a few rules for determining the eclipsing and ambiguity impacts on the aggregation results. The present study determined the model eclipsing and ambiguity problems using the criteria and guidelines of Uddin et al., (2022a). The details of the eclipsing and ambiguity assessment criteria are discussed in Uddin et al., (2022a). Details of the model eclipsing results can be found in Tables 7.S2 to Table 7.S9 (Appendix 7). Herein, Table 7.5 provides a comprehensive statistical summary of model eclipsing and ambiguity problems that were obtained from the rule of Uddin et al., (2022a) across various application domains. Details of the eclipsing and ambiguity results are discussed below:

(i) Eclipsing results

The eclipsing problem commonly occurs due to over estimation of the WQI score by the aggregation function (Uddin et al., 2021; 2022a). Usually, it occurs when the aggregation function estimates more than the higher index score, or even if one or more indicators have breached the guideline values, but the final index score does not reflect this circumstance (Uddin et al., 2022a). Form the data in table 7.5, it can be seen that the eclipsing problem can be found during summer season for most application domains with the exception of the Mulroy Bay, whereas it was found to be over the winter period. There were no eclipsing problem across various domains over the winter period except in Mulroy Bay. A number of monitoring sites were found to have the eclipsing problem across Dublin Bay (2 out of 24), Cork Harbour (5 out of 37), Galway Bay (only 1 out of 22) and Mulroy Bay (3 out of 14), respectively (Table 4). Compared to the existing WQI models, the IEWQI model-eclipsing rate is lower than other techniques (Uddin et al., 2022a). The results of the eclipsing problem in the present study are consistent with those of the authors' earlier studies (Uddin et al., 2022a;

2022b).

Table 7.5 The summary of statistics for the results of the IEWQI model eclipsing and ambiguity effects.

Attributes	Dublin Bay		Cork Harbour		Galway Bay		Mulroy Bay	
	Summer	Winter	Summer	Winter	Summer	Winter	Summer	Winter
Eclipsing	2 (8.3%)	0	5 (13.5%)	0	1 (4.5%)	0	0	3 (21.4%)
Ambiguity	4 (16.6%)	0	3 (8.1%)	0	0	0	0	1 (7.14%)
Total sites	**24**	**24**	**37**	**37**	**22**	**22**	**14**	**14**

(ii) Ambiguity results

Ambiguity is another crucial source of uncertainty in the WQI system that is associated with the sub-index and aggregation functions. It hides the real information about water quality contained in the initial components of the model input. Commonly, it may be categorized into two, like *Type-I* and *Type-II*. Details of the ambiguity and its measurement criteria can be found in Uddin et al., (2022a). Type-I ambiguity relates to the underestimation problem of the aggregation function, whereas Type-II is associated with the overestimation problem of the aggregation method. The present study determined the ambiguity problem according to the approach of Uddin et al., (2022a). Because this method is particularly useful in studying the assessment of model ambiguity in the WQI technique, details of the model ambiguity results can be found in Tables 7.S11 to 7.S18 (Appendix 7). The present study found a Type-II ambiguity problem across different waterbodies in Ireland. Like the eclipsing problem, an ambiguity problem was found for Dublin Bay (4 out of 24 monitoring sites) and Cork Harbour (3 out of 37 monitoring sites) during the summer season, whereas there was no impact found over the winter period across most domains except for Mulroy Bay (1 out of the 14 monitoring sites) (Table 7.5). During the study period, there was no ambiguity in Galway Bay. The ambiguity results show that the problem with ambiguity also affected the most eclipsed sites.

7.9 IEWQI prediction results

7.9.1 Model performance results

For the purposes of predicting the IEWQI score, the present study utilized the MLR technique. In order to evaluate the MLR performance, in this research, the10-fold cross-validation technique was utilized because it is a widely used method in machine learning studies. Figure 7.11 presents the various performance metrics of the MLR predictive model across various domains. Compared to the four domains, the lowest model prediction error (testing error) was found for Mulroy Bay (RMSE = 0.21, MSE = 0.045, MAE = 0.15 for summer, and RMSE = 0.36, MSE = 0.13, MAE = 0.32 for winter), and Galway Bay (RMSE = 0.23, MSE = 0.054, MAE = 0.19 for summer, and RMSE = 0.61, MSE = 0.38, MAE = 0.51 for winter), respectively during both seasons, whereas higher prediction errors were found for Dublin Bay (RMSE = 2.11, MSE = 4.45, MAE = 2.10 for summer, and RMSE = 1.72, MSE = 2.95, MAE = 1.45 for winter) and Cork Harbour (RMSE = 3.6, MSE = 12.96, MAE = 2.86 for summer, and RMSE = 3.69, MSE = 13.61, MAE = 3.63 for winter), respectively during model testing period (Figure 7.11). Moreover, a higher prediction error was found for those models during the training and testing periods. It can be seen from Figure 7.10 that the model performance has improved significantly during the testing period across the four domains over the study period. Compared to the temporal resolution of the WQI model, the lowest prediction error was found for the summer season across the four application domains. The MLR model's results are in line with the author's earlier research, which showed that the model performed better for predicting IEWQI scores during the winter (Uddin at al., 2022a; 2022b).

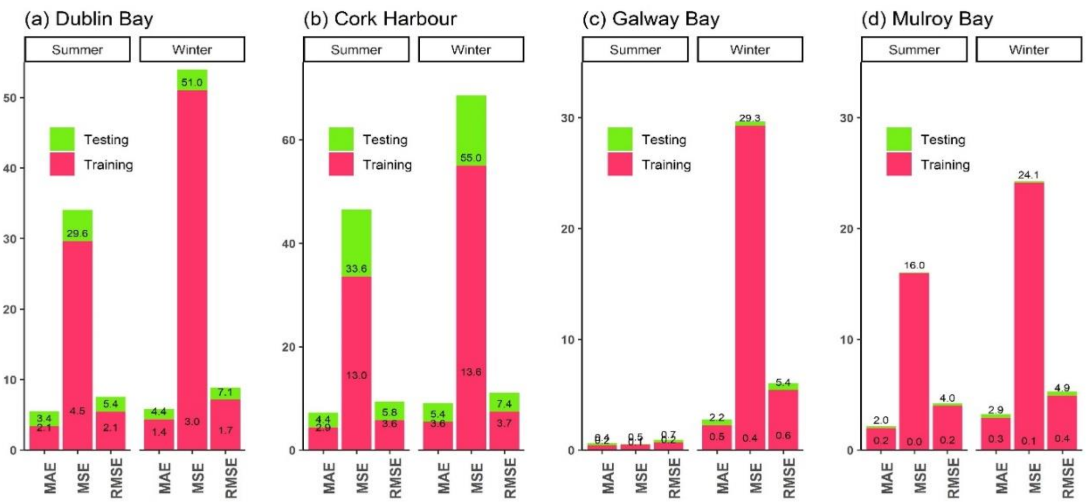


Figure 7.11. Comparison of model performance in predicting the IEWQI scores for four application domains using various statistical measures.

7.9.2 Comparison of IEWQI prediction results

Figure 8.8 shows the comparison results of WQI scores at each monitoring site across the four domains with a 95% confidence interval and a significant level of $p < 0.001$. Figure 7.7 (above) shows the summary statistics of actual and predicted WQI scores across various waterbodies over the study period. There was no significant difference between actual and predicted the WQI scores during both seasons (Figure 7.7). As can be seen from the figure 7.12 below, in Dublin Bay, the MLR predicted WQI score at each monitoring site accurately except for a single site during the summer season, whereas a relatively slight difference was found between the actual and predicted WQI score at most monitoring sites over the winter period (Figure 7.12a). In contrast to other domains, a significant difference was found between the actual and predicted WQI score at most monitoring sites in Cork Harbour during both the summer and winter seasons (Fig. 7.12b).

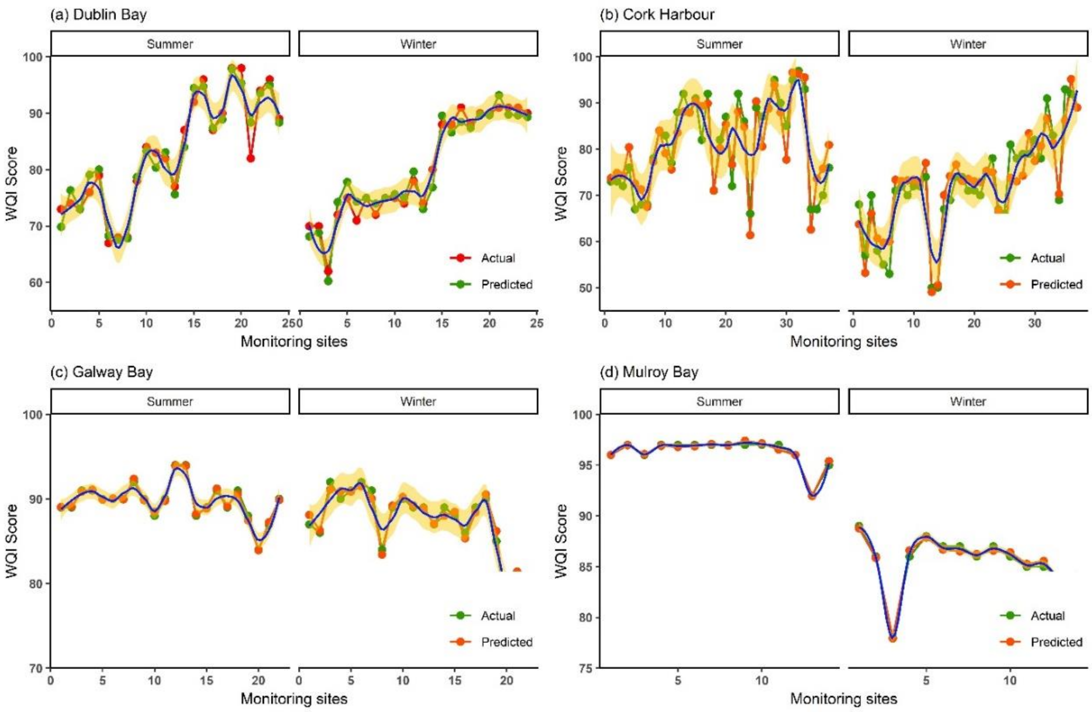


Figure 7.12. Point based comparison between actual and predicted IEWQI scores over the application domains with a 95% confidence interval at p <0.05, whereas the yellow shaded zone(s) indicates the uncertainty range of WQI scores.

As shown in the data in the figure, compared to the uncertainty interval at each site, higher uncertainty was found for the Cork Harbour during the summer season than in the winter period. During the summer, the MLR predicted WQI scores accurately at each monitoring site, whereas the model's prediction accuracy dropped during the winter period. Relatively, a slight difference was found between actual and predicted WQI scores with a higher uncertainty interval during the winter period (Figure 7.12c). On the other hand, in Mulroy Bay, from the data in figure 8d, the results indicate that there were no differences between actual and predicted WQI scores over both seasons (Figure 7.12d). The prediction results revealed that the IEWQI model assessed the water quality accurately in Mulroy Bay in terms of the uncertainty. The results of the point assessment show that the uncertainty interval could be useful for figuring out how much uncertainty may be contributed by the IEWQI model across various domains in terms of spatiotemporal resolution. However, the present study has found a lower level of uncertainty (≤ 2) in the final assessment of water quality across various domains. Details of the uncertainty results can be found in table 7.6 (below).

7.10 Model sensitivity results

For the purposes of sensitivity analysis of the IEWQI model in order to evaluate the model performance in terms of spatiotemporal resolution of various application domains, the present study utilized the coefficient of determination (R^2). Recently, several water research studies have used this technique to assess the model's sensitivity (Chaudhary and Hantush, 2017; Uddin et al., 2022a; 2022b). Commonly, it allows one to determine the relationship between model inputs (water quality indicators) and outputs (IEWQI score) using R^2 values. Its values range from 0 to1, with higher values, which are typically close to1, indicating the model's highest sensitivity to the input characteristics of the water quality of different domains. Figures 7.13 and 7.14 present the R^2 score for the IEWQI model across four application domains, respectively, for the summer and winter seasons. Based on the R^2 score, with the exception of the Cork Harbour, the highest sensitivity ($R^2 > 0.95$) was found for all domains during both seasons whereas relatively the lowest R2 was found for Cork Harbour during summer ($R^2 = 0.86$) and winter ($R^2 = 0.88$), respectively (Figure 7.12b; Figure 7.13b). The results of the R^2 values indicate that the IEWQI model is a good fit for assessing coastal water quality to any geospatial extent in Ireland with specific input attributes of water quality. Because in the majority of study cases, the IEWQI model can explain an average of 95% of input entities or the model converts all input attributes into the WQI score that presents the average of 95% of actual attributes of water quality indicators.

7.11 Model uncertainty results

In order to evaluate the IEWQI model uncertainty in assessing the coastal water quality, the present study utilized the inferential error bar technique with a 95%

confidence interval, whereas the t-statistics were used for validation of the results of the error bar analysis. Table 7.6 provides the results of t-statistics for the IEWQI model over the different domains, whereas figure 7.15 presents the uncertainty results of the IEWQI model for various application domains (mean WQI values of actual and predicted, standard error, and 95% confidence interval of actual and MLR predicted IEWQI scores). The results of t-statistics indicate that there were no significant differences between actual and predicted IEWQI scores over the four application domains during both the summer and winter seasons. Moreover, the results of error bar analysis also reveal that there were no significant differences between actual and predicted WQI scores across various application domains over the study period, with the exception of Cork Harbour and Dublin Bay.

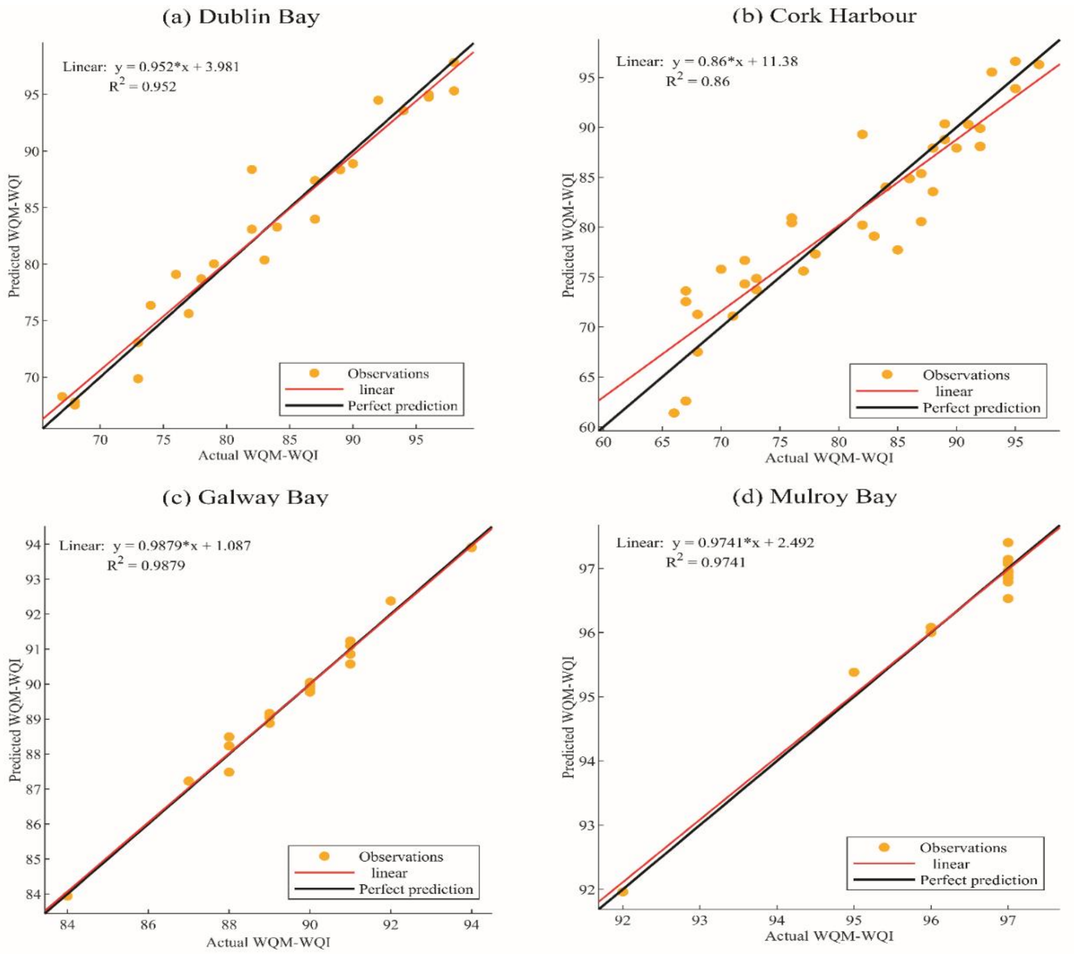


Figure 7.13. Relationship between actual and predicted IEWQI scores based on the testing datasets for four application domains over the summer season.

As shown in the figure below (figure 7.15), it can be seen clearly from the data that there was a slight difference in WQI score between actual and predicted scores during both seasons for both domains. Comparatively, the lowest standard error and standard deviation were found for Galway Bay and Mulroy Bay. The results of the uncertainty of the IEWQI model reflect the author's earlier studies (Uddin et al., 2022a; 2022c). However, the results of the t-statistics and error bar analysis indicate that the IEWQI model has no significant contribution to producing the uncertainty in the assessment of coastal water quality in terms of spatiotemporal resolution. Based on the uncertainty results, the proposed WQI model could be effective for assessing coastal water quality more accurately, and it can be used in any spatial domain with a high level of statistical confidence in terms of reducing model uncertainty.

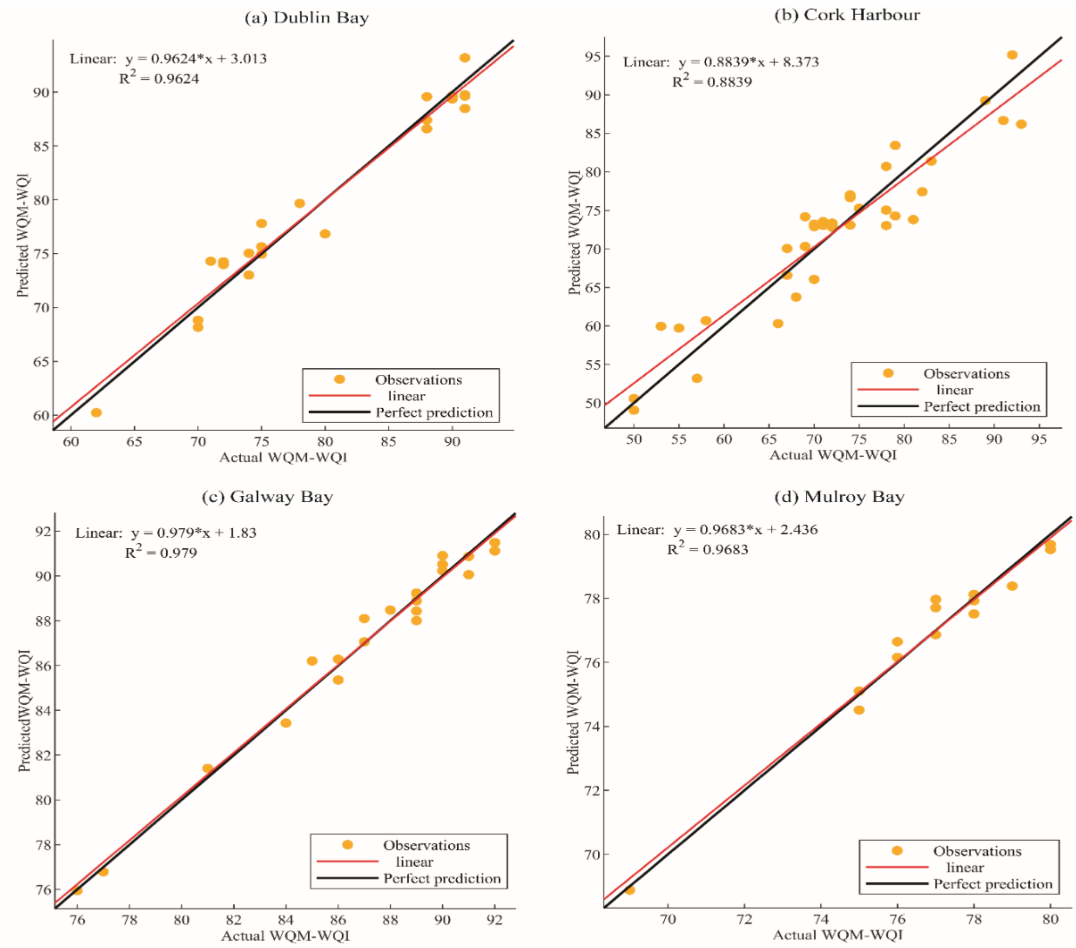


Figure 7.14. Relationship between actual and predicted IEWQI scores based on the testing datasets for four application domains over the winter season.

Table 7.6 t-statistics of IEWQI scores at p < 0 .000 across various domains over the study period.

Temporal resolution	t-statistics	Dublin Bay (df = 23)		Cork Harbour (df = 36)		Galway Bay (df = 21)		Mulroy Bay (df = 13)	
		Actual	Predicted	Actual	Predicted	Actual	Predicted	Actual	Predicted
Summer	t-value	41.34	42.36	50.71	57.68	193.09	194.27	260.54	263.98
	mean	82.95	82.96	81.30	81.29	89.77	89.77	96.28	96.28
	SE	2.00	1.95	1.60	1.48	0.46	0.46	0.40	0.36
	SD	9.83	9.59	9.75	9.04	2.18	2.17	1.38	1.36
Winter	t-value	43.32	44.15	40.64	43.23	93.55	94.54	104.45	124.73
	mean	80.04	80.04	72.11	72.11	87.18	87.18	76.78	85.08
	SE	1.84	1.81	1.77	1.67	0.93	0.92	0.74	0.68
	SD	9.05	8.88	10.79	10.15	4.37	4.32	2.75	2.56

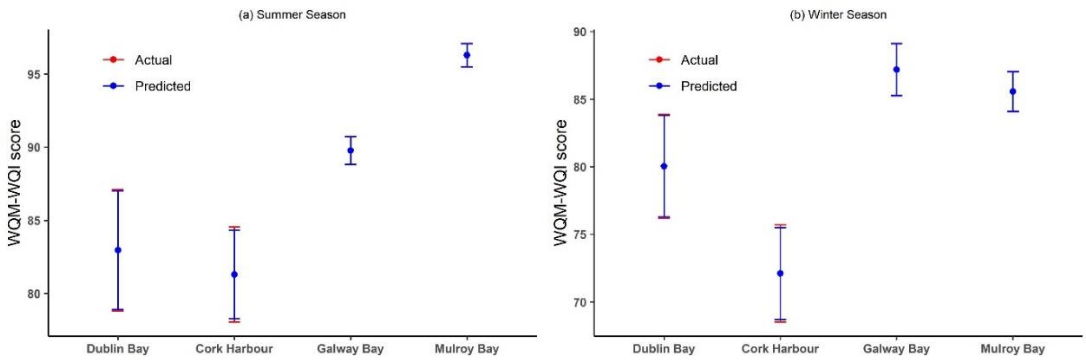


Figure 7.15**.** Statistical significance of IEWQI model uncertainty for various application domains with 95% confidence interval at < 0.005.

7.12 Model efficiency results

For the purposes of model efficiency analysis, the present study calculated the NSE and MEF using the actual and predicted IEWQI scores. Recently, a number of water research studies have utilized this tool to validate the model performance in terms of model efficiency (Guo et al., 2019; Izhar Shah et al., 2021; Jain and Sudheer, n.d.; Minh et al., 2022; Moriasi et al., 2015). Figure 7.16 shows the site-specific NSE and MSE results for the IEWQI model across the various application domains. Table 7.7 provides summary statistics of NSE and MEF over the study period. The site-specific results of the model efficiency reveal that a slight variation was found across the various domains during both the summer and winter seasons. According to the NSE and MSE values, the IEWQI model shows better performance across various application domains, with the exception of Cork Harbour (Figure 7.16) during both seasons. The model's efficiency was highest during the summer period when compared to its performance in terms of spatiotemporal resolution. In the case of each monitoring site assessment, the model was performed efficiently at each monitoring site across the application domains, whereas at a few monitoring sites the model showed poor performance.

In Dublin Bay, over the study periods, the model performed more efficiently at each monitoring site during both seasons, with the exception of the DB420 site. The model shows poor performance (NSE = - 0.28, and MEF = 1.13) at this point during the summer season. Relatively, higher NSE and MEF scores were calculated only for a few site-specific locations for the IEWQI model in Cork Harbour during both seasons. The results of NSE and MEF refer to the IEWQI model being over-fitted for predicting the WQI score in Cork Harbour. During both seasons, the models performed more efficiently at each monitoring site in both Galway Bay and Mulroy Bay, with the exception of the GY110 in Galway Bay and the MB050 in Mulroy Bay, respectively, during the winter period.

Table 7.7 Summary statistics of the IEWQI model efficiency for assessing transitional and coastal water quality across the various domains in Ireland.

Application domains	Summer				Winter			
	NSE		MEF		NSE		MEF	
	Min.	Max.	Min.	Max.	Min.	Max.	Min.	Max.
(i) Dublin bay	-0.28	1.00	0.00	1.13	0.00	0.99	0.00	1.00
(ii) Cork Harbour	-4.65	1.00	0.00	11.25	-4.83	17.90	0.00	2.41
(iii) Galway Bay	0.01	1.00	0.00	1.00	0.00	1.00	-0.78	0.92
(iv) Mulroy Bay	0.57	1.00	0.00	0.66	-3.87	1.52	0.00	1.51

However, the results of NSE and MEF reveal that, for the assessment of site-specific water quality, the IEWQI model was performed efficiently across all application domains, because the model can explain almost 95% of the variance for the actual water quality indicators in terms of their spatiotemporal resolution of various waterbodies. The results of the NSE of the present study are consistent with those of Guo et al., (2019) , who also applied this technique for assessing the impact of key factors on the temporal variation of water quality models.

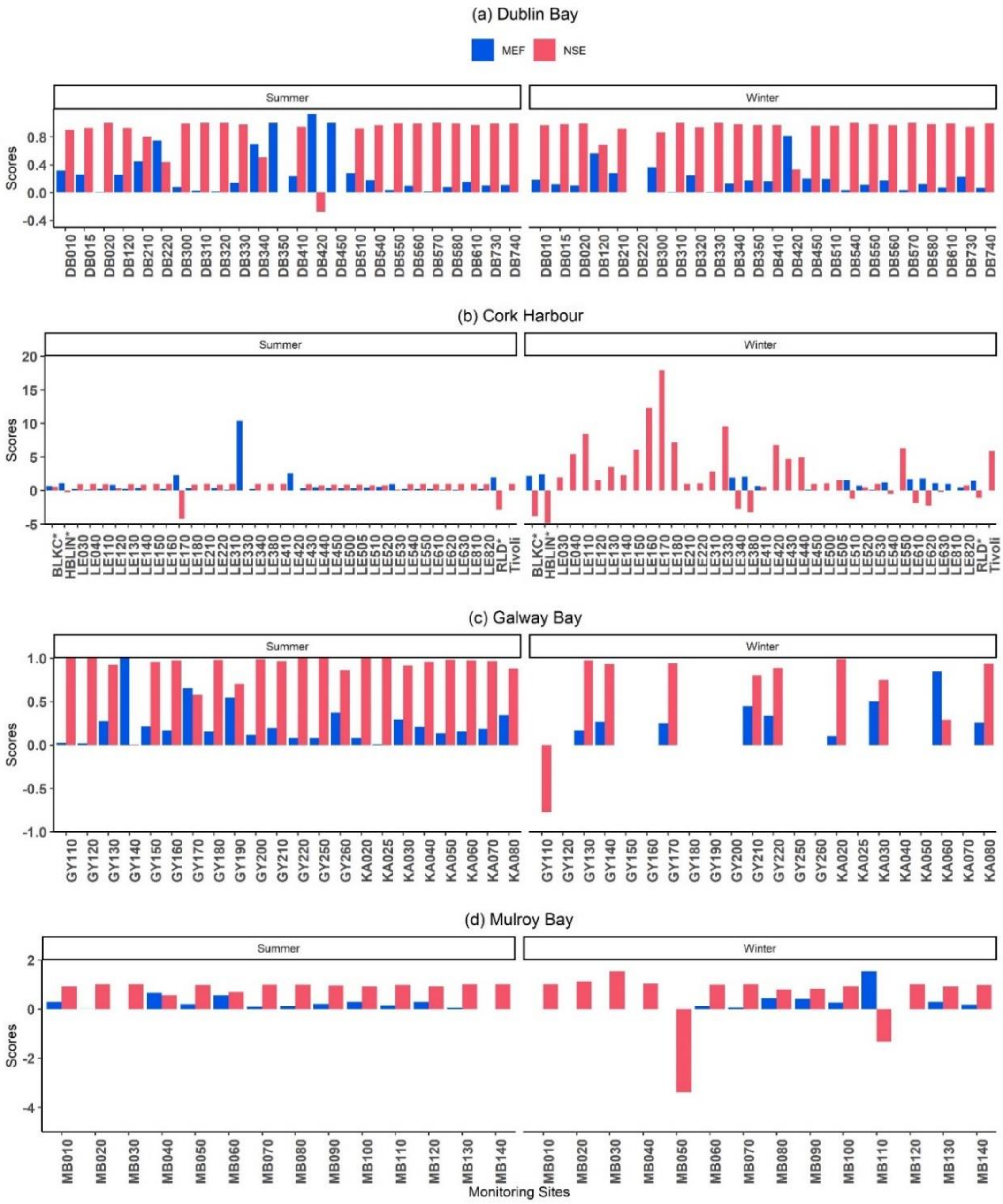


Figure 7.16. Results of the IEWQI model efficiency at each monitoring site across the different application domain in Ireland in terms of spatiotemporal resolution.

7.13 Assessment of water quality in Ireland

The ultimate goal of the IEWQI model is to assess and classify water quality using the specific classification scheme. For the classification of water quality, the present study used the improved classification scheme of Uddin et al., (2022a). Details of the classification are given in Table 7.2 above. Figure 7.17 presents a summary of the water quality status across the four application domains in Ireland. Details of the assessment results for each monitoring site in all domains can be found in Table 7.S2 to Table 7.S9 (Appendix 7), respectively, for Dublin Bay, Cork Harbour, Galway Bay, and Mulroy Bay. Figure 7.S2 and Figure 7.S3 present the water quality status at each monitoring site in terms of spatio-temporal resolution of water quality in various application domains. Table 7.S19 provides a comprehensive assessment of coastal and transitional water quality status over the various domains. The IEWQI model's results indicate that the two types of water quality dominated across the selected four domains through the study periods. From figure 7.17, it can be seen that water quality had "fair" and "good" classes across the domains during the summer and winter seasons.

There was a significant difference found between the summer and winter seasons in the water quality status across the domains. Relatively, most monitoring sites' water quality found "good" water quality during the summer season, whereas the quality degraded over the winter season across all domains (Figure 7.17). The IEWQI results indicated that the majority of monitoring sites' water quality status was "fair" through the winter season.

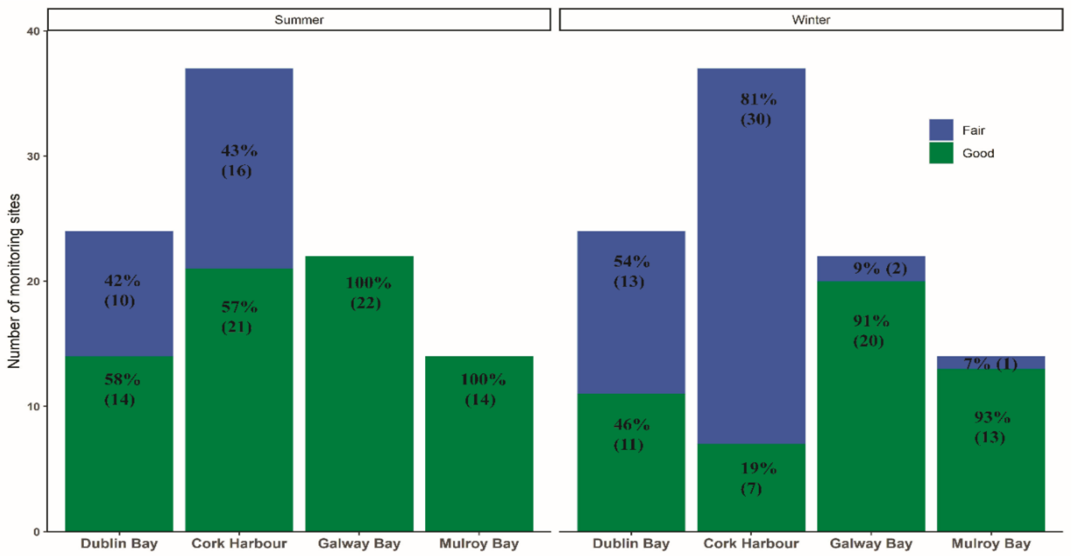


Figure 7.17. Statistical summary of water quality assessment results for four application domains over the study period.

Spatio-temporal variations of water quality and status at each monitoring site are presented in figures 7.S2 and 7.S3 (Appendix 7), respectively, for the summer and winter seasons across the application domains. There was a significant variation in water quality between summer and winter seasons across the application domains. Details of the results of the spatio-temporal assessment can be found in section 7.13.1

of the supplementary document as a continuation of section 7.13.

However, the IEWQI model results reflect actual scenarios of water quality across application domains under different pressures in the existing domain settings. Moreover. Moreover, the results of the present study are also in line with those of previous studies. The differences in water quality over the various domains between seasons may be due to the constituents of water quality indicators in terms of various factors like the geospatial setting of the domains, different pressures on water bodies etc.

7.14 Conclusion

An improved Irish Water Quality Index (IEWQI) model for assessing transitional and coastal waterbodies based on the legislation of Irish Water Guidelines was proposed. The developed model was tested in four identical waterbodies in Ireland to evaluate model performance by comparing the spatio-temporal attributes of various application domains, and model performance was analysis using three advanced statistical measures, including the coefficient of determination for sensitivity, inferential error analysis for uncertainty, and NSE and MEF for efficiency analysis, respectively. The key findings from the research are as follows:

(i) The sensitivity results of IEWQI indicate that the model outputs could be explained by more than 95% of the input entities, including less than 2% uncertainty with a 95% confidence interval at $p < 0.0001$.

(ii) The model performance validation results of NSE and MEF show that the IEWQI is superior for computing WQI scores at most monitoring sites across four application domains through the summer and winter periods.

(iii) All statistical measures of performance metrics also indicate that the IEWQI model is more effective for the prediction of WQI, whereas the lowest prediction errors were found during the testing phase for predicting WQI scores across four waterbodies during summer and winter.

(iv) The assessment results of water quality proved that the IEWQI model may be reliable for optimizing the model ambiguity and eclipsing problems.

(v) Moreover, the performance of IEWQI applications reveals that suggested indicators might be adequate and reliable to monitor the transitional and coastal waters with the improved model.

Although the present study was proposed the IEWQI model for transitional and coastal water quality, there is a high possibility that the IEWQI approach could be utilized to assess water quality in other waterbodies, particularly in rivers, lakes, and other bodies of water where saline water predominates. Despite the fact that the model was developed using water quality indicators for Cork Harbour, application results indicate that the IEWQI model could be used in any geospatial magnitude.

7.15 Declaration of competing interest

The authors confirm that they did not experience competing financial interests or personal interactions that could have had potential influences on this paper.

7.16 Acknowledgement

The authors gratefully acknowledge the editor's and anonymous reviewers' contributions to the improvement of this paper. This research was funded by the Hardiman Research Scholarship of the National University of Ireland Galway, which funded the first author as part of his PhD program. The authors would like to acknowledge support from MaREI, the SFI Research Center for Energy, Climate, and Marine research. The authors would like to thank the Environmental Protection Agency of Ireland for providing water quality data. The authors would also like to express their gratitude to Charles Sturt University for providing all necessary assistance to this PhD project through international co-supervision. The first author would like to sincerely thank Professor Azizur Rahman for his outstanding supervision support and methodological contributions to the PhD project. Moreover, the authors also sincerely acknowledge the Eco HydroInformatics Research Group (EHIRG), School of Engineering, College of Science and Engineering, University of Galway, Ireland, for providing computational laboratory facilities to complete this research.

7.17 References

Almeida, C., González, S.O., Mallea, M., González, P., 2012. A recreational water quality index using chemical, physical and microbiological parameters. Environmental Science and Pollution Research 19, 3400–3411. https://doi.org/10.1007/s11356-012-0865-5

Alphayo, S.M. and Sharma, M.P. (2018) Water Quality Assessment of Ruvu River in Tanzania Using NSFWQI. Journal of Scientific Research and Reports 20(3), 1-9.

Asadollah, S.B.H.S., Sharafati, A., Motta, D., Yaseen, Z.M., 2021. River water quality index prediction and uncertainty analysis: A comparative study of machine learning models. J Environ Chem Eng 9, 104599. https://doi.org/10.1016/j.jece.2020.104599

Barr, A., Mcelroy, E., 2019. WATER QUALIY RISK ASSESSMENT RPS Dublin Port Company Daniel Hogan Senior Scientist-Water Environment and Flood Risk Management WATER QUALIY RISK ASSESSMENT.

Bordalo, A.A., Teixeira, R. and Wiebe, W.J. (2006) A water quality index applied to an international shared river basin: The case of the Douro River. Environmental Management 38(6), 910-920.

Carsten Von Der Ohe, P., Prüß, A., Schäfer, R.B., Liess, M., de Deckere, E., Brack, W., 2007. Water quality indices across Europe - A comparison of the good ecological status of five river basins. Journal of Environmental Monitoring 9, 970–978. https://doi.org/10.1039/b704699p

Chaudhary, A., Hantush, M.M., 2017. Bayesian Monte Carlo and maximum likelihood approach for uncertainty estimation and risk management: Application to lake oxygen recovery model. Water Res 108, 301–311. https://doi.org/10.1016/j.watres.2016.11.012

Commowick, O., Warfield, S.K., 2010. Estimation of inferential uncertainty in assessing expert segmentation performance from STAPLE. IEEE Trans Med Imaging 29, 771–780. https://doi.org/10.1109/TMI.2009.2036011

Cumming, G., Fidler, F., Vaux, D.L., 2007. Error bars in experimental biology. Journal of Cell Biology 177, 7–11. https://doi.org/10.1083/jcb.200611141

Cumming, G., Finch, S., 2005. Inference by eye confidence intervals and how to read pictures of data. American Psychologist 60, 170–180. https://doi.org/10.1037/0003-066X.60.2.170

Cude, C.G. (2001) Oregon water quality index: A tool for evaluating water quality management effectiveness. Journal Of The American Water Resources Association.

Dadolahi-Sohrab, A., Arjomand, F., Fadaei-Nasab, M., 2012. Water quality index as a simple indicator of watersheds pollution in southwestern part of Iran. Water and Environment Journal 26, 445–454. https://doi.org/10.1111/j.1747-6593.2011.00303.x

de Rosemond, S., Duro, D.C. and Dubé, M. (2009) Comparative analysis of regional water quality in Canada using the Water Quality Index. Environmental Monitoring and Assessment 156(1-4), 223-240.

DUBLIN PORT COMPANY, 2021. DUBLIN PORT COMPANY.

Donnelly, M., 2017. An Investigation into Water Quality and the Ecological Status of the Canal System Present in Galway City, in Addition to the concentrations of Heavy Metals Present in the Claddagh Basin and Eglinton Canal.

Environmental Protection Agency, 2021. Bathing Water Quality in Ireland A report for the year 2021. 2021.

Environmental Protection Agency, 2020. Bathing Water Quality in Ireland.

Fathi, P., Ebrahimi Dorche, E., Zare Shahraki, M., Stribling, J., Beyraghdar Kashkooli, O., Esmaeili Ofogh, A. and Bruder, A. (2022) Revised Iranian Water Quality Index (RIWQI): a tool for the assessment and management of water quality in Iran. Environmental Monitoring and Assessment 194(7), 504.

Geurts, P., Ernst, D., Wehenkel, L., 2006. Extremely randomized trees. Mach Learn 63, 3–42. https://doi.org/10.1007/s10994-006-6226-1

Guo, D., Lintern, A., Webb, J.A., Ryu, D., Liu, S., Bende-Michl, U., Leahy, P., Wilson, P., Western, A.W., 2019. Key Factors Affecting Temporal Variability in Stream Water Quality. Water Resour Res 55, 112–129. https://doi.org/10.1029/2018WR023370

Guo, Q., Wu, W., Massart, D.L., Boucon, C., de Jong, S., 2002. Feature selection in principal component analysis of analytical data. Chemometrics and Intelligent Laboratory Systems 61, 123–132. https://doi.org/10.1016/S0169-7439(01)00203-9

Gradilla-Hernández, M.S., de Anda, J., Garcia-Gonzalez, A., Montes, C.Y., Barrios-Piña, H., Ruiz-Palomino, P. and Díaz-Vázquez, D. (2020) Assessment of the water quality of a subtropical lake using the NSF-WQI and a newly proposed ecosystem specific water quality index. Environmental Monitoring and Assessment 192(5), 296.

Gupta, A.K., Gupta, S.K. and Patil, R.S. (2003) A comparison of water quality indices for coastal water. Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering 38(11), 2711-2725.

Gupta, S., Gupta, S.K., 2021. A critical review on water quality index tool: Genesis, evolution and future directions. Ecol Inform 63. https://doi.org/10.1016/j.ecoinf.2021.101299

Hartnett, M., Nash, S., 2015. An integrated measurement and modeling methodology for estuarine water quality management. Water Science and Engineering 8, 9–19. https://doi.org/10.1016/j.wse.2014.10.001
Horton, R.K., 1965. An index-number system for rating water quality. J. Water Pollut. Control Fed. 37, 300–306. https://doi.org/10.2307/25035251
House, M.A., 1990. Water Quality Indices as Indicators of Ecosystem Changes. Environmental Monitoring and Assessment 15: 15, 255–263. https://doi.org/10.1007/BF00394892
House, M.A., 1980. A water quality index for rivers. Water Int 5, 16–21. https://doi.org/10.1080/02508068008685872
Huan, J., Li, H., Li, M., Chen, B., 2020. Prediction of dissolved oxygen in aquaculture based on gradient boosting decision tree and long short-term memory network: A study of Chang Zhou fishery demonstration base, China. Comput Electron Agric 175, 105530. https://doi.org/10.1016/j.compag.2020.105530
Ibrahim, S., Nazir, S., Velastin, S.A., 2021. Feature selection using correlation analysis and principal component analysis for accurate breast cancer diagnosis. J Imaging 7. https://doi.org/10.3390/jimaging7110225
Islam Khan, M.S., Islam, N., Uddin, J., Islam, S., Nasir, M.K., 2022. Water quality prediction and classification based on principal component regression and gradient boosting classifier approach. Journal of King Saud University - Computer and Information Sciences 34, 4773–4781. https://doi.org/10.1016/J.JKSUCI.2021.06.003
Islam Khan, M.S., Islam, N., Uddin, J., Islam, S., Nasir, M.K., 2021. Water quality prediction and classification based on principal component regression and gradient boosting classifier approach. Journal of King Saud University - Computer and Information Sciences. https://doi.org/10.1016/j.jksuci.2021.06.003
Izhar Shah, M., Alaloul, W.S., Alqahtani, A., Aldrees, A., Ali Musarat, M., Javed, M.F., 2021. Predictive modeling approach for surface water quality: Development and comparison of machine learning models. Sustainability (Switzerland) 13. https://doi.org/10.3390/su13147515
Jain, S.K., Sudheer, K.P., n.d. Fitting of Hydrologic Models: A Close Look at the Nash-Sutcliffe Index. https://doi.org/10.1061/ASCE1084-0699200813:10981
Jolliffe, I.T., 2007. Uncertainty and inference for verification measures. Weather Forecast. https://doi.org/10.1175/WAF989.1
Jha, D.K., Devi, M.P., Vidyalakshmi, R., Brindha, B., Vinithkumar, N.V. and Kirubagaran, R. (2015) Water quality assessment using water quality index and geographical information system methods in the coastal waters of Andaman Sea, India. Marine Pollution Bulletin.
Jiang, J., Tang, S., Han, D., Fu, G., Solomatine, D., Zheng, Y., 2020. A comprehensive review on the design and optimization of surface water quality monitoring networks. Environmental Modelling and Software 132, 104792. https://doi.org/10.1016/j.envsoft.2020.104792
Krueger, T., 2017. Bayesian inference of uncertainty in freshwater quality caused by low-resolution monitoring. Water Res 115, 138–148. https://doi.org/10.1016/j.watres.2017.02.061
Kumar, S., Chong, I., 2018. Correlation analysis to identify the effective data in machine learning: Prediction of depressive disorder and emotion states. Int J Environ Res Public Health 15. https://doi.org/10.3390/ijerph15122907
Liang, S., Jia, H., Xu, C., Xu, T., Melching, C., 2016. A Bayesian approach for evaluation of the effect of water quality model parameter uncertainty on TMDLs: A case study of Miyun Reservoir. Science of the Total Environment 560–561, 44–54. https://doi.org/10.1016/j.scitotenv.2016.04.001
Liou, S.M., Lo, S.L., Wang, S.H., 2004. A generalized water quality index for Taiwan. Environ Monit Assess 96, 35–52. https://doi.org/10.1023/B:EMAS.0000031715.83752.a1
Latinopoulos, D., Spiliotis, M., Ntislidou, C., Kagalou, I., Bobori, D., Tsiaoussi, V. and Lazaridou, M. (2021) “One Out–All Out” Principle in the Water Framework Directive 2000—A New Approach with Fuzzy Method on an Example of Greek Lakes.
Liou, S.M., Lo, S.L. and Wang, S.H. (2004) A generalized water quality index for Taiwan. Environmental Monitoring and Assessment 96(1-3), 35-52.
Li, Q., Liu, A., Yu, K., Yu, K.F., 2009. A weighted rank-sum procedure for comparing samples with multiple endpoints. Stat Interface 2, 197–201. https://doi.org/10.4310/sii.2009.v2.n2.a9
Ma, Z., Li, H., Ye, Z., Wen, J., Hu, Y. and Liu, Y. (2020) Application of modified water quality index (WQI) in the assessment of coastal water quality in main aquaculture areas of Dalian, China. Marine Pollution Bulletin 157(May).
McCuen, R.H., Knight, Z., Cutter, A.G., 2006a. Evaluation of the Nash–Sutcliffe Efficiency Index. J Hydrol Eng 11, 597–602. https://doi.org/10.1061/(asce)1084-0699(2006)11:6(597)

McCuen, R.H., Knight, Z., Cutter, A.G., 2006b. Evaluation of the Nash–Sutcliffe Efficiency Index. J Hydrol Eng 11, 597–602. https://doi.org/10.1061/(ASCE)1084-0699(2006)11:6(597)
McManus, S., Rahman, A., Horta, A., Coombes, J., 2020. Applied Bayesian Modeling for Assessment of Interpretation Uncertainty in Spatial Domains. Statistics for Data Science and Policy Analysis 3–13. https://doi.org/10.1007/978-981-15-1735-8_1
Minh, H.V.T., Tri, V.P.D., Ut, V.N., Avtar, R., Kumar, P., Dang, T.T.T., Hoa, A. van, Ty, T. van, Downes, N.K., 2022. A Model-Based Approach for Improving Surface Water Quality Management in Aquaculture using MIKE 11: A Case of the Long Xuyen Quadangle, Mekong Delta, Vietnam. Water (Switzerland) 14. https://doi.org/10.3390/w14030412
Misaghi, F., Delgosha, F., Razzaghmanesh, M. and Myers, B. (2017) Introducing a water quality index for assessing water for irrigation purposes: A case study of the Ghezel Ozan River. Science of The Total Environment 589, 107-116.
Mladenović-Ranisavljević, I.I., Žerajić, S.A., 2018. Comparison of different models of water quality index in the assessment of surface water quality. International Journal of Environmental Science and Technology 15, 665–674. https://doi.org/10.1007/s13762-017-1426-8
Moriasi, D.N., Gitau, M.W., Pai, N., Daggupati, P., 2015. Hydrologic and water quality models: Performance measures and evaluation criteria. Trans ASABE 58, 1763–1785. https://doi.org/10.13031/trans.58.10715
Naghibi, S.A., Hashemi, H., Berndtsson, R., Lee, S., 2020. Application of extreme gradient boosting and parallel random forest algorithms for assessing groundwater spring potential using DEM-derived factors. J Hydrol (Amst) 589, 125197. https://doi.org/10.1016/j.jhydrol.2020.125197
Neary, B., Cash, K., Hebert, S., Khan, H., Saffran, K., Swain, L., Williamson, D., 2001. Canadian Water Quality Guidelines for the Protection of Aquatic Life CCME Water Quality Index 1.0 Technical Report. Canadian Council of Ministers of the Environment.
News Releases 2022 | Environmental Protection Agency [WWW Document], n.d. URL https://www.epa.ie/news-releases/news-releases-2022/78-of-irelands-bathing-sites-have-excellent-water-quality-.php (accessed 9.22.22).
Odu, G.O., 2019. Weighting methods for multi-criteria decision making technique. Journal of Applied Sciences and Environmental Management 23, 1449. https://doi.org/10.4314/jasem.v23i8.7
Parween, S., Siddique, N.A., Mahammad Diganta, M.T., Olbert, A.I., Uddin, Md.G., 2022. Assessment of urban river water quality using modified NSF water quality index model at Siliguri city, West Bengal, India. Environmental and Sustainability Indicators 16, 100202. https://doi.org/10.1016/j.indic.2022.100202
Prato, S., La Valle, P., De Luca, E., Lattanzi, L., Migliore, G., Morgana, J.G., Munari, C., Nicoletti, L., Izzo, G. and Mistri, M. (2014) The "one-out, all-out" principle entails the risk of imposing unnecessary restoration costs: A study case in two Mediterranean coastal lakes. Marine Pollution Bulletin 80(1), 30-40.
Roszkowska, E., 2013. Rank Ordering Criteria Weighting Methods – a Comparative Overview. Optimum. Studia Ekonomiczne 5, 14–33. https://doi.org/10.15290/ose.2013.05.65.02
Said, A., Stevens, D.K., Sehlke, G., 2004. An innovative index for evaluating water quality in streams. Environ Manage. https://doi.org/10.1007/s00267-004-0210-y
Seifi, A., Dehghani, M., Singh, V.P., 2020. Uncertainty analysis of water quality index (WQI) for groundwater quality evaluation: Application of Monte-Carlo method for weight allocation. Ecol Indic 117. https://doi.org/10.1016/j.ecolind.2020.106653
Sharif, O., Hasan, M.Z., Rahman, A., 2022. Determining an effective short term COVID-19 prediction model in ASEAN countries. Sci Rep 12, 1–11. https://doi.org/10.1038/s41598-022-08486-5
Singh, P.K., Panigrahy, B.P., Verma, P., 2018. Evaluation of the Surface Water Quality Index of Jharia Coal Mining Region and Its Management of Surface Water Resources, in: Environmental Pollution. Springer Nature Singapore Pte Ltd.2018, pp. 429–437. https://doi.org/10.1007/978-981-10-5792-2_34
Sim, S.F., Ling, T.Y., Lau, S. and Jaafar, M.Z. (2015) A novel computer-aided multivariate water quality index. Environ Monit Assess 187(4), 181-181.
Smith, D.G., 1990. A better water quality indexing system for rivers and streams. Water Res. https://doi.org/10.1016/0043-1354(90)90047-A
Strobl, R.O., Robillard, P.D., 2008. Network design for water quality monitoring of surface freshwaters: A review. J Environ Manage 87, 639–648. https://doi.org/10.1016/j.jenvman.2007.03.001
Song, B., Kang, S., 2016. A Method of Assigning Weights Using a Ranking and Nonhierarchy Comparison. Advances in Decision Sciences 2016. https://doi.org/10.1155/2016/8963214

Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2018. Development of a water quality index for rivers in West Java Province, Indonesia. Ecol Indic 85, 966–982. https://doi.org/10.1016/j.ecolind.2017.11.049

Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2017. Using the Analytic Hierarchy Process to identify parameter weights for developing a water quality index. Ecol Indic 75, 220–233. https://doi.org/10.1016/j.ecolind.2016.12.043

Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2016. Development of river water quality indices—a review. Environ Monit Assess. https://doi.org/10.1007/s10661-015-5050-0

Tao, X.-F., Huang, T., Li, X.-F., Peng, D.-P., 2016. Application of a PCA based water quality classification method in water quality assessment in the Tongjiyan Irrigation Area, China 118–125. https://doi.org/10.2991/iceep-16.2016.20

Thi Minh Hanh, P., Sthiannopkao, S., The Ba, D., Kim, K.-W., 2010. Development of Water Quality Indexes to Identify Pollutants in Vietnam’s Surface Water. Journal of Environmental Engineering. https://doi.org/10.1061/(asce)ee.1943-7870.0000314

Toner, P., Bowman, J., Clabby, K., Lucey, J., Mc, McGarrigle, M., Concannon, C., Clenaghan, C., Cunningham, P., J., D., O’Boyle, S., MacCárthaigh, M., Craig, M., Quinn, R., 2005. Water Quality in Ireland 2001-2003.

Tomas, D., Čurlin, M. and Marić, A.S. (2017) Assessing the surface water status in Pannonian ecoregion by the water quality index model. Ecological Indicators 79(April), 182-190.

Touzani, S., Granderson, J., Fernandes, S., 2018. Gradient boosting machine for modeling the energy consumption of commercial buildings. Energy Build 158, 1533–1543. https://doi.org/10.1016/j.enbuild.2017.11.039

Trodd, W., Shane, O., 2018. Water quality in Ireland: an indicators report 1–66.

Uddin, Md.G., Moniruzzaman, Md., Khan, M., 2017. Evaluation of Groundwater Quality Using CCME Water Quality Index in the Rooppur Nuclear Power Plant Area, Ishwardi, Pabna, Bangladesh. American Journal of Environmental Protection. https://doi.org/10.12691/env-5-2-2

Uddin, M.G., Moniruzzaman, M., Quader, M.A., Hasan, M.A., 2018. Spatial variability in the distribution of trace metals in groundwater around the Rooppur nuclear power plant in Ishwardi, Bangladesh. Groundw Sustain Dev 7. https://doi.org/10.1016/j.gsd.2018.06.002

Uddin, M.G., Olbert, A.I., Nash, S., 2020a. Assessment of water quality using Water Quality Index (WQI) models and advanced geostatistical technique, in: Civil Engineering Research Association of Ireland (CERAI). Civil Engineering Research Association of Ireland (CERAI), Cork Institute of Technology, Cork, pp. 594–599.

Uddin, M.G., Stephen Nash, Olbert, A.I., 2020b. Application of Water Quality Index Models to an Irish Estuary, in: Civil and Environmental Research. Civil Engineering Research Association of Ireland (CERAI), pp. 576–581.

Uddin, G., Nash, S., Olbert, A.I., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol Indic 122, 107218. https://doi.org/10.1016/j.ecolind.2020.107218

Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022a. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment. Water Res 219, 118532. https://doi.org/10.1016/j.watres.2022.118532

Uddin, Md.G., Nash, S., Talas, M., Diganta, M., Rahman, A., Olbert, A.I., 2022b. Robust machine learning algorithms for predicting coastal water quality index, Journal of Environmental Management. https://doi.org/https://doi.org/10.1016/j.jenvman.2022.115923

Uddin, Md.G., Nash, S., Rahman, A., Olbert, A.I., 2022c. A novel approach for estimating and predicting uncertainty in water quality index model using machine learning approaches.

Uddin, G., Nash, S., Rahman, A., Olbert, A.I., 2022d. Assessing optimization techniques for improving water quality model.

Uddin, MD.G., Nash, S., Rahman, A., Olbert, A.I., 2022e. Performance Analysis of the Water Quality Index Model for Classification of Coastal Water Quality Using Machine Learning Techniques. SSRN Electronic Journal. https://doi.org/10.2139/ssrn.4197032

Uddin, G., Nash, S., Olbert, A.I., 2022f. Optimization of Parameters in a Water Quality Index Model using Principal Component Analysis, in: Proceedings of the 39th IAHR World Congress. Proceedings of the 39th IAHR World Congress.

Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022g. Development of a water quality index model - a comparative analysis of various weighting methods, in: Çiner, Prof.Dr.A. (Ed.), Mediterranean Geosciences Union Annual Meeting (MedGU-21). Spinger, Istanbul, pp. 1–6.

Vergara, J.R., Estévez, P.A., 2014. A review of feature selection methods based on mutual information. Neural Comput Appl 24, 175–186. https://doi.org/10.1007/s00521-013-1368-0

Wall, B., Cahalane, A., Derham, J., 2020. Ireland's Environment - An Integrated Assessment.

Zaghloul, M.S., Achari, G., 2022. Application of machine learning techniques to model a full-scale wastewater treatment plant with biological nutrient removal. J Environ Chem Eng 10, 107430. https://doi.org/10.1016/j.jece.2022.107430

Zotou, I., Tsihrintzis, V.A. and Gikas, G.D. (2019) Performance of Seven Water Quality Indices (WQIs) in a Mediterranean River. Environmental Monitoring and Assessment 191(8).

Zotou, I., Tsihrintzis, V.A., Gikas, G.D., 2018. Comparative Assessment of Various Water Quality Indices (WQIs) in Polyphytos Reservoir-Aliakmon River, Greece. Proc West Mark Ed Assoc Conf 2, 611. https://doi.org/10.3390/proceedings2110611

8. Robust machine learning algorithms for predicting coastal water quality index

This chapter was published in the **"Journal of Environmental Management"** on August 19, 2022. Details can be found at the following web resource:
https://doi.org/10.1016/j.jenvman.2022.115923

8.1 Chapter highlights

- The research utilized eight widely used ML algorithms to determine the most reliable and robust ML algorithm(s) to anticipate WQIs at each monitoring point instead of repeatedly employing SI and weight values in order to reduce model uncertainty.
- Develop a robust algorithm with optimized hyperparameters for predicting the newly developed weighted quadratic mean (WQM) WQI model for assessing coastal water quality most accurately at each monitoring site in Cork Harbour, Ireland.
- For the purposes of the model performance analysis, a range of statistical measures were utilized.
- Tree based algorithms, the DT, ExT, XGB, and RF models, showed excellent performance, respectively, in order to predict the WQM-WQI score.
- A higher percent of relative index prediction errors was found for the SVM models (+22.7 to −75).
- Compared to the other algorithms in terms of the model overfitting problem, the XGB showed the best outperformance for predicting WQI scores at each monitoring site, whereas the lowest training (RMSE = 3.3, MSE = 10.91, MAE = 1.67, and R2 = 1.0) and testing (RMSE = 0.0, MSE = 0.0, MAE = 0.02, and R2 = 1.0) errors were found, respectively.
- Based on the uncertainty results, relatively higher prediction uncertainty was found at the upper monitoring sites in Cork Harbour.
- The results of this research could be effective in developing the prediction model for assessing coastal water quality using the new WQI approach, which may be helpful for improving the water monitoring program.

8.2 Abstract

Coastal water quality assessment is an essential task to keep "good water quality" status for living organisms in coastal ecosystems. The Water quality index (WQI) is a widely used tool to assess water quality but this technique has received much criticism due to the model's reliability and inconsistence. The present study used a recently developed improved WQI model for calculating coastal WQIs in Cork Harbour. The aim of the research is to determine the most reliable and robust machine learning (ML) algorithm(s) to anticipate WQIs at each monitoring point instead of repeatedly employing SI and weight values in order to reduce model uncertainty. In this study, we compared eight commonly used algorithms, including Random Forest (RF), Decision Tree (DT), K-Nearest Neighbors (KNN), Extreme Gradient Boosting (XGB), Extra Tree (ExT), Support Vector Machine (SVM), Linear Regression (LR), and Gaussian Naïve Bayes (GNB). For the purposes of developing the prediction models, the dataset was divided into two groups: training (70%) and testing (30%), whereas the models were validated using the 10-fold cross-validation method. In order to evaluate the models' performance, the RMSE, MSE, MAE, R^2, and PREI metrics were used in this study. The tree-based DT (RMSE = 0.0, MSE = 0.0, MAE = 0.0, R^2 =1.0 and PERI = 0.0) and the ExT (RMSE = 0.0, MSE = 0.0, MAE = 0.0, R^2 =1.0 and PERI = 0.0) and ensemble tree-based XGB (RMSE = 0.0, MSE = 0.0, MAE = 0.0, R^2 = 1.0 and PERI = +0.16 to -0.17) and RF (RMSE = 2.0, MSE = 3.80, MAE = 1.10, R^2 = 0.98, PERI = +3.52 to -25.38) models outperformed other models. The results of model performance and PREI indicate that the DT, ExT, and GXB models could be effective, robust and significantly reduce model uncertainty in predicting WQIs. The findings of this study are also useful for reducing model uncertainty and optimizing the WQM-WQI model architecture for predicting WQI values.

Keywords: Robust machine learning algorithms; Coastal Water quality Index model; Coastal water quality; Uncertainty, Cork Harbour

8.3 Introduction

In any aquatic ecosystem, freshwater is an important bio-indicator for living organisms and therefore, the new challenge for the world's future is to maintain "good water quality status”. Recently a few studies have revealed that around 50 marine species including 48 fish species, crustaceans, shellfish, and five types of seaweed living in Irish waters are under threat of extinction due to the water quality and functional changes of habitat of aquatic system (Fogarty P., 2017). Water quality deteriorates over time due to a variety of factors, one of which is human intervention. Industrialization and urbanization have accelerated day by day to ensure a better quality of life. As a consequence, freshwater consumption has significantly increased over many decades (Gikas et al., 2020; Uddin et al., 2018). Therefore, both anthropogenic and natural events have gradually accumulated, resulting in fast degradation of surface and groundwater quality (Aschonitis et al., 2012; Uddin et al., 2021, 2020).

Water resources management is a critical process involving various components, including institutional framework, skilled labour, legislation, financial freedom and resource availability. Several countries have formulated management and action plans to maintain their good water quality. However, due to resource availability, they face a few common problems in implementing or adopting the management program. In Europe, Water Framework Directive (WFD) is an effective tool for managing water and its ecosystem (Uddin et al., 2022). It recommended adopting the monitoring program to investigate water quality by all member states as already; many countries have been suffering its challenges and trying to overcome that issue (Zotou et al., 2020).

Thus far, several tools and techniques have been developed for assessing water quality. The water quality index is one of them. Recently, this technique has been extensively used to evaluate water quality. Its application has increased rapidly due to its ability to convert a vast amount of water quality information into a unitless numerical expression using simple mathematical functions. Commonly, this technique consists of four crucial elements: (i) selecting water quality indicator; (ii) sub-index process; (iii) weighting of water quality indicators; and (iv) aggregation function. Further details of the WQI models and their uses are available in the literature (e.g., Uddin et al., 2021). Recently, several studies have revealed that the WQI model produced considerable uncertainty in its modeling process (Abbasi and Abbasi, 2012; Juwana et al., 2016; Rezaie-Balf et al., 2020; Sutadian et al., 2016; Uddin et al., 2021). As a result, the WQI model does not reflect accurate water quality attributes. Many researchers have proposed a range of modified WQIs for optimizing this issue, but unfortunately, several recent studies have revealed that those models have experienced similar problems (Abbasi and Abbasi, 2011; Chang et al., 2020; Smith, 1990; Stoner, 1978; Yan et al., 2016).

Also, this method is much more sensitive to eclipsing and ambiguity problems. The "eclipsing" problem can be occurred due to inappropriate sub-indexing rules, parameter weightings, or inappropriate aggregation functions that do not reflect the real information of water quality (Sutadian et al., 2016; Uddin et al., 2021). Recently, a few studies have revealed that the "eclipsing" problem occurs due to overestimation of the WQI index by the aggregation function (Uddin et al., (2022). Like eclipsing, ambiguity is another important source of the WQI model uncertainty. It hides the actual water quality information by underestimation and overestimation of WQI values (Uddin et al, 2021; 2022). Details of the eclipsing and ambiguity problems discussed by Uddin et al., 2022. In the WQI model, several studies have considered the effects of ambiguity and eclipsing issues of sub-index and aggregation functions (Smith, 1990; Abbasi and Abbasi, 2012). Details of the ambiguity and eclipsing problems, sources and impact on WQI model of them can be found in Uddin et al. (2022). To determine their effects, Uddin et al. (2022) compared eight WQI models (four weighted and four unweighted) to evaluate the ambiguity and eclipsing problems for assessing coastal water quality in his study. This study recommended that the WQM-WQI model could be effective and reliable for assessing coastal water quality in terms of reducing uncertainty in the WQI model.

Due to the inconsistency of existing WQI techniques, a few researchers have recently used the ML technique to reduce model uncertainty and attempt to predict WQIs accurately (Babbar and Babbar, 2017; Bui et al., 2020; Gao et al., 2020; Hassan et al., 2021; Kouadri et al., 2021; Rezaie-Balf et al., 2020; Wang et al., 2017). Several studies have applied a variety of ML algorithms such as extreme gradient boosting, Naïve Bayes, support vector machine, random forest, and decision tree algorithms for the comparison of algorithms performance in order to predict WQIs correctly (Ahmad et al., 2017; Bui et al., 2020; Deng et al., 2022; Khan and See, 2016; Leong et al., 2019; Othman et al., 2020) . A summary of the various ML techniques in predicting water quality is provided in Appendix (a). Bui et al. (2020) compare sixteen algorithms to identify the robust model for predicting WQIs accurately. They suggest that tree-based algorithms are practical for predicting WQIs. Some studies recommend that ensemble tree-based algorithms such as extreme gradient boosting (XGB) and random forest (RF) are potentially useful for predicting WQIs (Grbčić et al., 2021; Haghiabi et al., 2018; Khan et al., 2021; Khullar and Singh, 2021). Moreover, researchers successfully applied AI-based algorithms like support vector machine (SVM), least square SVM (LSVM) and artificial neural network for predicting WQIs (Aldhyani et al., 2020; Haghiabi et al., 2018; Pham et al., 2019; Prasad et al., 2022; Wu and Wang, 2022). However, most studies have focused on the river/lake or groundwater quality index utilizing the existing WQI models while most studies have been carried out on only the prediction of WQIs, no studies have been found to improve the WQI model architecture. Compared to other studies, the present research widely explores, for the first time, to improve the newly developed WQM-WQI model architecture using ML techniques in order to reduce the model uncertainity.

This study aims to identify the robust ML algorithm with optimizing the hyperparameters for predicting WQIs correctly at each monitoring site in Cork Harbour, Ireland, comparing eight widely used ML algorithms Decision Tree (DT), Extra Tree (ExT), Extreme Gradient Boosting (XGB), Random Forest (RF), Support Vector Machine (SVM), K-Nearest Neighbors (KNN), Linear Regression (LR), and Gaussian Naïve Bayes (GNB). We use these algorithms to determine outperformed models to reduce the WQI model prediction uncertainty and improve the model architecture especially coastal WQIs.

The paper is developed as follows: Section 8.4 presents the details of the nature of Cork Harbour and its environmental significance. Section 8.5 - 8.6 describes the details overview of various ML algorithms, validation processes and other statistical methods for assessing model, Section 8.7 provides in depth of the prediction results and discusses the output of the prediction models, and Section 8.8 - 8.9 summarizes the findings, recommendations, limitations and future direction of this research.

8.4 Application domain- a case study in Cork Harbour

The present study was conducted in Cork Harbour as Special Protection Area (SPA), that is relatively the deepest and longest (17.72 km) surface waterbodies in Ireland

(Hartnett and Nash, 2015; Nash et al., 2011). The Harbour has covered with large surface area (85.85 km^2) and brackish estuary on the south coast of Ireland (Nash et al., 2011). It is a macro-tidal with a typical spring tide range of 4.2 m at the entrance to the Harbour (Uddin et al., 2022). Relatively, the Cork city is the well-known as an industrial hub of Ireland and the surrounding hinterlands are dominated with extensive agricultural practices which influence water quality in the region directly due to the using chemical fertilizers for developing crops (EPA, 2017). Recently, several annual environmental reports of EPA has revealed that the Cork and Donegal received the highest raw discharge waste water directly without any treatment (EPA, 2017). Moreover, the Cork Harbors' geological patterns are vital for Harbour area's ecosystem and fresh water quality. It has been identified as a Special Protection Area (SPA) under the 1979 Wild birds Directive (79/409/EEC).

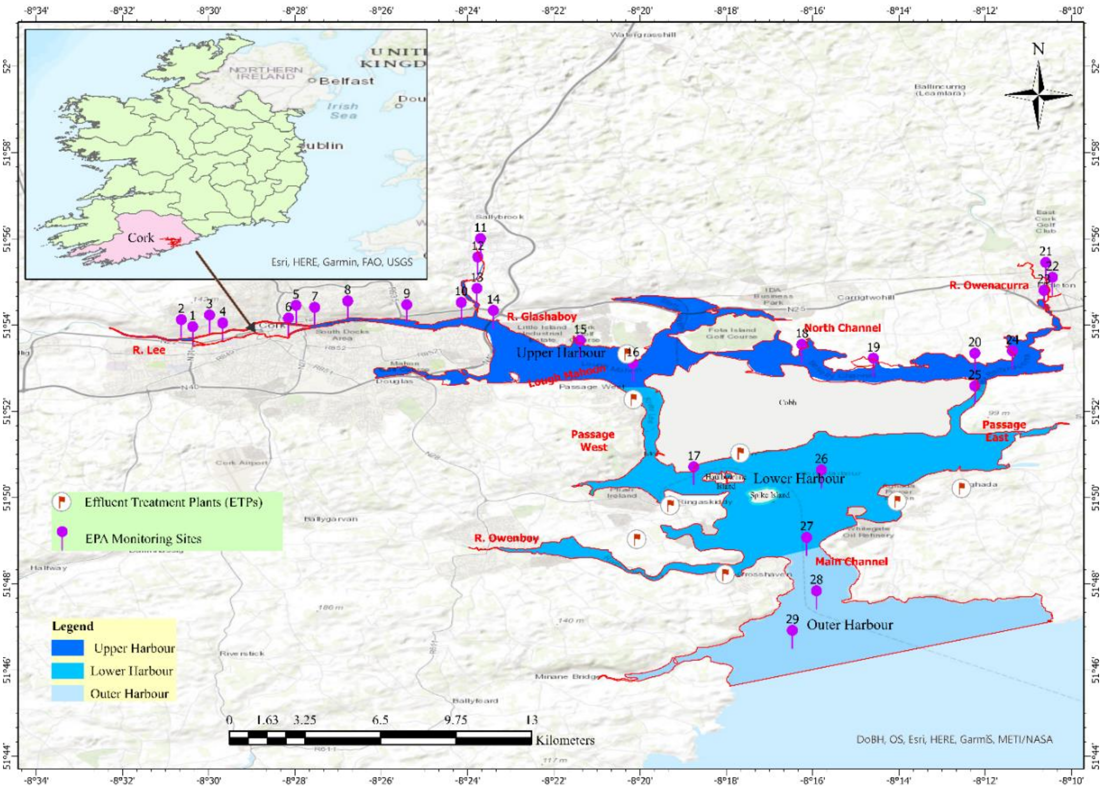


Figure 8.1. Study domain: EPA water quality monitoring sites and effluent treatment plants (ETPs) in Cork Harbour, Ireland.

8.5 Methods and materials

8.5.1 Data obtaining process

Water quality data was retrieved from the Irish Environmental Protection Agency

(EPA) water quality monitoring database for Cork Harbour. The details of the data are available at https://www.catchments.ie/data. Typically, the EPA monitors the water quality of Habour frequently. A total of 29 monitoring locations out of 32 were considered for this study. Details of the monitoring sites and their descriptions are provided in Table 8.S2. Figure 8.1 provides the details of the monitoring locations in Cork Harbour. This study uses eleven water quality variables for the WQI calculation: temperature (TEMP), total organic nitrogen (TON), ammonia (AMN), dissolved oxygen (DOX), ammoniacal nitrogen (AMN), pH, salinity (SAL), molybdate reactive phosphorus (MRP), biological oxygen demand (BOD), transparency (TRAN), and *Chlorophyll a* (CHL). Selected WQ indicators data was considered from 1 m depth at each monitoring site in Cork Harbour. Table 8.1 provides an overview of the studied water quality indicators unit; standard threshold and Table 8.S3 supply the details of the indicator monitoring data at each site, respectively. Water quality indicators were considered for this study based on the availability of data variables in the monitoring database 2020, considering the fine dissemination of monitoring sites. For further analysis, averaged concentrations (from January 2020 to December 2020) of indicators were used in this research for further analysis (Table 8.S3).

Table 8.1 Water quality parameters, units and standard threshold for coastal water quality accordance to Uddin et al., (2022).

Parameter	Unit	Standard threshold	
		Lower	Upper
CHL*(i)*	mg/m^3	0.0	14.2
DOX*(i)*	% sat	72	128
MRP*(i)*	mg/l as P	0.0	0.05
DIN*(i)*	mg/l	0.0	1.20
AMN*(ii)*	mg/l	0	1.5
BOD*(ii)*	mg/l	0	7
pH*(iii)*	-	5	9
TEMP*(ii)*	˚C	-	25
TON*(iv)*	mg/l as N	0.0	2
TRAN*(v)*	m/depth	> 1	-
SAL*(ii)*	psu	12	38

(xi) ATSEBI guide values, indicators standard values was obtained based on median value of salinity. In this study, SAL median value was found 20.47 (see details in Appendix 1d)
(xii) EPA, Ireland (2001), recommended values for the surface water.
(xiii) pH and Alkalinity Monitoring Manual for estuary , EPA,USA
(xiv) the European Communities regulations for quality of surface water intended for the abstraction of drinking water, 1989 (S.I. No. 294/1989).
(xv)EPA' bathing Water Quality Regulations 2008, (Ref. No. 79/2008).

8.5.2 WQI calculation

A range of WQI models has been used to calculate the WQI values. Its application has increased sequentially due to its simple mathematical functions and ease of use. However, the existing literature on WQI models is extensive and focuses mainly on details of WQI models and their services (Gupta and Gupta, 2021; Uddin et al., 2021) without checking their statistical accuracy. Hence, this research enhances the accuracy of the WQM based WQI model outputs by estimating more precise and statistically reliable water quality index scores. Typically, an ideal WQI model comprises four components such as water indicators selection, sub-index (SI) function, indicators weight generation and aggregation function. Details of these components with statistical functions are available in the literature (e.g., Rahman and Harding, 2016; Uddin et al., 2022; Uddin et al., 2022a, 2022b) . In this study, the WQIs was calculated based on the improvement methodology proposed by Uddin et al., (2022) because this approach is one of the more practical and effective for assessing coastal water quality. In details, the weighted quadratic mean (WQM) WQI methodology can be found in Uddin et al., 2022.

8.5.2.1 Evaluation of WQIs

Currently, various classification schemes are used to evaluate the WQIs in literature. Several recent studies have claimed that the WQIs model results do not reflect the actual information on water quality due to the various classification schemes for similar data attributes (e.g., see Uddin et al. 2022). Uddin et al., (2022) proposed unique classification schemes for assessing coastal water quality, and we used these schemes in this research. Table 8.2 provides the details of the classification schemes.

Table 8.2 Classification scheme for coastal water quality.

Classification scheme	Range of score	Description
Good	80-100	Water quality is suitable to use for any purposes.
Fair	50-79	A few indicators meet the guide values and the water quality is safe with a minor observation.
Marginal	30-49	Most of the indicators does not fall into the criteria; water quality is unsafe, which may be harmful for aquatic life.
Poor	0-29	Each indicators failed to meet all the criteria; water quality is completely unsafe and not suitable for many certain uses.

8.5.3 Data pre-processing

8.5.3.1 Data standardization

Prior to the training of ML algorithms, it is essential to standardize data variables. Commonly, in ML technique, this method used for converting all data variables into a uniform scale in order to optimize the model training errors (Rahman, 2020, 2019; Solanki et al., 2015). In this study, water quality data variables were standardized using z score normalization process. Z score can be presented as follows:

$$\boldsymbol{z} = \frac{x_i - \bar{x}}{\sigma} \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots. (8.\mathbf{1})$$

Where, z is the standardize score, x_i is the ith data variable, $\bar{x}$ refers to the mean of data variable and σ is the standard deviation of data.

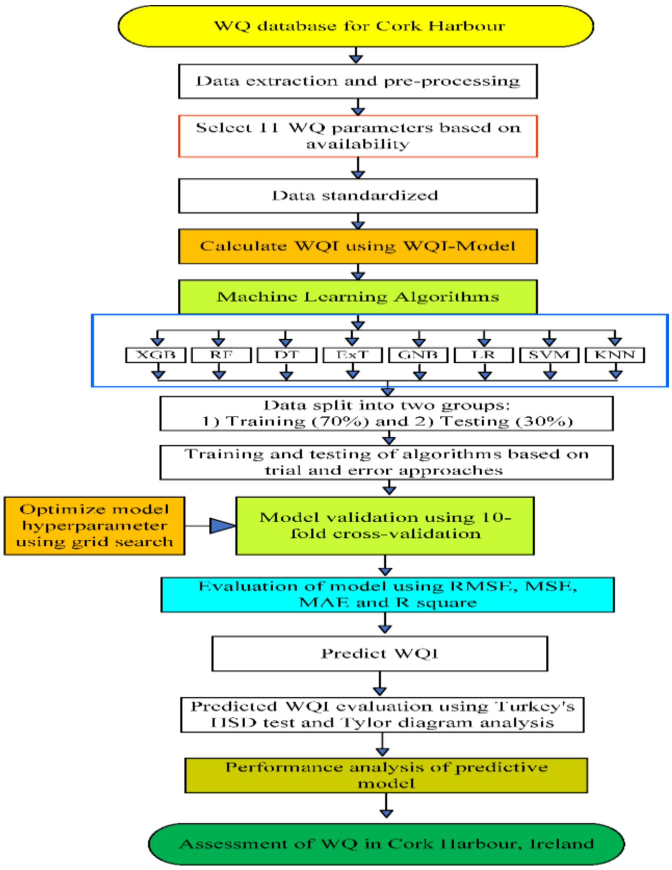


Figure 8.2. A comprehensive framework for the assessment of predicting WQIs.

8.5.3.2 Data splitting

Before, training the ML algorithms, data was divided into training [70% (20 monitoring sites)] and testing [30% (9 monitoring sites)] sets. After splitting data, eight ML algorithms were trained and tested using training and testing data sets respectively. Model performance was evaluated for both phases.

8.6 Machine learning algorithms

ML technique is widely used to predict unknown objects. Recently, this technique has been utilized in different branches of research. For example, research on predicting water quality has revealed that the ML algorithm could be more effective in evaluating water quality than other traditional methods (Aldhyani et al., 2020; Azrour et al., 2021; Babbar and Babbar, 2017; Di et al., 2019; Haghiabi et al., 2018; Mohammed et al., 2018; Prakash et al., 2018; Solanki et al., 2015; Xiong et al., 2020). Several studies have effectively used machine learning approaches to predict WQI (Ahmad et al., 2017; Bui et al., 2020; Grbčić et al., 2021; Hassan et al., 2021; Kadam et al., 2019; Kouadri et al., 2021; Leong et al., 2019; Venkata Vara Prasad et al., 2020; Wang et al., 2017). This research utilised eight ML algorithms to identify robust algorithms for predicting WQM-WQIs. The details methodological procedures of this study are presented in figure 8.2. The details of various ML algorithms can be found in the Appendix 8 as a continuation of 8.6.1.

8.6.2 Model hyper-parameterization

Hyper-parameters tuning of ML technique is performed to obtain higher level model accuracy (Elgeldawi et al., 2021; Villalobos-Arias et al., 2020). In ML approaches, numerous methods are used to hyper-parameterise the predictive model. Most of the studies in the literature used grid search and random search techniques to optimise the model hyper-parameters (Shekar and Dagnew, 2019). The grid search technique is widely used because this technique evaluates model accuracy for each grid position (Elgeldawi et al., 2021; Shekar and Dagnew, 2019). Compared to the typical hyper-parametrization process, the grid search is more efficient method than the random search (Villalobos-Arias et al., 2020). Thus, this research uses the grid search technique to optimise the model parameters. Table 8.3 presents hyper-parameters for various ML models the during model training phase.

Table 8.3 Optimized hyper-parameters of various ML models during testing period.

Model parameters	XGB	RF	DT	ExT	LR	KNN	SVM	GNB
n_estimators	100	100	100	100	100	-	30	200
learning_rate	0.2	-	-	-	-	-	-	-
max.depth	20	10	10	20				-
gamma	0	-	-	-	-	-	auto	-
booster	gbtree	-	-	-	-	-		-
Kernel		-	-	-	-	-	RBF	-
subsample	1	-	-	-	-	-	-	-
colsample_bytree	1	-	-	-	-	-	-	-
base_score	0.5	-	-	-	-	-	-	-
reg_lamda	1	-	-	-	-	-	-	-
bootstrap	True	True	-	True	-	-	-	-
cv.folds	10		-	-	-	-	-	-
random_state	1	1	-	1	-	-	-	-
Objective	reg.linear		-	-	-	-	-	-
criterion	-	Squared_error	-	Squared_error	-	-	-	-
max_leaf_nodes		5	10	5	-	30	-	-
min_samples_leaf		1	5	1	-	-	-	-
epsilon	-	-	-	-	-	-	0.1	-
shrinking	-	-	-	-	-	-	True	-
fit_intercept	-	-	-	-	TRUE	-	-	-
n_neighbors	-	-	-	-	-	5	-	-
weight	-	-	-	-	-	uniform	-	-
metrics	-	-	-	-	-	minkowski	-	-
power_parameters	-	-	-	-	-	2	-	-

8.6.3 Model performance analysis

8.6.3.1 Cross-validation approaches

Cross-validation (CV) is the most common procedures to evaluate the ML models for small datasets. To assess the performance of ML predictive model, the present study is used the random CV technique to compare the model performance. In this study, 10-fold CV technique was utilized including widely used four evaluation criteria: mean square error (MSE), root mean square error (RMSE), mean absolute error (MAE), and coefficient of determination (R^2). Details technique can be found in Xiong et al., (2020). Except for R^2, the performance criteria expect a predictive model's performance to be as small as possible. In general, the R^2 value refers to assessing the models how well fitted the model with predicted data. It should be close to 1 (He et al., 2015; Sharif et al., 2022) . Model evaluation criteria are measured as follows:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (8.8)$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (8.9)$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (8.10)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \hat{y})^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (8.11)$$

Where y_i and $\hat{y}$ are the *i^th^* observed and mean of the predicted values respectively. *n* is the number of observations.

8.6.3.2 Prediction uncertainty analysis

For the purposes of uncertainty analysis in the predictive WQIs of various ML models, several techniques are used, such as Monte Carlo simulation, ML algorithms, etc. In this study, the percent of relative error index (PREI) was utilized to evaluate the prediction error at each observation location because this technique has recently been used for the assessment of predictive bias in predicting ML models (Bui et al., 2020). The result is given in percentage (%). The optimal value of PBIAS is 0.0, with low-magnitude values refers accurate model simulation. Positive values indicate underestimated bias, whereas negative values represent model overestimation bias. Figure 8.11 presents the prediction percentage of bias and percent of relative error index, respectively. The PREI are can be defined as follows:

$$\boldsymbol{PREI = \left(\frac{y_i - \hat{y}_i}{y_i}\right) \times 100} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (\mathbf{8.12})$$

where y_i actual WQIs for i^{th} observation and $\hat{y}_i$ is the mean predicted WQIs.

In addition, the present study utilized the inferential error bars analysis technique because many studies have utilized this method to evaluate the uncertainty of various datasets or groups. The details of the methodology can be found in Cumming et al., (2007). Figure 8.11 presents the uncertainty results of the WQI scores obtained from the various prediction models.

8.6.3.3 Comparative analysis of predictive models

In this study, predictive model bias was analysed by comparing eight ML models using the Tylor diagram. This technique is commonly used to compare various methods, techniques, or models in terms of data deviation. It is effective to identify an appropriate model because it allows three statistical measures, including the correlation between observations and predictions, the root-mean-square deviation (RMSD) and their standard deviations (SD) which help in understanding the model reliability (Calim et al., 2018). Recently, several studies have applied this method to compare the bias among models (Seifi et al., 2020; Xu et al., 2016). Figure 8.14 presents the summary of statistics for various ML predictive models.

8.7 Results

8.7.1. Physico-chemical assessment of water quality

Figure 8.3 presents the descriptive statistics for the studied 11 physico-chemical water quality indicators in Cork Harbour. Basic statistics were obtained using Whisker's box-plot technique, where a black solid line and a red point indicated the median and mean values of water quality indicators, respectively. For the determination of correlation among water quality indicators, the significant associations among the water quality indicators were analysed through the Pearson's correlation test at a 99% confidence level, and the results of the correlation between indicators are presented in Figure 8.4.

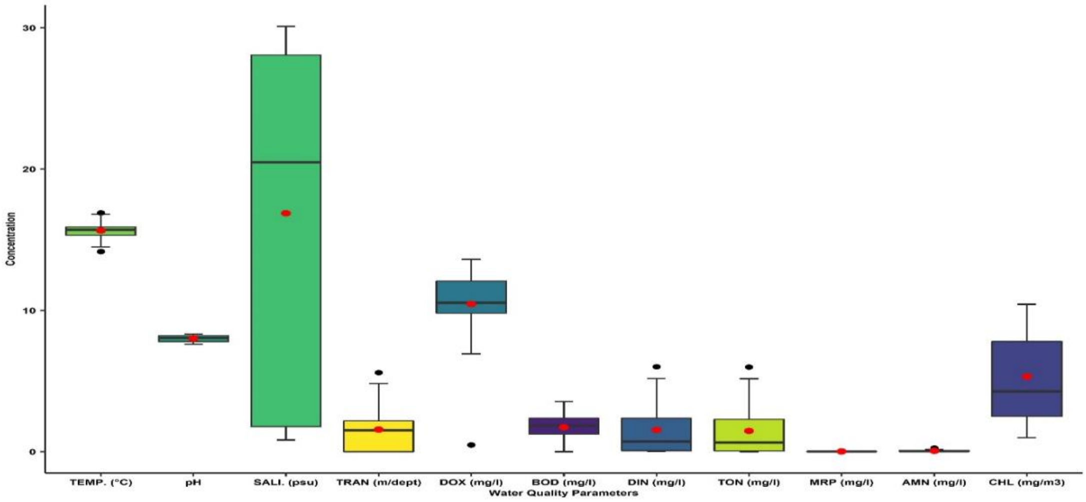


Figure 8.3. Physico-chemical attributes of water quality in Cork Harbour.

In this study, water TEMP, pH, CHL, and AMN were found within the standard threshold values of coastal water quality. The details of the standard thresholds are provided in Table 8.1 above. The highest water TEMP was found at 16.90˚C and the lowest at 13.90˚C with a mean and median value of 15.58˚C and 15.7˚C, respectively throughout the study period, implying a negative skew (mean < median) within the data (Figure 8.3). Similarly, water pH also showed a negative skew, having a mean value of 8.00 and a median value of 8.05 (Figure 8.3). The CHL ranged from 1.00 mg/m^3 to 10.43 mg/m^3 with a mean value of 5.32 mg/m^3, whereas the AMN's mean concentration was found to be 0.07 mg/l across the monitoring sites in Cork harbour. The values of TRAN were ranged from 0.00 m/depth to 5.60 m/depth with a positive skew within the dataset (mean > median) and showed a significant moderate positive relationship with water pH ($r = 0.60$, $p < 0.01$) (Figure 8.4). A significant variation of SAL concentration was observed across the monitoring sites in this research. It varied from 0.83 to 30.1 psu with a mean value of 16.87 psu (Figure 8.3). It is noted that SAL concentration is only used to determine the standard threshold of coastal water quality for MRP, DOX, CHL and DIN. The details of the procedures can be found in Uddin et al., (2022). Excessive dissolved oxygen concertation is harmful for aquatic species (Chiang et al., 2021). DOX concentration was found in the North-channel of the upper Harbour, it was 13.61 mg/l (exceed), whereas the lowest concentration (6.93 mg/l) was found in River Lee of the upper Harbour (Appendix 1(c)). The DOX showed a significant, strong positive association with water pH ($r = 0.86$, $p < 0.01$) (Figure 8.4). The data for BOD showed a higher median value (1.86 mg/l) than the mean value (1.74

mg/l), and it varied between 0.00 mg/l and 3.55 mg/l (Figure 8.3).

Figure 8.4. Pearson’s correlation of physico-chemical indicators in Cork Harbour.

More than 40% of monitoring sites' DIN concentrations exceeded the upper threshold limit of 1.20 mg/l, with a mean value of 1.54 mg/l (Figure 8.3). TON also showed positive skewness across the monitoring sites in Harbour while around 34% of the data points exceeded the upper guideline value of 2 mg/l (Figure 8.3). As shown in figure 8.4, a significant strong negative association was found for both DIN and TON with water pH and TRAN, respectively ($r = -0.77$, $p < 0.01$) and ($r = - 0.70$, $p < 0.01$). Likely, MRP concentration exceeded the standard threshold of coastal water quality; it ranged from 0.01 mg/l to 0.06 mg/l. The MRP showed a moderate positive relationship with both DIN and TON ($r = 0.59$, p 0.01) (Figure 8.4). In this research, a positive correlation was observed between CHL and water pH ($r = 0.82$, $p < 0.01$) and DOX ($r = 0.80$, $p < 0.01$), and a negative relationship was associated with DIN and TON ($r = 0.61$, $p < 0.01$) (Figure 8.4).

8.7.2 Assessing water quality using WQM-WQI models

Water resource management is critical for all states to maintain "good water quality" status. Now a day, the WQI model is widely used to evaluate water quality due to its simple application and easy to evaluate the outcomes of the model. Table 8.S3 provide the details WQIs for each monitoring sites in Cork Harbour. For the evaluation of coastal water quality, the present study was utilized the WQM-WQI model to calculate the WQIs values. It ranged from 33 to 73, with an average of 56.19. Water quality status was evaluated using the coastal water quality classification scheme that are provided in Table 8.2 above. Water quality status are provided in Table 8.4 below. Two types of water quality were found in Cork Harbour. These varied from "marginal" to "fair" categories. From Table 4, it can be obtained that in total, 13 (44.82%) of monitoring sites' water quality was found to be "fair", whereas 16 (55.18%) were assessed as "marginal" in Cork Harbour, respectively.

Table 8.4 Point evaluation of water quality in Cork Harbour using WQM model.

Model	Total monitoring locations	Water quality status			
		Good	Fair	Marginal	Poor
WQM-WQI	29	0	44.82 % (13)	55.18% (16)	0

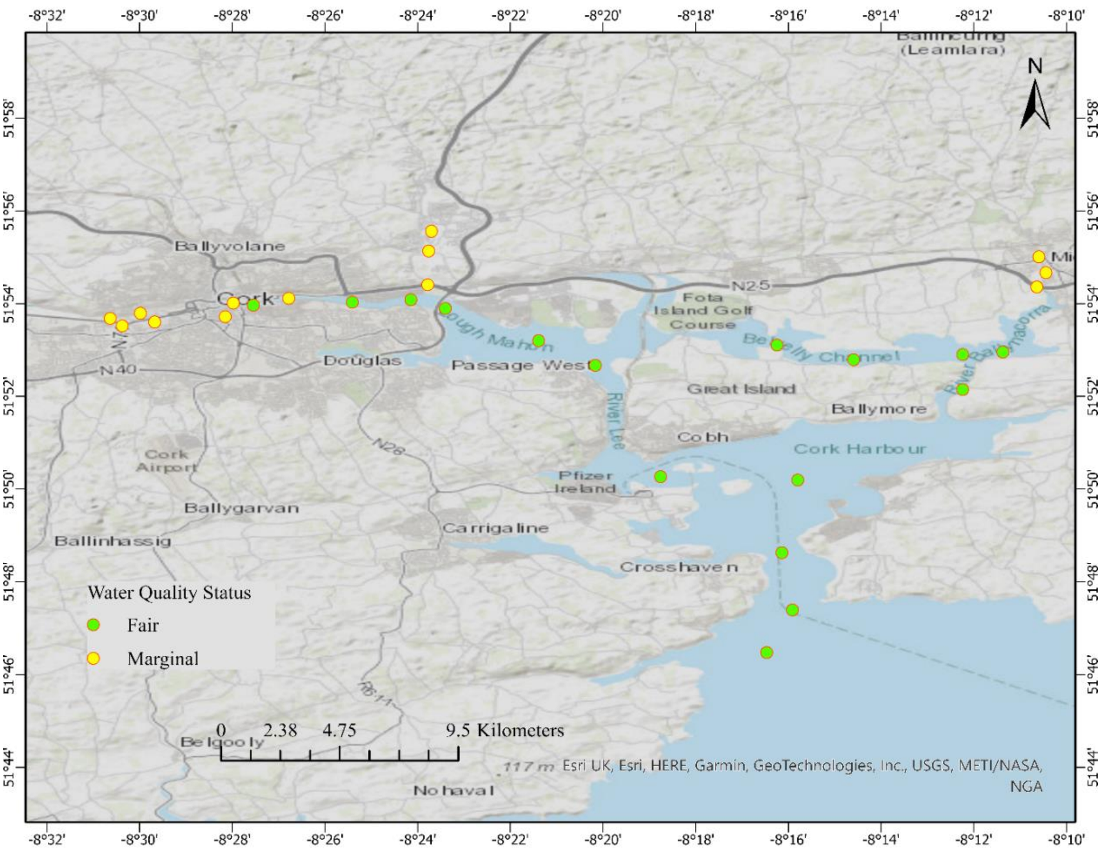


Figure 8.5. Water quality status in Cork Harbour using WQM-WQI model.

Figure 8.5 (above) presents water quality status at each monitoring location in Cork Harbour over the study period. As can be seen from figure below, the Harbour water quality was dominated by the “fair” category, most of the monitoring locations water quality were evaluated as fair quality. The “marginal” class water quality was evaluated in the upper Lee estuary and the upper part of the river Owenacurra (Midleton). The results of the WQM-WQIs also in line with our earlier observations, which showed that the upper Harbour water quality was worst compared to the other parts of the Harbour (Uddin, et al., 2022).

8.7.3 Comparative analysis of various ML regression models

In this study, we applied eight ML regression algorithms to predict the WQM-WQIs values in Cork Harbour. Table 8.S5 provides the predicted WQM-WQIs for various ML models. In order to validate the predictive results of various ML algorithms, the CV approaches was utilized. Figure 8.6 presents the CV results (RMSE, MSE and MAE) for the eight ML models. According to the cross-validation results, the XGB, RF, DT and ExT have the highest prediction perform among the algorithms. The lowest prediction errors belonged to the XGB, DT, and ExT algorithms, but during the training and testing periods the lowest errors were found for the XGB model, whereas the lowest training (RMSE = 3.3, MSE = 10.91, and MAE = 1.67) and testing (RMSE = 0.0, MSE = 0.0, and MAE = 0.02) errors were found for the XGB model. Compared to best algorithms, relatively, higher prediction errors were found for the DT (RMSE = 3.97, MSE = 15.82 and MAE =2.62) and the ExT (RMSE = 3.60, MSE = 12.96 and MAE = 2.29), respectively during model training period. Interestingly, there was no prediction errors (RMSE, MSE and MAE were found 0 respectively) during testing period, whereas both algorithms were predicted WQI values at each monitoring sites properly. Similar finding also revealed by Chicco et al., (2021). Contrary, the RF also had a very low prediction error, while the GNB and KNN algorithms had higher prediction errors, it ranged from 0.02 to ± 3.75. These algorithms did not predict each WQI value accurately at each monitoring site in Harbour. Compared to other algorithms, the SVM performance had very poor over the study period. The large error was found for the SVM model, whereas testing (RMSE, MSE and MAE were 13.40, 179.61 and 12.77 respectively) and training errors also (RMSE, MSE and MAE were 12.68, 160.93 and 11.59 respectively) had higher than other algorithms (Figure 8.6).

For the identification of the best algorithms, the present research was also utilized the determination of coefficient (R^2) to evaluate the model performance. Usually, the R^2 refers to the correlation and performance reliability between predictors and response variables, which helps to identify the best algorithm.

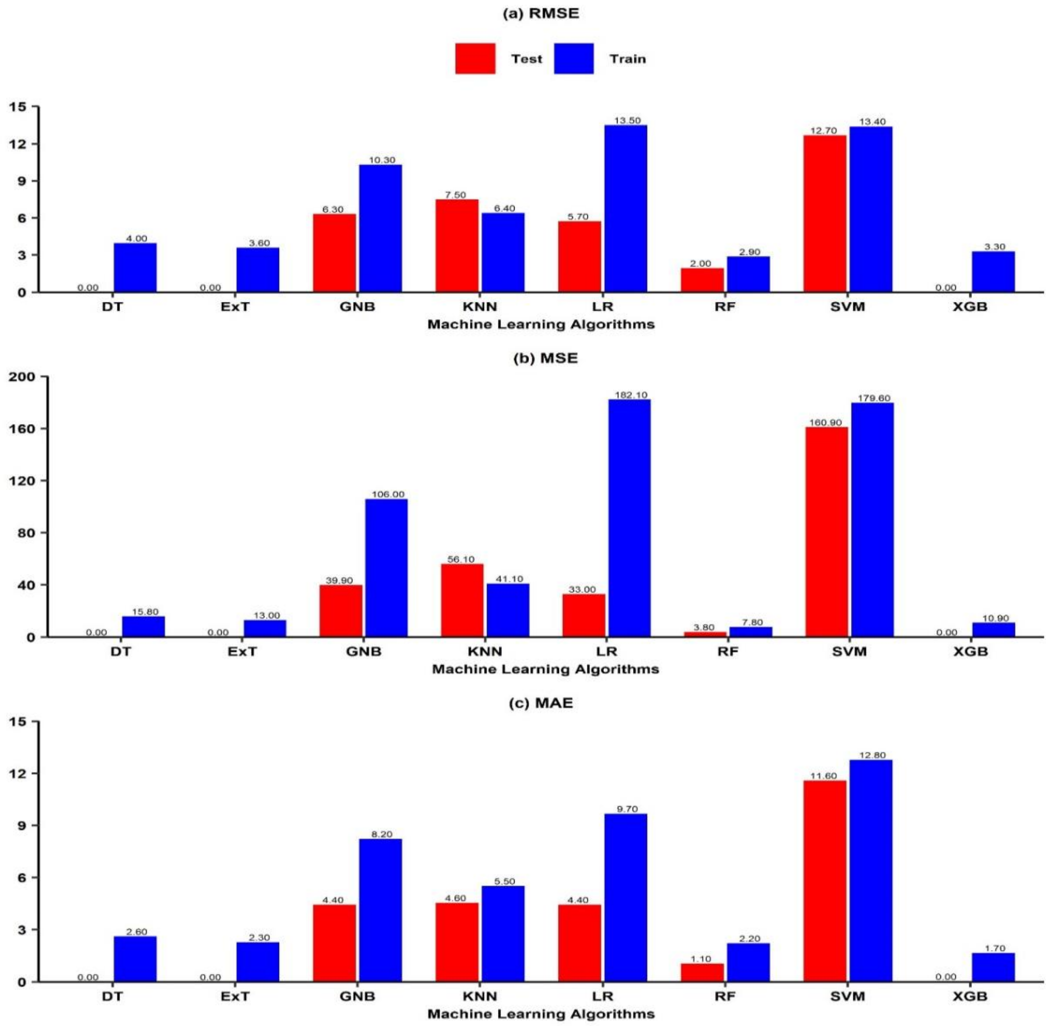


Figure 8.6. 10-fold cross-validation results of various ML algorithms.

Figure 8.7 presents the R^2 value for the various ML algorithms. As discussed above, the XGB, DT and ExT algorithms had lower prediction errors. Those algorithms predicted WQI values at each monitoring sites properly. For these algorithms, R^2 values were found 1, where relative close to 1 (0.98) found for the RF (Figure 8.7d). It can be seen from the Figure 8.7g, there were no relationship between predictors and response for the SVM model whereas the R^2 value had less than 50% (0.43). Although, the LR algorithm had higher R^2 values (0.81) but this algorithm did not predict WQI values at each point properly (Figure 8.7f). On the other hand, the KNN and the GNB showed moderate relationship between actual and predicted WQI values (Figure 8.7b; Figure 8.7h). Therefore, results of R^2 also indicates that the XGB, DT and ExT algorithms had higher predictive capabilities for predicting WQI values.

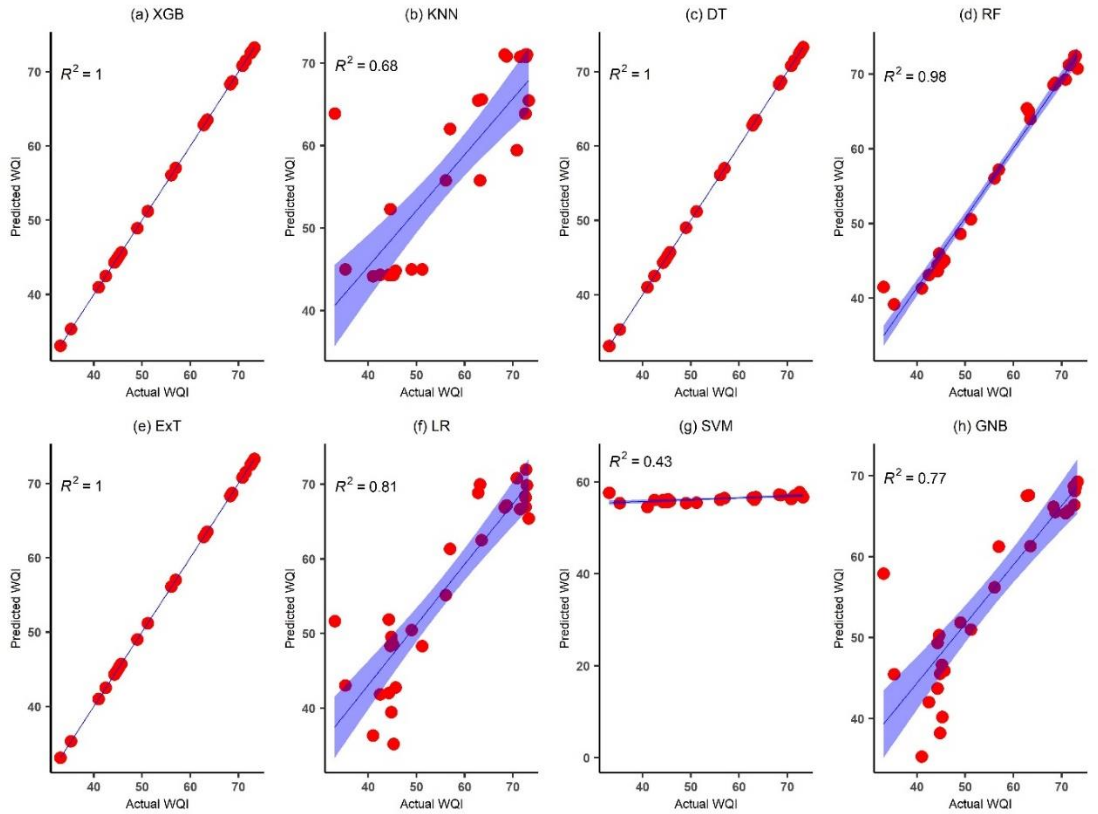


Figure 8.7. Scatter plots of actual vs predicted WQI values based on the model testing dataset of different ML regression algorithms for validation purposes.

However, based on the prediction errors, the XGB, DT and ExT were predicted at each WQI values properly. Figure 8.8 shows a comparison scenario between actual and predicted WQIs at each monitoring site in Cork Harbour. As can be seen from Figure 8.8, all algorithms performed well, except the SVM. Unlike, it showed the worst performed and did not follow the trend to the actual WQI values at each monitoring sites.

In addition, an overview of statistical summary for the predicted WQIs and actual WQIs for various ML models are presented in the Figure 9. Whereas boxplots show differences in predicted WQI values among ML models in line with the actual WQI (Figure 8.9a). The Figure 8.8 also reveals that there has been a slight statistical variation among ML algorithms predicted WQIs except XGB, DT and ExT. As shown in Figure 8.9a, compared to all prediction models, there were no significant statistical variation between actual and predictive WQI values for the XGB, DT and ExT models at $p < 0.05$. Completely, different trend was found for the SVM predicted and actual WQI values over the study period, whereas a slight variation was found for the KNN and LR models (Figure 8.9a). The Cumulative Distribution Function (CDF) results of the predicted ML models are shown in Figure 8.9b. The CDF results indicated that 95% of monitoring sites were predicted correctly except the SVM methods.

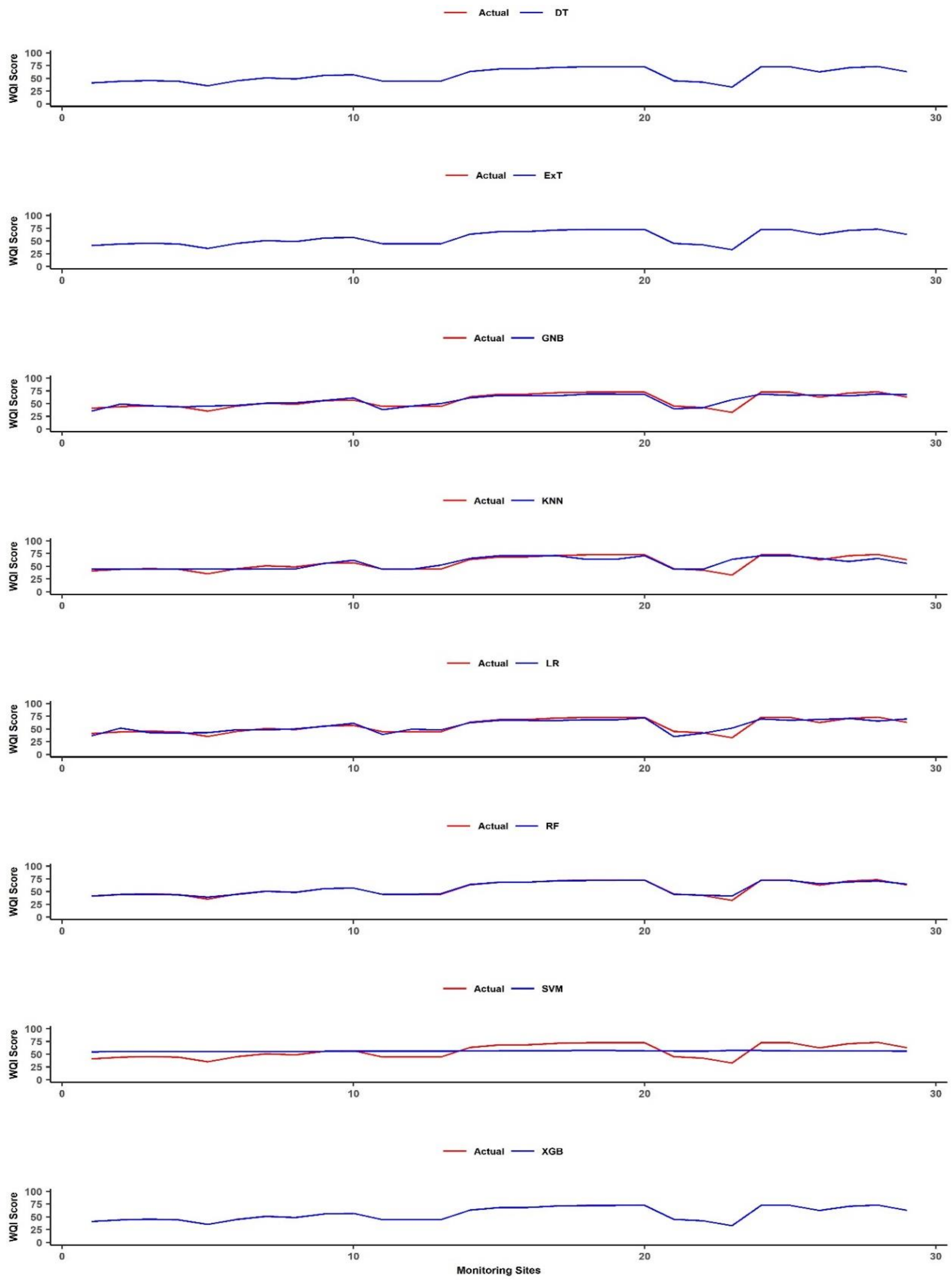


Figure 8.8. Comparison of the model testing performance between predicted and actual WQI values at each monitoring sites.

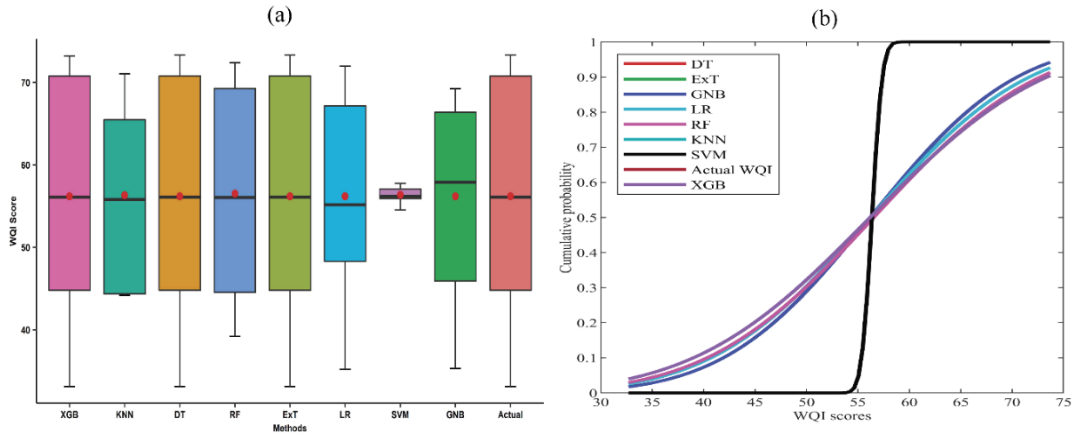


Figure 8.9. Comparison of predicted WQI from various ML models: (a) Boxplots show a comparison between actual and predicted WQI scores and (b) CDF comparison of predicted WQI scores of various ML.

Here, we compared several ML models using Tukey's HSD comparison technique. Figure 8.10 presents the overall and pair-wise comparison among ML models with a 95% confidence level. The results of Tukey's reveal that there were no statistically significant difference among models. Moreover, the 95% individual confidence level also indicates that predicted WQI values of all models were found between -10 to +10 that means all pairs of predicted means included zero, which indicates that the differences are not statistically significant.

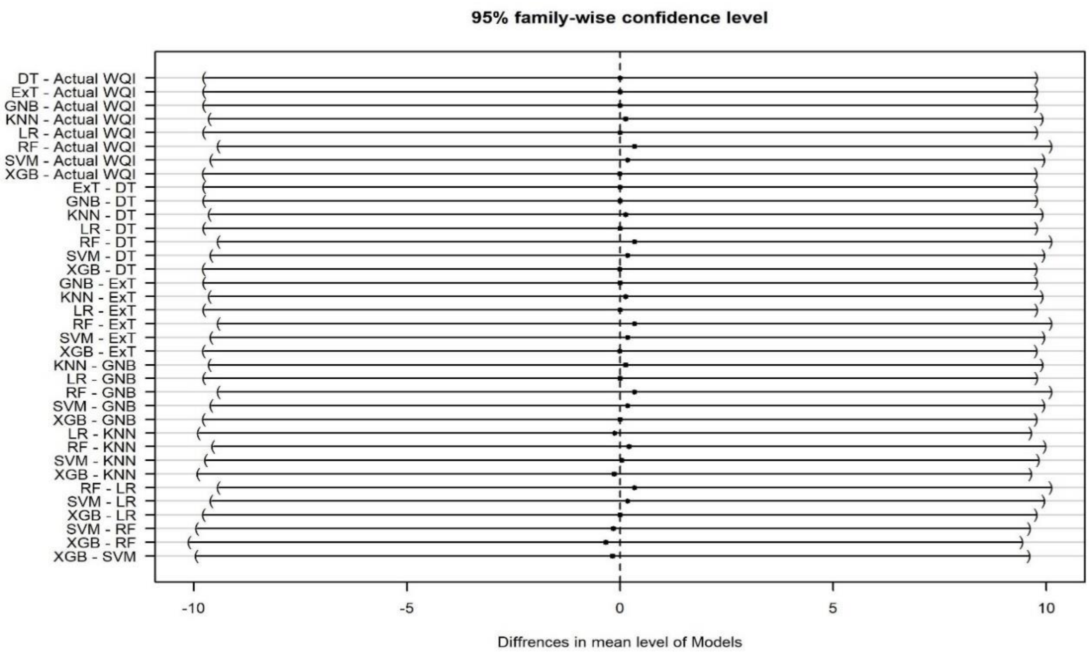


Figure 8.10. Multiple comparison results of pair-wise ML models with 95% CI from Tukey's HSD, the vertical dashed line indicates the point where the difference between

the means is equal to zero or similarity of model statistics, the 0 refers to the means are equal of both models.

8.7.4 Assessment of uncertainty in predicting WQIs

Based on the CV and HSD analysis, it is hard to determine the best algorithm for predicting WQIs. Here, we utilized PREI, whereas PREI allows comparing the prediction capabilities of models based on their tendency to over or underestimate the WQIs at each observation. It offers an opportunity to examine the prediction power of the model at each data point. Figure 8.11 presents the PREI of various predictive models at each location in Cork Harbour.

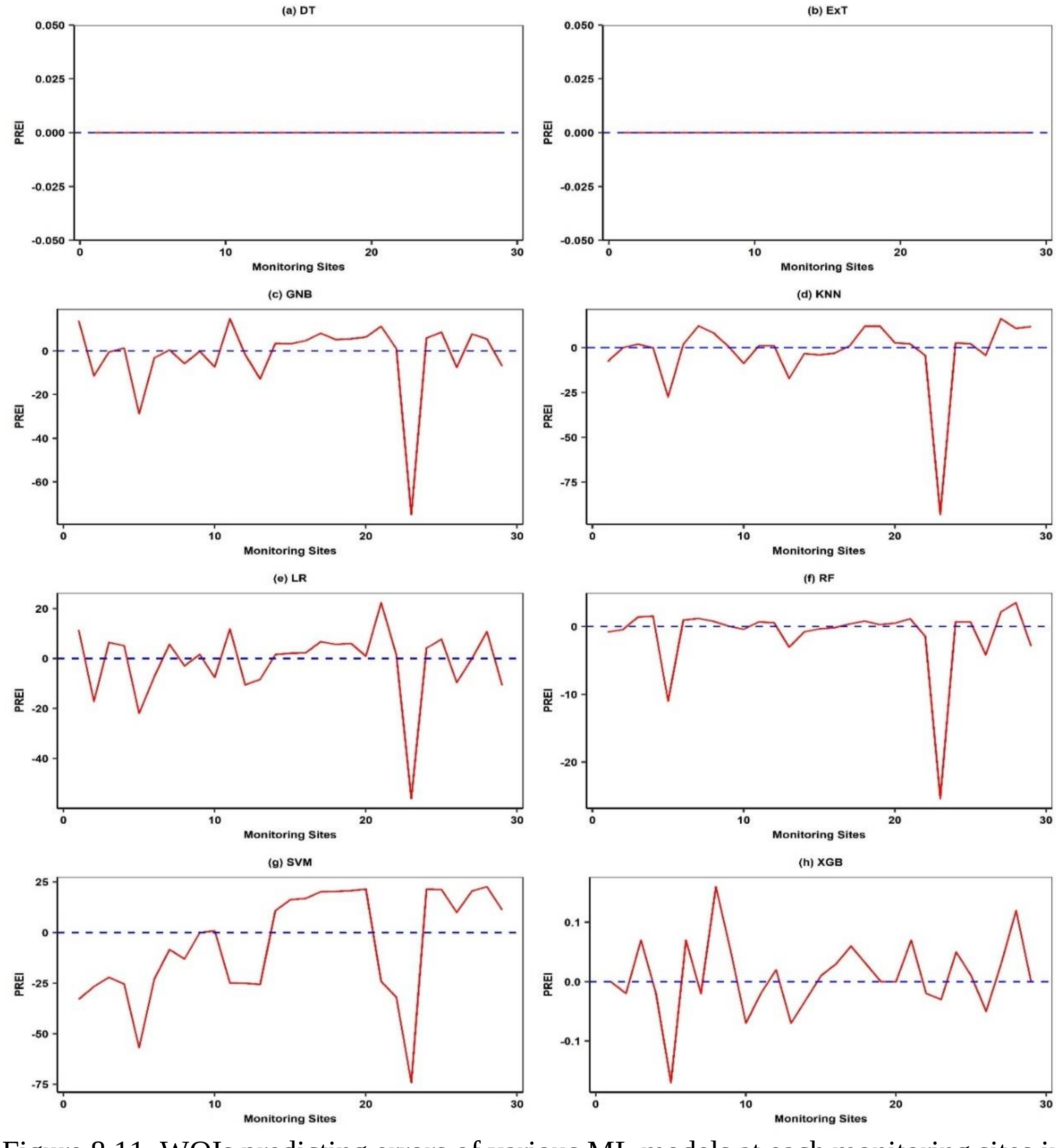


Figure 8.11. WQIs predicting errors of various ML models at each monitoring sites in Cork Harbour.

Compared to among ML algorithms, the lowest error was found for the DT, ExT, XGB, and RF models, respectively. As shown in Figure 8.11, underestimating and overestimating biases highly influenced the GNB (+14.71 to -74.9), KNN (+16 to -93), LR (+22.30 to -56.1), RF (+3.52 to -25.38), and SVM (+22.7 to -75) models, respectively. The lowest underestimate and overestimate were found for the XGB model. It ranged from +0.16 to -0.17; whereas there was no bias for DT and ExT in predicting WQIs at each monitoring site. Except XGB, most of the algorithms had overestimated problems in predicting WQIs at monitoring sites in the upper-Eastern part of the Harbour.

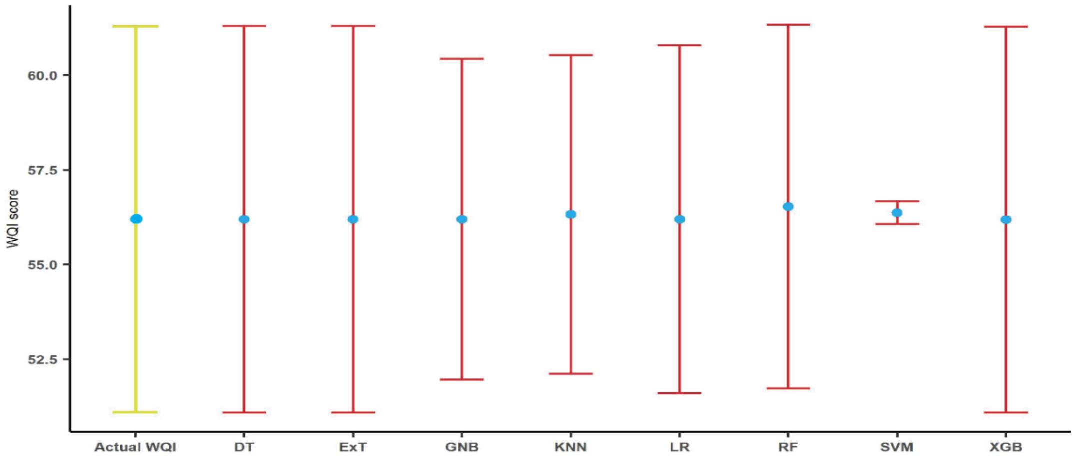


Figure 8.12**. S**tatistical significance of predicting uncertainty in WQIs for various ML models with 95% CI. Here, 95% CI where n is 29, $p < 0.0001$. Green error bar represent the measured (actual) WQIs using WQM-WQI model.

However, this study also utilized the 95% confidence interval analysis of predicted WQIs for various ML models. Above, Figure 8.12 reveals that similar data discrepancies had the DT, ExT, and XGB models in predicting WQIs. It can be easily figured out from the figure above that there was no data variation between actual (green error bar) and predicted WQIs for these models. In contrast, the GBN, KNN, and LR showed similar errors in predicting WQIs. Unlike GBN, KNN, and LR, comparatively low errors were made in predicting WQIs for the RF model. The SVM algorithm shows completely different results from others. It had higher data variation between actual and predicted WQIs.

Based on the model errors, this study found three based (DT and ExT) and ensemble tree based (XGB and RF) are more robust and reliable than other algorithms. These algorithms perform better when predicting WQIs for the coastal water quality. The finding are in line with those observed in earlier studies (Bui et al., 2020; Ghorbani et al., 2018; Khosravi et al., 2018; Kouadri et al., 2021). As seen from Figure 8.13 below, DT and ExT models were predicted WQIs correctly at each monitoring sites whereas small variation was found between predicted and actual WQIs for the XGB and RF models. The results of the predictive WQIs indicate that DT and ExT models had overfitting problems because tree-based models are developed based on a single tree without any control (Biebler et al., 2009; Ying, 2019).

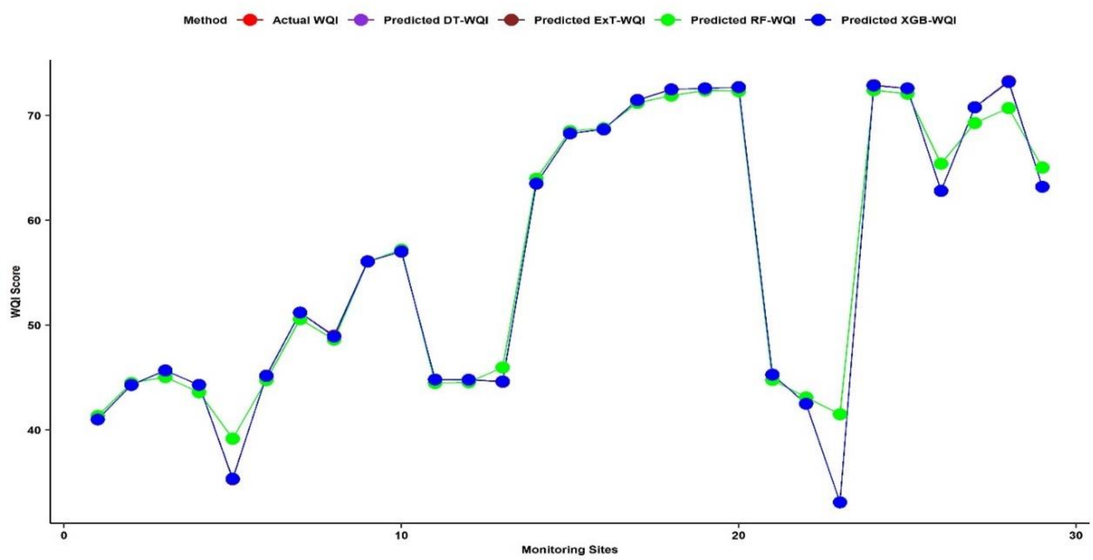


Figure 8.13. Comparison among the outperformed machine learning algorithms.

8.7.5 Justification of prediction errors of various model

To justify the model bias in predicting WQIs, the Tylor diagram analysis was utilized in this research. Recently, this approach is widely used to compare various methods/datasets/models in terms of data variances (Kärnä and Baptista, 2016; Xu et al., 2016). Figure 8.13 provides an insight into how the model performed in terms of three statistical measures, where, statistics were obtained from various ML techniques by using actual and predicted WQI values in Cork Harbour respectively.

As can be seen from Figure 8.14, a significant statistical difference was found among ML models with $p < 0.05$. As shown in Figure 8.10, it can be clearly defined that the SVM model significantly differed from the other ML algorithms. Comparatively, the lowest RMSD, SD, and higher correlation were found for the XGB, DT and ExT algorithms respectively. In addition, relatively the RF algorithms shows well performance compare than remaining algorithms.

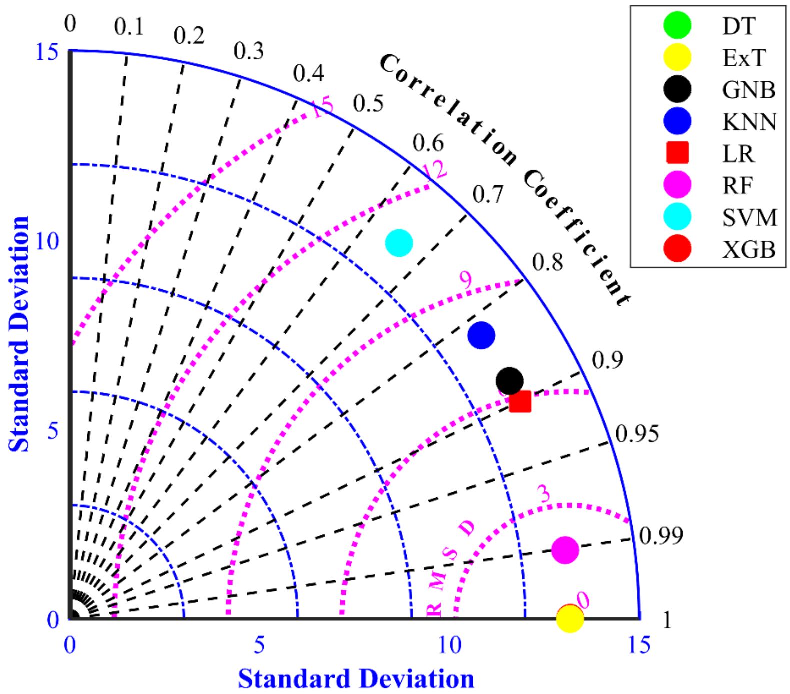


Figure 8.14. Various predictive ML models comparison using Tylor diagram.

However, the present study compared various ML algorithms using the cross-validation results, coefficient of determination, analysis. In terms of bias between actual and predicted WQIs, the results of Tukey's HSD test and Tylor diagram reveal that there were no statistically significant differences between predicted and actual WQI values for all algorithms except SVM. In order to evaluate the predictive performance, the CV results indicate that the XGB, DT, and ExT algorithms had the lowest prediction errors compared to other models.

Therefore, the results of this research reveal that the DT, ExT, XGB, and RF models might be effective and robust for predicting coastal WQIs in terms of reducing the WQI model uncertainty. On the other hand, it is not easy to conclude which algorithm is "better" or "worst". The present study was observed to perform well for other models except SVM.

8.8 Discussion

WQI model is a widely used tool to assess water quality by employing straightforward mathematical functions. Computing WQI values is relatively complex using SI and indicator weight values (Leong et al., 2019). Because, recently, several studies have revealed that these components provide a considerable uncertainty to the final assessment (Uddin et al., 2021; 2022). In this circumstance, many studies utilized the ML technique for predicting WQI values, except for SI and weight values. In this research, we used eight ML algorithms for predicting the newly developed WQM-WQI model in order to identify the most robust technique in terms of assessing coastal water quality. In this research, the WQM-WQI revealed that the water quality in Cork Harbour can be classified into two categories: "fair" and "marginal" over the study period (Table 8.4). Comparatively, better water quality found in the lower and the outer Harbour than in the upper part (Figure 8.5). The past decade has setup an increase in the use of ETPs in this area. Recently, several annual reports of the EPA's Ireland revealed that the ETPs could contribute to raw wastewater discharges into the estuary directly without any modification of water attributes (Hartnett and Nash, 2015; Figure 8.1). As a result, it is expected that the water quality in the upper part of the Harbour's associated with relatively downgraded water quality due to the extremely loaded the wastewater.

In the present study, eight widely used algorithms tested in order to identify the most robust model. Details of the prediction results are provided in Figure 8.8 and Table 8.S5. Based on the model performance metrics, compared to the models, DT and Ext showed the outperformed capabilities to predict WQM-WQIs. However, model overfitting problems were found for these algorithms over the testing period due to the small dataset (Song and Lu, 2015; Vabalas et al., 2019) . Compared with other algorithms like SVM and KNN, the DT provides better results that are effective for the prediction (Huynh-Cam et al., 2021). Unlike the decision tree model, ensemble based bagging RF and boosting XGB algorithms outperformed in predicting WQM-WQIs during both training and testing periods. Recently, several studies have also revealed that the XGB algorithm is effective for predicting WQIs (Grbčić et al., 2021; Huan et al., 2020; Islam Khan et al., 2021; M. G. Uddin et al., 2022b). Because the ensemble based algorithms combine multiple DTs and consider the average of the output of all DTs for the prediction (Malek et al., 2022). In contrast, non-parametric KNN, Gaussian based GNB, and LR algorithms showed better performance than the SVM model. In this study, the worst performance found for the SVM during both the training and testing periods (Figure 8.6). Mostly, the SVM model performance is influenced by the distribution of input variables and the number of inputs (Vabalas et al., 2019). As shown in Figure 8.3, model inputs DOX, DIN, TON, and CHL had a negative left skew data distribution, whereas the remaining inputs had a normal distribution. The SVM model performance was worst during the testing period due to input variation because the SVM model prediction results are highly sensitive to the significant features (Kaliappan et al., 2021; Veropoulos et al., 1999). In addition, Akbani et al., (2004) point out three causes of performance loss in the SVM prediction model: (i) positive points lying further from the ideal boundary (Wu and Chang, 2003); (ii) weakness of soft-margins (Veropoulos et al., 1999); and (iii) imbalanced support vector ratio (Wu and Chang, 2003). Details of the contorlling factors of the sensitivity of the SVM model are discussed by (Akbani et al., 2004) and Veropoulos et al., (1999). In this study, the SVM model performance dropped during the testing period due to the imbalanced support vector ratio. Moreover, the lowest prediction errors (PREI) found for the DT, ExT, XGB and RF, respectively (Figure 8.11). The results of this study show that the DT, EXT, XGB, and RF algorithms are efficient for predicting WQM-WQIs in terms of the lowest prediction errors when compared to other models. However, the findings of this research could be helpful for monitoring and assessing coastal water quality using the WQM-WQI model incorporating robust ML technique(s).

8.9 Conclusion

The goal of this research was to determine the robust algorithm for predicting the coastal water quality index (CWQI) accurately in terms of model uncertainty. To achieve this goal, eight ML algorithms (DT, RF, XGB, KNN, SVM, ExT, LR, and GNB) were tested and validated for predicting CWQI in Cork Harbour. Predictive models were validated using a number of validators such as RMSE, MSE, MAE, R^2 and PREI. The findings of this study can be summarized as follows:

- Compared to CV results, the XGB showed the best outperformed, whereas the lowest training (RMSE = 3.3, MSE = 10.91, MAE = 1.67, and R2 = 1.0) and testing (RMSE = 0.0, MSE = 0.0, MAE = 0.02, and R2 = 1.0) errors were found, respectively.
- The lowest prediction errors were found for the DT (PREI = 0), ExT (PREI = 0), and XGB (PERI = + 0.1 to - 0.1). They perform better in predicting WQIs at each of the monitoring sites in Cork Harbour.

- Unlike the remaining models, the RF showed better performance; its errors ranged from +1.0 to -25), whereas the remaining models had higher underestimate and overestimate problems.
- Although the Tukey's HSD family wise multi-comparison results reveal that, there were no significant difference between actual and predicted WQIs among ML models except the SVM.

Therefore, it can be concluded, based on the results of this study, that tree-based (DT and ExT) and ensemble-based (XGB and RF) algorithms could be effective and robust for predicting the CWQI. The findings of this research would also have been much more useful in predicting WQIs at each monitoring site more accurately in order to reduce the uncertainty in the WQI model. This study's inadequacy to assess the water quality in terms of temporal resolution constitutes one of its limitations. Further studies should be carried out in order to validate the other algorithms in terms of predicting WQIs using temporal variability of data attributes.

8.10 Declaration of competing interest

The authors confirm that they did not experience competing financial interests or personal interactions that could have had potential influences on this paper.

8.11 Acknowledgement

The authors gratefully acknowledge the editor's and anonymous reviewers' contributions to the improvement of this paper. This research was funded by the Hardiman Research Scholarship of the National University of Ireland Galway, which funded the first author as part of his PhD program. The authors would like to thank the Environmental Protection Agency of Ireland for providing water quality data. The authors would like to acknowledge support from MaREI, the SFI Research Centre for Energy, Climate, and Marine research. The authors also sincerely acknowledge Charles Sturt University for providing all necessary supports to this PhD project through the international co-supervision.

8.12 References

Abbasi, T., Abbasi, S., 2012. Water Quality Indices, Water Quality Indices. https://doi.org/10.1016/C2010-0-69472-7

Abbasi, T., Abbasi, S.A., 2011. Water quality indices based on bioassessment: The biotic indices. J.

Water Health. https://doi.org/10.2166/wh.2011.133
Ahmad, Z., Rahim, N.A., Bahadori, A., Zhang, J., 2017. Improving water quality index prediction in Perak River basin Malaysia through a combination of multiple neural networks. Int. J. River Basin Manag. 15, 79–87. https://doi.org/10.1080/15715124.2016.1256297
Akbani, R., Kwek, S., Japkowicz, N., 2004. Applying Support Vector Machines to Imbalanced Datasets, in: European Conference on Machine Learning. San Antonio, USA, pp. 39–50. https://doi.org/10.1007/978-3-540-30115-8_7
Aldhyani, T.H.H., Al-Yaari, M., Alkahtani, H., Maashi, M., 2020. Water Quality Prediction Using Artificial Intelligence Algorithms. Appl. Bionics Biomech. 2020. https://doi.org/10.1155/2020/6659314
Aschonitis, V.G., Mastrocicco, M., Colombani, N., SalemiE., Kazakis, N., Voudouris, K., Castaldelli, G., 2012. Assessment of the intrinsic vulnerability of agricultural land to water and nitrogen losses via deterministic approach and regression analysis. Water. Air. Soil Pollut. 223, 1605–1614. https://doi.org/10.1007/s11270-011-0968-5
Babbar, R., Babbar, S., 2017. Predicting river water quality index using data mining techniques. Environ. Earth Sci. 76, 1–15. https://doi.org/10.1007/s12665-017-6845-9
Biebler, K.E.E., Jäger, B.P., Wodney, M., 2009. Basic principles of data mining, Social Implications of Data Mining and Information Privacy: Interdisciplinary Frameworks and Solutions. https://doi.org/10.4018/978-1-60566-196-4.ch015
Bui, D.T., Khosravi, K., Tiefenbacher, J., Nguyen, H., Kazakis, N., 2020. Improving prediction of water quality indices using novel hybrid machine-learning algorithms. Sci. Total Environ. 721, 137612. https://doi.org/10.1016/j.scitotenv.2020.137612
Calim, M.C., Nobre, P., Oke, P., Schiller, A., Siqueira, L.S.P., Castelão, G.P., 2018. A new tool for model assessment in the frequency domain – Spectral Taylor Diagram : application to a global ocean general circulation model with tides. Geosci. Model Dev. https://doi.org/10.5194/gmd-2018-5
Chang, N., Luo, L., Wang, X.C., Song, J., Han, J., Ao, D., 2020. A novel index for assessing the water quality of urban landscape lakes based on water transparency. Sci. Total Environ. 735, 139351. https://doi.org/10.1016/j.scitotenv.2020.139351
Chiang, L.C., Wang, Y.C., Chen, Y.K., Liao, C.J., 2021. Quantification of land use/land cover impacts on stream water quality across Taiwan. J. Clean. Prod. 318, 128443. https://doi.org/10.1016/j.jclepro.2021.128443
Chicco, D., Warrens, M.J., Jurman, G., 2021. The coefficient of determination R-squared is more informative than SMAPE, MAE, MAPE, MSE and RMSE in regression analysis evaluation. PeerJ Comput. Sci. 7, e623. https://doi.org/10.7717/peerj-cs.623
Cumming, G., Fidler, F., Vaux, D.L., 2007. Error bars in experimental biology. J. Cell Biol. 177, 7–11. https://doi.org/10.1083/jcb.200611141
Deng, T., Duan, H.-F., Keramat, A., 2022. Spatiotemporal characterization and forecasting of coastal water quality in the semi-enclosed Tolo Harbour based on machine learning and EKC analysis. Eng. Appl. Comput. Fluid Mech. 16, 694–712. https://doi.org/10.1080/19942060.2022.2035257
Elgeldawi, E., Sayed, A., Galal, A.R., Zaki, A.M., 2021. Hyperparameter tuning for machine learning algorithms used for arabic sentiment analysis. Informatics 8, 1–21. https://doi.org/10.3390/informatics8040079
EPA, 2017. Urban Waste Water Treatment, Official Journal of the European Union.
Fogarty P., 2017. Protecting Our Ocean’s Wealth-a proposal for legal protection of threatened marine species. Dublin.
Gao, Y., Qian, H., Ren, W., Wang, H., Liu, F., Yang, F., 2020. Hydrogeochemical characterization and quality assessment of groundwater based on integrated-weight water quality index in a concentrated urban area. J. Clean. Prod. 260, 121006. https://doi.org/10.1016/j.jclepro.2020.121006
Ghorbani, M.A., Deo, R.C., Karimi, V., Yaseen, Z.M., Terzi, O., 2018. Implementation of a hybrid MLP-FFA model for water level prediction of Lake Egirdir, Turkey. Stoch. Environ. Res. Risk Assess. 32, 1683–1697. https://doi.org/10.1007/s00477-017-1474-0
Gikas, G.D., Sylaios, G.K., Tsihrintzis, V.A., Konstantinou, I.K., Albanis, T., Boskidis, I., 2020. Comparative evaluation of river chemical status based on WFD methodology and CCME water quality index. Sci. Total Environ. 745, 140849. https://doi.org/10.1016/j.scitotenv.2020.140849
Grbčić, L., Družeta, S., Mauša, G., Lipić, T., Lušić, D.V., Alvir, M., Lučin, I., Sikirica, A., Davidović, D., Travaš, V., Kalafatović, D., Pikelj, K., Fajković, H., Holjević, T., Kranjčević, L., 2021. Coastal water quality prediction based on machine learning with feature interpretation and spatio-temporal analysis.

Haghiabi, A.H., Nasrolahi, A.H., Parsaie, A., 2018a. Water quality prediction using machine learning methods. Water Qual. Res. J. Canada 53, 3–13. https://doi.org/10.2166/wqrj.2018.025
Haghiabi, A.H., Nasrolahi, A.H., Parsaie, A., 2018b. Water quality prediction using machine learning methods. Water Qual. Res. J. 53, 3–13. https://doi.org/10.2166/wqrj.2018.025
Hartnett, M., Nash, S., 2015. An integrated measurement and modeling methodology for estuarine water quality management. Water Sci. Eng. 8, 9–19. https://doi.org/10.1016/j.wse.2014.10.001
Hassan, Md. Mehedi, Hassan, Md. Mahedi, Akter, L., Rahman, M.M., Zaman, S., Hasib, K.M., Jahan, N., Smrity, R.N., Farhana, J., Raihan, M., Mollick, S., 2021. Efficient Prediction of Water Quality Index (WQI) Using Machine Learning Algorithms. Human-Centric Intell. Syst. 1, 86. https://doi.org/10.2991/hcis.k.211203.001
He, X., Gou, W., Liu, Y., Gao, Z., 2015. A Practical Method of Nonprobabilistic Reliability and Parameter Sensitivity Analysis Based on Space-Filling Design. Math. Probl. Eng. 2015, 1–12. https://doi.org/10.1155/2015/561202
Huan, J., Li, H., Li, M., Chen, B., 2020. Prediction of dissolved oxygen in aquaculture based on gradient boosting decision tree and long short-term memory network: A study of Chang Zhou fishery demonstration base, China. Comput. Electron. Agric. 175, 105530. https://doi.org/10.1016/j.compag.2020.105530
Huynh-Cam, T.T., Chen, L.S., Le, H., 2021. Using decision trees and random forest algorithms to predict and determine factors contributing to first-year university students' learning performance. Algorithms 14. https://doi.org/10.3390/a14110318
Islam Khan, M.S., Islam, N., Uddin, J., Islam, S., Nasir, M.K., 2021. Water quality prediction and classification based on principal component regression and gradient boosting classifier approach. J. King Saud Univ. - Comput. Inf. Sci. https://doi.org/10.1016/j.jksuci.2021.06.003
Juwana, I., Muttil, N., Perera, B.J.C., 2016. Uncertainty and sensitivity analysis of West Java Water Sustainability Index - A case study on Citarum catchment in Indonesia. Ecol. Indic. 61, 170–178. https://doi.org/10.1016/j.ecolind.2015.08.034
Kaliappan, J., Srinivasan, K., Mian Qaisar, S., Sundararajan, K., Chang, C.Y., Suganthan, C., 2021. Performance Evaluation of Regression Models for the Prediction of the COVID-19 Reproduction Rate. Front. Public Heal. 9, 1–12. https://doi.org/10.3389/fpubh.2021.729795
Kärnä, T., Baptista, A.M., 2016. Evaluation of a long-term hindcast simulation for the Columbia River estuary. Ocean Model. 99, 1–14. https://doi.org/10.1016/j.ocemod.2015.12.007
Khan, Y., See, C.S., 2016. Predicting and analyzing water quality using Machine Learning: A comprehensive model. 2016 IEEE Long Isl. Syst. Appl. Technol. Conf. LISAT 2016. https://doi.org/10.1109/LISAT.2016.7494106
Khosravi, K., Mao, L., Kisi, O., Yaseen, Z.M., Shahid, S., 2018. Quantifying hourly suspended sediment load using data mining models: Case study of a glacierized Andean catchment in Chile. J. Hydrol. 567, 165–179. https://doi.org/10.1016/j.jhydrol.2018.10.015
Khullar, S., Singh, N., 2021. Machine learning techniques in river water quality modelling: A research travelogue. Water Sci. Technol. Water Supply 21. https://doi.org/10.2166/ws.2020.277
Kouadri, S., Elbeltagi, A., Islam, A.R.M.T., Kateb, S., 2021. Performance of machine learning methods in predicting water quality index based on irregular data set: application on Illizi region (Algerian southeast). Appl. Water Sci. 11, 1–20. https://doi.org/10.1007/s13201-021-01528-9
Leong, W.C., Bahadori, A., Zhang, J., Ahmad, Z., 2019. Prediction of water quality index (WQI) using support vector machine (SVM) and least square-support vector machine (LS-SVM). Int. J. River Basin Manag. 0, 1–8. https://doi.org/10.1080/15715124.2019.1628030
Malek, N.H.A., Wan Yaacob, W.F., Md Nasir, S.A., Shaadan, N., 2022. Prediction of Water Quality Classification of the Kelantan River Basin, Malaysia, Using Machine Learning Techniques. Water. https://doi.org/10.3390/w14071067
Nash, S., Hartnett, M., Dabrowski, T., 2011. Modelling phytoplankton dynamics in a complex estuarine system. Proc. Inst. Civ. Eng. - Water Manag. 164, 35–54. https://doi.org/10.1680/wama.800087
Othman, F., Alaaeldin, M.E., Seyam, M., Ahmed, A.N., Teo, F.Y., Ming Fai, C., Afan, H.A., Sherif, M., Sefelnasr, A., El-Shafie, A., 2020. Efficient river water quality index prediction considering minimal number of inputs variables. Eng. Appl. Comput. Fluid Mech. 14, 751–763. https://doi.org/10.1080/19942060.2020.1760942
Pham, B.T., Prakash, I., Khosravi, K., Chapi, K., Trinh, P.T., Ngo, T.Q., Hosseini, S. V., Bui, D.T., 2019. A comparison of Support Vector Machines and Bayesian algorithms for landslide susceptibility modelling. Geocarto Int. 34, 1385–1407. https://doi.org/10.1080/10106049.2018.1489422
Prasad, D.V.V., Venkataramana, L.Y., Kumar, P.S., Prasannamedha, G., Harshana, S., Srividya, S.J., Harrinei, K., Indraganti, S., 2022. Analysis and prediction of water quality using deep learning

and auto deep learning techniques. Sci. Total Environ. 821, 153311. https://doi.org/10.1016/j.scitotenv.2022.153311
Rahman, A., 2020. Statistics for Data Science and Policy Analysis, Statistics for Data Science and Policy Analysis. Springer Singapore. https://doi.org/10.1007/978-981-15-1735-8
Rahman, A., 2019. Statistics-Based Data Preprocessing Methods and Machine Learning Algorithms for Big Data Analysis | Rahman | International Journal of Artificial Intelligence™. Int. J. Artif. Intell. 17, 44–65.
Rahman, A., Harding, A., 2016. Small area estimation and microsimulation modeling, 1st ed, Small Area Estimation and Microsimulation Modeling. CRC Press. https://doi.org/10.1201/9781315372143/SMALL-AREA-ESTIMATION-MICROSIMULATION-MODELING-AZIZUR-RAHMAN-ANN-HARDING
Rezaie-Balf, M., Attar, N.F., Mohammadzadeh, A., Murti, M.A., Ahmed, A.N., Fai, C.M., Nabipour, N., Alaghmand, S., El-Shafie, A., 2020. Physicochemical parameters data assimilation for efficient improvement of water quality index prediction: Comparative assessment of a noise suppression hybridization approach. J. Clean. Prod. 271. https://doi.org/10.1016/j.jclepro.2020.122576
Seifi, A., Dehghani, M., Singh, V.P., 2020. Uncertainty analysis of water quality index (WQI) for groundwater quality evaluation: Application of Monte-Carlo method for weight allocation. Ecol. Indic. 117, 106653. https://doi.org/10.1016/j.ecolind.2020.106653
Sharif, O., Hasan, M.Z., Rahman, A., 2022. Determining an effective short term COVID-19 prediction model in ASEAN countries. Sci. Rep. 12, 1–11. https://doi.org/10.1038/s41598-022-08486-5
Smith, D.G., 1990. A better water quality indexing system for rivers and streams. Water Res. 24, 1237–1244. https://doi.org/10.1016/0043-1354(90)90047-A
Solanki, A., Agrawal, H., Khare, K., 2015. Predictive Analysis of Water Quality Parameters using Deep Learning. Int. J. Comput. Appl. 125, 29–34. https://doi.org/10.5120/ijca2015905874
Song, Y.Y., Lu, Y., 2015. Decision tree methods: applications for classification and prediction. Shanghai Arch. Psychiatry 27, 130–135. https://doi.org/10.11919/j.issn.1002-0829.215044
Stoner, J.D., 1978. Water-Quality Indices for Specific Water Uses. Geol. Surv. Circ.
Sutadian, A.D. hany, Muttil, N., Yilmaz, A.G. okhan, Perera, B.J.C., 2016. Development of river water quality indices-a review. Environ. Monit. Assess. 188, 58. https://doi.org/10.1007/s10661-015-5050-0
Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2018. Development of a water quality index for rivers in West Java Province, Indonesia. Ecol. Indic. 85, 966–982. https://doi.org/10.1016/j.ecolind.2017.11.049
Uddin, G., Nash, S., Olbert, A.I., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol. Indic. 122, 107218. https://doi.org/10.1016/j.ecolind.2020.107218
Uddin, M.G., Moniruzzaman, M., Quader, M.A., Hasan, M.A., 2018. Spatial variability in the distribution of trace metals in groundwater around the Rooppur nuclear power plant in Ishwardi, Bangladesh. Groundw. Sustain. Dev. 7. https://doi.org/10.1016/j.gsd.2018.06.002
Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment. Water Res. 118532. https://doi.org/10.1016/J.WATRES.2022.118532
Uddin, G., Nash, S., Olbert, A.I., 2022a. Optimization of Parameters in a Water Quality Index Model using Principal Component Analysis.
Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022b. Development of a water quality index model - a comparative analysis of various weighting methods, in: Çiner, P.D.A. (Ed.), Mediterranean Geosciences Union Annual Meeting (MedGU-21). Istanbul, pp. 1–6.
Uddin, M.G., Stephen Nash, Olbert, A.I., 2020. Application of Water Quality Index Models to an Irish Estuary, in: Kieran Runae, V.J. (Ed.), Civil and Environmental Research. Civil and Environmental Research, Cork, Ireland, pp. 576–581.
Vabalas, A., Gowen, E., Poliakoff, E., Casson, A.J., 2019. Machine learning algorithm validation with a limited sample size. PLoS One 14, e0224365. https://doi.org/10.1371/journal.pone.0224365
Veropoulos, K., Campbell, C., Cristianini, N., Others, 1999. Controlling the sensitivity of support vector machines, in: Proceedings of the International Joint Conference on Artificial Intelligence. pp. 55–60.
Villalobos-Arias, L., Quesada-López, C., Guevara-Coto, J., Martínez, A., Jenkins, M., 2020. Evaluating hyper-parameter tuning using random search in support vector machines for software effort estimation. PROMISE 2020 - Proc. 16th ACM Int. Conf. Predict. Model. Data Anal. Softw. Eng. Co-located with ESEC/FSE 2020 31–40. https://doi.org/10.1145/3416508.3417121

Wang, X., Zhang, F., Ding, J., 2017. Evaluation of water quality based on a machine learning algorithm and water quality index for the Ebinur Lake Watershed, China. Sci. Rep. 7, 1–18. https://doi.org/10.1038/s41598-017-12853-y

Wu, G., Chang, E.Y., 2003. Class-boundary alignment for imbalanced dataset learning. ICML Work. Learn. from Imbalanced Data Sets II 49–56.

Wu, J., Wang, Z., 2022. A Hybrid Model for Water Quality Prediction Based on an Artificial Neural Network, Wavelet Transform, and Long Short-Term Memory. Water (Switzerland) 14. https://doi.org/10.3390/w14040610

Xiong, Z., Cui, Y., Liu, Z., Zhao, Y., Hu, M., Hu, J., 2020. Evaluating explorative prediction power of machine learning algorithms for materials discovery using k-fold forward cross-validation. Comput. Mater. Sci. 171, 109203. https://doi.org/10.1016/j.commatsci.2019.109203

Xu, Z., Hou, Z., Han, Y., Guo, W., 2016. A diagram for evaluating multiple aspects of model performance in simulating vector fields. Geosci. Model Dev. 9, 4365–4380. https://doi.org/10.5194/gmd-9-4365-2016

Yan, F., Qiao, D., Qian, B., Ma, L., Xing, X., Zhang, Y., Wang, X., 2016. Improvement of CCME WQI using grey relational method. J. Hydrol. 543, 316–323. https://doi.org/10.1016/j.jhydrol.2016.10.007

Ying, X., 2019. An Overview of Overfitting and its Solutions. J. Phys. Conf. Ser. 1168. https://doi.org/10.1088/1742-6596/1168/2/022022

9. An improved methodology for the assessment of trophic status for coastal and transitional waters using machine learning and artificial intelligence approaches

This chapter was submitted in the Journal of **“Water Research”.** Under Review.

9.1 Chapter highlights

- The trophic status index (TSI) is one of the most extensively used methods for determining trophic status.
- To date, a variety of TSI models used for assessing trophic states have been developed. Recently, several studies have revealed that the existing TSI model produces a significant amount of uncertainty in the trophic assessment due to the inappropriate water quality indicators.
- Most TSI methods recommend a series of water quality indicators for the assessment of trophic states without any specific guidelines/framework.
- The research found that the existing TSI system’s inputs were highly influenced by the data redundancy problem.
- Due to the selection of inappropriate model input, the current techniques have produced a significant amount of uncertainty in measurement.
- For the conversion of the various indicator values into the uniform scale, there are no specific functions; most methods use log transformation functions for that purpose.
- In addition, the existing TSI system used a range of classification schemes for rating trophic status. Consequently, different techniques provided various ranks of trophic levels for the same water quality attributes.
- An improved methodology was developed for the assessment of trophic status for coastal and transitional waters using Cork Harbour as a case study.
- The proposed ATSI model consists of three components, including (i) the important indicator election process, (ii) the indicator conversion function, and (iii) the rating scheme, as follows with the improvement technique(s):
    1. Crucial indicators were selected using ML and AI techniques in order to avoid the data redundancy problem in the input.

(2) A linear rescaling function was developed for converting various water quality indicators into the ATSI score.
(3) A brand new classification scheme is proposed for determining the trophic state based on the OSPAR convention.

- The developed model was tested in four Irish waterbodies for assessing the trophic status.
- The model outcomes were validated using the EPA's water quality monitoring data.
- Model sensitivity was analyzed in terms of the spatial resolution of waterbodies.
- A series of statistical, mathematical, ML, and AI approaches were utilized to evaluate model performance as well as estimate model uncertainty.
- A comparative analysis was carried out between the newly developed ATSI model and the existing ATSEBI system of Ireland in order to determine the model's performance in terms of model uncertainty.
- A considerable amount of variation was found between the ATSI and ATSEBI models, whereas the results of the ATSI model are in line with the earlier studies.
- To the best of our knowledge, it was the first initiative to develop a systematic approach incorporating ML and AI approaches that takes care of the input data redundancy issue and model uncertainty.
- The results of this study could contribute to further advancements in the TSI model's state-of-the-art.

9.2 Abstract

Here, we present an improved methodology for the assessment of trophic status in transitional and coastal (TrC) waters using Cork Harbour, Ireland, as the case study in order to optimize the data redundancy problem of existing trophic assessment techniques. In this research, we proposed an assessment trophic status index (ATSI) model consisting of three crucial components: (i) selection process for water quality (WQ) indicators, (ii) function for obtaining the ATSI score, and (iii) classification scheme for translating the ATSI score. For the development of the ATSI model, ten WQ indicators for which data were available were initially considered, including water pH, transparency, temperature, dissolved inorganic nitrogen, biological oxygen demand, chlorophyll a (CHL), dissolved oxygen, total organic nitrogen, molybdate reactive phosphorus, and salinity. The crucial inputs for the ATSI model were selected using machine learning (ML) and artificial intelligence (AI) techniques in order to optimize input data redundancy. Prior to calculating the ATSI score, CHL prediction model was developed from the selected crucial dataset using the ten ML and AI algorithms to accurately predict the CHL. Compared to ten algorithms, the XGBoost showed excellent performance during both the training (RMSE = 0.0 , MSE = 0.0, MAE = 0.01) and testing (RMSE = 0.0, MSE = 0.0, MAE = 0.01) periods. Once the CHL prediction values were obtained, the ATSI scores were calculated using a linear rescaling interpolation function that was newly developed in this research. For ranking trophic status, a brand new classification scheme was proposed for TrC waters. The developed ATSI model was applied in four TrC waterbodies in Ireland for the assessment of trophic status in terms of the spatial sensitivity of the model, whereas the model's sensitivity and efficiency were evaluated using the coefficient of determination (R^2) and the NSE and MEF, respectively. The results of the model R^2 indicate that the model sensitivity was higher (R^2 = 1) across all application domains. The model efficiency and uncertainty results also reveal that the ATSI model efficiency was excellent in calculating the ATSI score across four domains in terms of reducing model uncertainty. The trophic assessment results of the ATSI model were found to be consistent with those earlier studies. In comparison to the existing ATSEBI system that is widely used in Ireland for the assessment of trophic status in TrC waters, a significant difference was found between the ATSI and ASTEBI systems across all domains except Mulroy Bay. However, the findings from the research could be helpful for further improving the trophic assessment techniques and monitoring of marine ecosystems.

Keywords: new methodology; ML and AI approach; ATSI model; trophic status assessment; coastal and transitional waters; Cork Harbour.

9.3. Introduction

Eutrophication is one of the major concerns for monitoring and assessing coastal and transitional (TrC) waters. Due to the abundance of nutrient components in the waterbodies, the eutrophication process accelerates (Andricevic et al., 2021; Frolov et al., 2013a; Giordani et al., 2009; Glibert, 2017; Parparov, 2010; Wurtsbaugh et al., 2019). Recently, a number of studies have revealed that the eutrophication process occurs tremendously in waterbodies and may be caused by natural and anthropogenic activities like urban wastewater, agricultural activities, domestic waste water, industrial waste water etc. (Devlin et al., 2011; Hartnett et al., 2012; O'Boyle et al., 2013; Uddin et al., 2018; 2022a; Uddin et al., 2022b; Uddin et al., 2020a). Algal blooms are the crucial indicator for the development of eutrophication, which is closely linked to the productivity rate of chlorophyll a and other phytoplanktons in the TrC ecosystem (Frolov et al., 2013; Glibert, 2017; Heisler et al., 2008; Wurtsbaugh et al., 2019). Gradually, the TrC ecosystem has become more complex due to the various functional activities in aquatic ecosystems (Frolov et al., 2013; Hartnett et al., 2012).

Therefore, in order to manage the TrC environment, it is essential to monitor and assess the trophic health of the ecosystems. For the purposes of the assessment of the ecosystem status, several tools and techniques have widely used in the literature, and the trophic status index (TSI) is one of them. In the recent years, many countries/organizations/researchers has been developed a number of TSI for assessing the trophic status in TrC waters, like as OSPAR model developed by the Oslo Paris Conventions for protecting the Northeast Atlantic marine environment (Devlin et al., 2011; Fiori et al., 2016; Hartnett et al., 2012; O'Boyle et al., 2013; Pettine et al., 2007; Wasmund et al., 2001), Assessment of Estuarine Trophic Status (ASSETS) developed based on a series of acts including the clean water act, coastal zone management act, harmful algae and hypoxia research and control act, and also the ocean act for conservation of the marine and coastal environment (Devlin et al., 2011; Ferreira et al., 2007; Xiao et al., 2007), environmental protection agency national coastal assessment system (EPA NCA) (Fergus et al., 2021; Gillett et al., 2015; Hale et al., 2016; Yurista et al., 2016), UK water framework directive (WFD) system (Carsten Von Der Ohe et al., 2007; Zotou et al., 2018), trophic status index (TRIX) (Andricevic et al., 2021; Fiori et al., 2016; Giovanardi and Vollenweider, 2004; Pettine et al., 2007; Primpas and Karydis, 2011; Yucel-Gier et al., 2011), Carlson Index (Carlson, 1984; El-Serehy et al., 2018), simple trophic status index (STSI) (O'Boyle et al., 2013), and assessment of trophic status of estuaries and bays in Ireland (ATSEBI) System developed based on OSPAR criteria for assessing trophic status in Ireland (O'Boyle et al., 2013; Toner et al., 2005). Commonly, the existing TSI model(s) consist of three identical components, including (i) WQ indicator selection, (ii) converting the indicator's measured value into a numerical scale, and (iii) determining trophic state using the respective indicator guidelines values, like the Carlson Index, TRIX, STSI, etc. Contrary, a few techniques only use two identical steps to determine the trophic state: (i) indicator selection, and (ii) determining the trophic state by comparing guideline values like the ATSEBI system, OSPAR comprehensive procedure (Devlin et al., 2011; O'Boyle et al., 2013; Toner et al., 2005). Recently, many studies have revealed that the existing TSI model(s) contributed a significant amount of uncertainty to the final assessment due to the variability of the model architecture (Carlson, 1984; Devlin et al., 2011; El-Serehy et al., 2018; Gupta, 2014; Hartnett et al., 2012; Liu et al., 2022; O'Boyle et al., 2013; Toner et al., 2005).

In terms of selecting WQ indicators, existing tools and techniques have widely used the common WQ indicators including chlorophyll-a, dissolved oxygen, total phosphorus, dissolved inorganic nitrogen, total nitrogen, dissolved inorganic phosphorus, phytoplankton, suspended particulate matter, Secchi depth, or transparency for the assessment of trbophic status in TrC waters (Bricker et al., 2003; Carlson, 1984; El-Serehy et al., 2018; Gupta, 2014; Hartnett et al., 2012; Hollister et al., 2016; Koussourdevis et al., 1989; O'Boyle et al., 2013; Pettine et al., 2007; Saluja and Garg, 2017; Tugrul et al., 2019; Xu and Jiao, 2018). A detailed list of WQ indicators for various trophic status assessment techniques is described in Devlin et al., (2011). A few studies have argued that the entire TSI model uses the multi-indicators approach for determining the trophic state (Carlson, 1984). These were useless techniques because of the number of indicators that must be measured or monitored by the typical monitoring programme (Carlson, 1984). The typical monitoring programme is relatively complex process involving a series of elements, including expert labour, infrastructural framework, legislation, sufficient funding and resources availability (Uddin et al., 2021; Uddin et al., 2022a). In addition, recently, several studies have revealed that the existing techniques produce a considerable amount of uncertainty in the final assessment due to the inappropriate selection of WQ indicators (Uddin et al., 2022a; 2022b; 2022d). To the best of the author's knowledge, there are no specific guidelines for selecting relevant/significant WQ indicators for the development of the trophic status methodology/tools/technique. Most studies have considered the WQ indicators based on the various WQ management policies/directives/frameworks like EU directives (for examples, the Water Framework Directive, the Habitats Directive, the Marine Strategy Framework Directive, the Urban Waste Water Directive, and the Nitrates Directive), OSPAR Convention, the USEPA NCA etc. without any statistical or mathematical justifications. A few studies have used the correlation technique for selecting the WQ indicator for assessing trophic status in TrC waters (Bennett et al., 2017; El-Serehy et al., 2018; Fiori et al., 2016; Kärcher et al., 2020; Matus-Hernández et al., 2018; Morgan et al., 2006; Nguyen et al., 2019). Many studies have only used nutrients, including CHL, for determining the ecological status (Carlson, 1984; Mnyango et al., 2022; Toner et al., 2005), whereas a few studies have used only water pH and DOX in order to assess the ecological environment (Gupta, 2014; Malek et al., 2011; O'Boyle et al., 2013). It is noted that, recently, a few studies have used only CHL for assessing the trophic state in coastal waterbodies (Duan et al., 2007; El-Serehy et al., 2018; Fu et al., 2016; Jamshidi et al., 2011; Lake et al., 2013; Malek et al., 2011; Mamun et al., 2021; Watanabe et al., 2015; Zhou et al., 2021). In addition, several studies have utilized machine learning and artificial intelligence techniques for assessing the trophic status and incorporating CHL prediction model(s) (Aldhyani et al., 2020; Khatri et al., 2021; Liu et al., 2022; Li et al., 2017; Matus-Hernández et al., 2018; Wei et al., 2019).

Moreover, a few studies have utilized the multiple linear regression (MLR) approaches for extracting the important indicators for determining the ecosystem environment (Almeida et al., 2021; Farnaz Nojavan et al., 2019; Hagy et al., 2022; Mamun et al., 2021 Parparov, 2010). Recently, several studies have revealed that the model performance significantly reduced in a MLR or ML models due to the data redundancy problems (Danasingh et al., 2020; Li et al., 2018; Westad and Marini, 2022). It might be associated in regression model from the multicollinearity problem of input variables. Commonly, it occurs when a number of dependent variables are highly correlated among them in a regression model (Danasingh et al., 2020; Westad and Marini, 2022). Therefore, it is essential to remove input redundancy from the MLR or ML models (Kim, 2019; Kraha et al., 2012; Shrestha, 2020). Due to the fact that the majority of current TSI models, particularly those that use multiple indicators, like the ATSEBI system, ASSETS, TRIX, and OSPAR comprehensive procedure, were suggested using the highly correlated WQ indicators as input variables for assessing the trophic status, these models have multicollinearity issues. A few studies have addressed the similar issue in literatures (Carlson, 1984; Liu et al., 2022; Markad et al., 2019; O'Boyle et al., 2013; Xu and Jiao, 2018). This problem can be clarified using an example, here, the authors considered the ATSEBI system for the analysis of multicollinearity, which is a model widely used for assessing the trophic status in Ireland. The model suggested four identical indicators, including dissolved oxygen, dissolved inorganic nitrogen, molybdate reactive phosphorus (MRP), and chlorophyll a (O'Boyle et al., 2013; Toner et al., 2005). In this research, an extensive multicollinearity problem was found among input indicators in terms of predicting CHL (see figure 4). Details of the ATSEBI system can be found in Section 2.7 below. Other TSI models that are currently in use have also been linked to the multicollinearity problem, which has a significant impact on the model's performance (Liu et al., 2022). Considering the mentioned circumstance of existing TSI techniques. The present study is proposed a novel approach for selecting crucial WQ indicators in developing the Assessment of Trophic Status Index (ATSI) model, incorporating multiple linear regression (MLR) and ML approaches in order to diagnose input data redundancy or multicollinearity issues (see section 9.4.4.1).

Another crucial component is the aggregation/transformation functions of the TSI models that is commonly used to calculate the TSI score by transferring various indicators information into a single numerical value (Andricevic et al., 2021; Fiori et al., 2016; Mnyango et al., 2022). Commonly, the index model used various types of aggregation functions, including weighted, unweighted, multiplicative, combined, etc. for converting different WQ indicator information into a unit-less numerical expression without losing or hiding any crucial information from the original data (Parween et al., 2022; Uddin et al., 2022a; 2022c; 2022d;2023a; 2023b; 2021). In the case of the trophic status index (TSI) model, most approaches utilize the logarithmic function for calculating the TSI score (Carlson, 1984; El-Serehy et al., 2018; Kumar and Mahajan, 2020; Li et al., 2021; Liu et al., 2022; Mamun and An, 2017; O'Boyle et al., 2013; Pérez-Ruzafa et al., 2019; Sathishkumar et al., 2022; Tugrul et al., 2019). A few studies have directly used indicator information to determine trophic status by comparing measured and guideline values (O'Boyle et al., 2013; Toner et al., 2005). To the best of the author's knowledge, there are no specific conversion function(s) for transferring different WQ indicators into a numerical value. Recently, a number of studies have revealed that the existing TSI models produced considerable uncertainty due to the inappropriate aggregation/transformation functions (Carlson, 1984; Kulshreshtha and Shanmugam, 2018; Rueda et al., 2007; Uddin et al., 2023a; Zhou et al., 2021). It should be revised and improved in order to improve the model's reliability while maximizing the model's uncertainty in the aggregation process.

Another crucial component is classification scheme for determining trophic status in marine ecosystems (Carlson, 1984; Devlin et al., 2011). A number of classification schemes have utilized the existing TSI system in order to obtain the trophic status in TrC waters. Details of the various classification schemes for different TSI models can be found in in Devlin et al., (2011). Recently, many studies have revealed that the entire trophic classification scheme(s) is very complex to determine the trophic state using a range of WQ criteria (Carlson, 1984; O'Boyle et al., 2013). A few studies have reported that the existing TSI models are contributed to the metaphoring problem (different interpretation for similar attributes of indicator due to the variability of classification schemes) of the model (Uddin et al., 2021; 2023b). Details of the metaphoring problem is described in (Uddin et al., 2023b)

However, the aims of this research is to develop an improved methodology for assessing trophic status in TrC waters using cutting-edge machine learning and artificial intelligence techniques in terms of reducing model uncertainty and improving reliability. The aims of this research were obtained by follows:

(i) In order to obtain the robust WQ indicators, the present study was utilized the MLR and ML techniques for avoiding the input redundancy problem (see Section 9.4.4.1)

(ii) After obtaining model input, a newly developed linear rescaling interpolation function was used to calculate the ATSI score without losing any significant information (see section 9.4.4.2).

(iii) Once the ASTI scores were calculated, trophic status was assessed using a brand new classification scheme that was developed based on the OSPAR criteria for assessing trophic status in marine ecosystems (see section 9.4.4.3).

(iv) When achieving trophic state, the present study also evaluated the model's efficiency and uncertainty in terms of the correct assessment of trophic state, which is the first initiative in developing a model for assessing trophic state.

(v) Finally, In order to assess the model's sensitivity with respect to the spatial resolution of application domains, an improved ATSI model was applied to four TrC waterbodies in Ireland for determining the trophic state.

This research paper is divided into six main sections. Rest of the paper, section 9.4 – 9.7 a brief overview of this study, discusses a new set of tools and techniques that are applied to develop the ATSI model and its uncertainty. The results and findings in developing the ATSI model are provided in section 9.8, the ATSI model applications and results are presented in section 9.9 – 9.10 and finally in section 9.11 conclusions are drawn from this study.

9.4. Materials and methods

9.4.1 Model application domain

For the purposes of the development of the ATSI model, the present study selected the Cork Harbour based on the two consideration (i) it is the most heavily populated and largest natural Harbour in Ireland and (ii) full suite WQ monitoring data availability. Moreover, recently, several studies have revealed that the ecological status and water quality in Cork Harbour significantly depleted due to the various natural and anthropogenic pressures like river waste pressures, river agricultural pressures, run-off pressures, etc. Details of the pressures are graphically visualized in Figure 9.14. The Harbour is designated as a Special Protection Area (SPA) under the 1979 Wild birds Directive (79/409/EEC), and it is Ireland's deepest and longest (17.72 km) surface water body (Hartnett and Nash, 2015; Uddin et al., 2022a; 2022b; 2022c). It is located at the mouth of the River Lee in Cork City. It is the longest river, including larger reservoirs that inflow the main stream into the Harbour (Uddin et al., 2022a; 2022b; 2023b).

The city of Cork is the industrial hub of the southwest Irish region, and the surrounding hinterlands are subject to relatively intense agricultural activities that influence Harbor’s water quality and the ecological environment in the region (Hartnett et al., 2012). The area adjacent to the Harbour is also one of Ireland's most economically promising zones (Hartnett et al., 2012). Moreover, the Harbour receives large quantities of effluent from various sources each year, such as industries and domestic and municipal waste, which results in variable water quality throughout the Harbour (Hartnett et al., 2012; Nash et al., 2011; Uddin et al., 2022a; 2022b; 2020a; 2020b). It should be noted that a considerable amount of raw effluent discharges enter the Harbour directly from the seven wastewater treatment plants (WWTPs) (Uddin et al., 2023a; 2022a; 2022b). Details of the WWTPs location and WQ monitoring sites are presented in figure 9.1. Moreover, the geological components of the Harbour' are enriched with more nutrient elements, they are essential for maintaining the ecosystem and fresh water quality. After developing, the ATSI model was tested in three waterbodies, including (i) Dublin Bay, (ii) Galway Bay, and (iii) Mulroy Bay, in order to assess the sensitivity of the model in terms of spatiotemporal resolution. Details of the application domains are presented in Figure 9.1.

9.4.2 Data description

To the development of the ATSI model, the water quality (WQ) data was achieved from the Environmental Protection Agency (EPA), Ireland' WQ monitoring database. Commonly, the EPA collects WQ data monthly from number of particular monitoring sites in several national and local water bodies. Details of the WQ data attributes can be found in cloud based database at https://www.catchments.ie/data/). For the development to the ATSI model, initially ten WQ indicators were obtained of Cork Harbour from the database 2021 including 37 monitoring sites. Details of the monitoring sites and Harbour attributes are presented in Figure 9.1 and Table 7.S1. The average concentration of ten indicators including salinity (SAL), biological oxygen demand (BOD), dissolved oxygen (DOX), chlorophyll a (CHL), molybdate reactive phosphorus (MRP), water pH, total oxidised nitrogen (TON), water transparency (TRAN), dissolved inorganic nitrogen (DIN) and water temperature (TEMP) were used in this research. Details of the WQ indicators, unit and their guideline values are provided in Table 9.S1 and Figure 9.3 presents a statistical summary of WQ indicators, respectively.

For the purposes of testing the ATSI model, similar WQ attributes were obtained from the EPA's database for Dublin Bay, Galway Bay and Muroy Bay. Details of the monitoring sites and physical attributes of Bays are presented in Figure 9.1. Average concentration of selected ten WQ indicators concentration can be found in Table 9.S1.

For consistency of data attributes, only 1 m depth samples from the water surface were considered in this study.

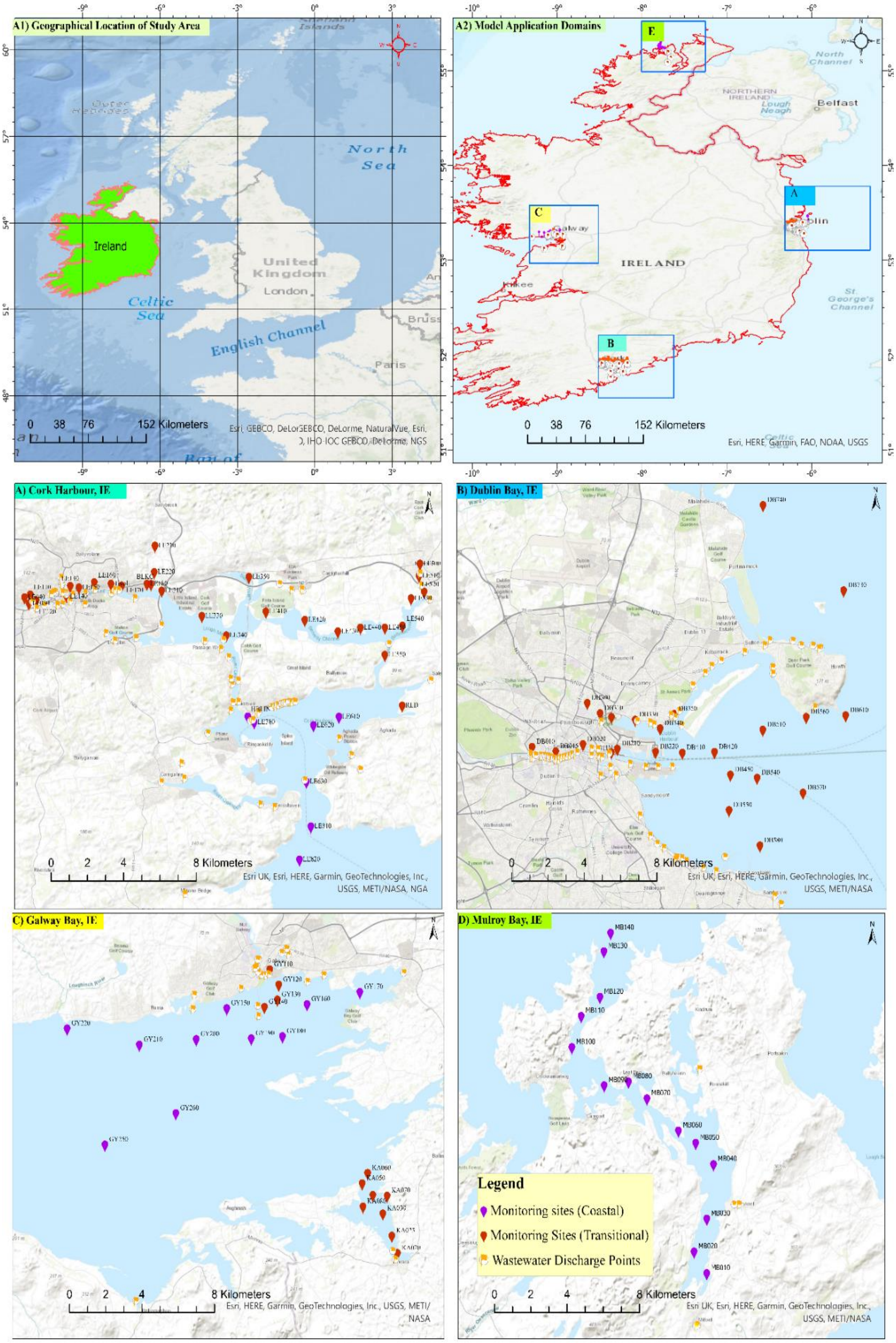


Figure 9.1. Model development and tested domains in Ireland.

9.4.3 Data standardization

Prior to the further analysis, WQ data standardization is an important task to avoid unexpected any biasness in analysis or minimizing the training errors in a prediction models (Md. G. Uddin et al., 2022g). Commonly, this techniques allows converting WQ data into a uniform scale (Rahman, 2020; Rahman and Harding, 2016; Uddin et al., 2022b). In order to standardize data, the present study was utilized the approach of Uddin et al., (2022b). Details of the procedures can be found in Uddin et al., (2022b).

Table 9.1 Standard thresholds (guideline) of water quality indicators for coastal and transitional waters.

	General Indicators	unit	Standard threshold (summer)	
			Lower	Upper
	BOD5$^{(ii)}$	mg/l	0	7
	pH$^{(iii)}$	-	5	9
	TEMP$^{(ii)}$	^{0}C	-	25
	TON$^{(iv)}$	mg/l as N	0.0	2
	TRAN$^{(v)}$	m/depth	>1	-
(a) Cork Harbour	Nutrients indicators		*thresholds for SAL median value of 31*	
	DOX$^{(i)}$	% sat	78	122
	MRP$^{(i)}$	mg/l as P	0.0	0.044
	DIN$^{(i)}$	mg/l	0.0	0.51
	CHL	µg/l	11.1	22.2
(b) Dublin Bay			*thresholds for SAL median value of 31*	
	DOX$^{(i)}$	% sat	78	122
	MRP$^{(i)}$	mg/l as P	0.0	0.044
	DIN$^{(i)}$	mg/l	0.0	0.51
	CHL	µg/l	11.1	22.2
(c) Galway Bay			*thresholds for SAL median value of 29*	
	DOX$^{(i)}$	% sat	77	123
	MRP$^{(i)}$	mg/l as P	0.0	0.047
	DIN$^{(i)}$	mg/l	0.0	0.630
	CHL	µg/l	11.7	23.3
(d) Mulroy Bay			*thresholds for SAL median value of 33*	
	DOX$^{(i)}$	% sat	79	121
	MRP$^{(i)}$	mg/l as P	0.0	0.042
	DIN$^{(i)}$	mg/l	0.0	0.380
	CHL	µg/l	10.6	21.1

9 *ATSEBI standards, determine the standard values based on median value of Salinity (see details* (Toner et al., 2005b)*, pp. 72 – 76).*
10 *EPA, Ireland (2001), recommended values for the surface water/freshwater/river water/aquatic life.*
11 *Estuary Monitoring Manual for pH and Alkalinity, EPA,USA*
12 *The European Communities (Quality of surface water intended for the abstraction of drinking water) regulations, 1989 (S.I. No. 294/1989).*
13 *Bathing Water Quality Regulations 2008, (S.I. No. 79/2008).*

9.4.4 Methodology for assessment of tropic status index (ATSI) model

Typically, most TSI models were developed using the simple linear regression model (Clarke et al., 1997; Mamun and An, 2017; Nguyen et al., 2019). In this paper, we proposed a new approach for the assessment of trophic status that is called as "ATSI" model. It consist three components including (i) input selection process, (ii) ATSI function and (iii) ATSI scores translation scheme. A schematic framework of the ATSI development process is presented in Figure 9.2. These are now described for the developed ATSI model below.

9.4.4.1 Indicator selection technique

Input selection is a crucial component in developing a model because irrelevant input attributes can produces model uncertainty or biasness to the final assessment (Uddin et al., 2022a; 2022d; 2023a; 2021)**.** For developing the robust model, it is essential to select the crucial WQ indicators. A number of tools and techniques including principal components analysis, correlation technique, multiple linear regression (MLR) analysis etc. have utilized to select the important indicators in developing water quality model like water quality index model (Uddin et al., 2022d). Recently, many studies have used cutting edge of the machine learning and artificial intelligence techniques for selecting the crucial variables or indicators from a given dataset to enhance the model performance (Uddin et al., 2022a; 2022d). To the development of the ATSI model, the present study was utilized a comprehensive approach incorporating MLR and machine learning techniques for selecting important WQ indicators.

Before developing any model, input selection is an important step. Recently, many studies have reported that model performance could be affected due to inappropriate input selection (Uddin et al., 2022a; 2022d, 2022e; 2021). A number of problems have been associated with the inappropriate selection of model input; the multicollinearity problem is one of them (Yoo and Cho, 2019; Yu et al., 2015; J. Zhang et al., 2022). Because multicollinearity problems can reduce the model's performance in MLR or any other prediction models, it occur when multiple independent variables are highly correlated with one another in a regression model (Filstrup and Downing, 2017; Ogorodnyk et al., 2019; Park et al., 2022; Shin et al., 2020). Due to the multicollinearity problem, regression model performance drops significantly because it reduces the model regression coefficient with small changes in the model inputs

(Rahman, 2019; Yoo and Cho, 2019; Yu et al., 2015). Recently, several studies have revealed that the multicollinearity problem has significantly reduced the model's accuracy and also caused the overfitting problem in machine learning or prediction model studies of CHL (Filstrup and Downing, 2017; Kim and Ahn, 2022a; Park et al., 2022; Shin et al., 2020; Yoo and Cho, 2019; J. Zhang et al., 2022). A few studies suggested that it is essential to check the multicollinearity problem before developing any model(s) (Yoo and Cho, 2019; Yu et al., 2015). Commonly, the multicollinearity problem is identified using several tools and techniques, like the variance inflation factor (VIF), Pearson correlation, Eigen value, condition index, etc (Daoud, 2018; Dormann et al., 2013; J. Zhang et al., 2022). The VIF technique provides detailed information on highly correlated independent variables and measures multicollinearity in regression analysis. This technique is widely used for identifying the multicollinearity problem in data science studies, including water research. Recently, a number of studies have utilized this technique for developing a water quality prediction model in terms of selecting the crucial WQ indicators. In this research, we used the VIF test and Pearson correlation analysis techniques for selecting crucial indicators in order to develop the ATSI model in terms of avoiding the multicollinearity problem in model input. For the purposes of multicollinearity analysis, two identical techniques were utilized in this research including-

(i) Variance inflation factor (VIF) analysis

The VIF is a statistical measure of multicollinearity that helps to estimate how much the variance of a regression coefficient is inflated due to multicollinearity in the MLR model (Ogorodnyk et al., 2019; Shin et al., 2020; Yu et al., 2015; J. Zhang et al., 2022). The VIF can be defined as:

$$\boldsymbol{VIF_i = \frac{1}{1 - R_i^2}} \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots..(\mathbf{9.1})$$

Where $\boldsymbol{R_i^2}$ indicates that the coefficient of determination between the i^{th} water quality indicators and all others indicators in a MLR model, $\boldsymbol{VIF_i}$ refers variance inflation factor of the i^{th} explanatory variable.

(ii) Pearson correlation technique

Correlation analysis is a widely used statistical measure for determining the relationship between or among variables. Commonly, the Pearson product moment correlation coefficient is most widely used in any research, including research on water resources. Its score ranges from -1 to +1, where values close to 1 indicate a strong correlation (negative or positive) and values close to 0 indicate a weak negative or positive relationship (Kothari et al., 2021; Schober and Schwarte, 2018). In this research, the Pearson correlation analysis was utilized in order to determine the degree of relationship between or among water quality indicators and CHL. The Pearson correlation expression can be follows:

$$r = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}} \quad \dots\dots\dots\dots\dots (9.2)$$

Where n is the number of observation, r is Pearson correlation, x_i is the ith water quality indicator, whereas $\bar{x}$ refer to the mean value of *x,* similarly, y_i presents the ith target water quality indicator and $\bar{y}$ is the mean value of *y*.

9.4.4.1.1 MLR model

For the purposes of the effect analysis of multicollinearity on the CHL predictive model, the present study used the multiple linear regression analysis (MLR) method. Recently, several studies have utilized this technique for assessing the impact of multicollinearity on the prediction models in literature (Dias Curto and Castro Pinto, 2007; Kraha et al., 2012; P. Obite et al., 2020; Rahman, 2020; Rahman et al., 2013; Shrestha, 2020; Yoo and Cho, 2019). In addition, many water research studies have extensively used this approach to develop an efficient prediction model with the best possible input (Band et al., 2020; Best et al., 2008; Cho and Lee, 2018; Mohd Zebaral Hoque et al., 2022; Siddik, 2022; Sokolova et al., 2022). In order to perform the MLR analysis, prior to commencing the MLR, multicollinearity analysis was conducted using the VIFs and Pearson correlation techniques these are mentioned in earlier section. After obtaining the multicollinearity results, seven MLR models were developed using seven sets of input; these were selected based on the VIFs and correlation results. Table 4 presents the details of the MLR models, various sets of input (predictors), and their formulating criteria and response (CHL). Once the MLR models were constructed, the best possible set of input was selected for the CHL prediction model based on the three evaluation metrics including mean square error (MSE), root mean square error (RMSE), and coefficient of determination

(R^2). root MSE, MSE and R^2. In this study, the model performance metrics were calculated using the methodology of Uddin et al., (2022a). Details of the various performance metrics can be found in Uddin et al., (2022b). Table 5 provides the different MLR models' performance metrics. Robust algorithm(s) was/were selected by comparing ten widely used machine learning (ML) algorithms for predicting CHL in TrC waters using the best input for the development of an effective CHL prediction model. Details of the ML approaches are described in Section 9.4.4.1.2.

9.4.4.1.2 Prediction approaches

Commonly, the ML algorithm(s) are widely used to predict unknown objects in terms of reducing the computational cost and uncertainty (Uddin et al., 2022b, 2022d). Recently, several studies have utilized this approach to predict CHL for the assessment of trophic status (Abdi et al., 2020; Aldhyani et al., 2020; Angel and McCabe, 2022; Bonansea et al., 2015; Kärcher et al., 2020; Kim and Ahn, 2022; Malek et al., 2011; Matus-Hernández et al., 2018; Mozo et al., 2022; Wei et al., 2019). Moreover, a number of water research studies have revealed that the ML techniques could be effective in minimizing input data redundancy (Ahmad et al., 2017; Kouadri et al., 2021; Uddin et al., 2022a; 2022b, 2022d). Many studies have used this approach for detecting the multicollinearity problem in a prediction model for the assessment of water quality in the literature. It is noted that, recently, the authors have revealed that the ML approach is an effective and reliable tool for reducing water quality model uncertainty in terms of minimizing the input variables (Degenhardt et al., 2019; Speiser et al., 2019; Uddin et al., 2022a; 2022b). Therefore, the present study utilized this technique to achieve the following goals: (i) to validate the optimal input for developing the CHL prediction model in terms of predicting CHL accurately, and (ii) to identify the best algorithm(s) and optimize the parameters for developing a CHL prediction model for assessing the tropic status in TrC waters.

(i) Preparing training and testing datasets

Prior to the development of the ML models, WQ dataset was divided into two sets (i) 70 % (26) of training and 30% (11) of testing. The details of ML input datasets are given in Table 9.S1.

(ii) Constructed ML models

After preparing datasets, for the purposes of obtaining the goals of the ML approaches, the present study was utilized ten widely used ML algorithms including Extreme Gradient Boosting (XGBoost), CatBoost, deep neural network (DNN), Random Forest (RF), Decision Tree (DT), Extra Tree (ExT), K-Nearest Neighbors (KNN), Support Vector Machine (SVM), Gaussian Naïve Bayes (GNB) and multiple linear regression (MLR) for predicting CHL. Details of the algorithms are discussed in an earlier study by the authors, Uddin et al., (2022b). These algorithms were selected in this research based on the recommendations of literatures, because many studies have used widely for predicting water quality as well as CHL prediction. Moreover, recently, several studies have revealed that tree based (like DT and ExT) and ensemble tree based algorithms (like RF, XGBoost, CatBoost) showed better performance than other methods (Bui et al., 2020; Kouadri et al., 2021; Uddin et al., 2022a; 2022b; 2022d).

(iii) Hyper-parameters tuning technique

Commonly, tuning the hyper-parameters is an essential step to obtaining the higher performance of ML models in predicting results (Elgeldawi et al., 2021; Uddin et al., 2022a; 2022b; Villalobos-Arias et al., 2020). A number of techniques are widely utilized in ML studies in order to obtain the best possible set of hyperparameters for the algorithm(s); the grid search technique is one of them (Ghawi and Pfeffer, 2019; Jiang and Xu, 2022; Shekar and Dagnew, 2019; Uddin et al., 2022a; 2022b; 2022d). In addition, a few studies have revealed that the grid search technique is effective for avoiding the over-fitting problem (Elgeldawi et al., 2021; Yao et al., 2015). Therefore, the present study utilized the grid search technique in order to obtain the optimal hyperparameters and their values for developing a robust CHL prediction model according to the methodology of Uddin et al., (2022b). Details of the optimal parameters for various ML models are provided in Table 9.S3.

9.4.4.2 Aggregation function

In the present study, a linear rescaling interpolation function was proposed to convert the model input into a numerical form without losing any real information about the input’s indicators. It ranges from 0 to 100, where 0 indicates the "worst" trophic status and 100 is "excellent" status. The proposed linear rescaling function was developed based on the standard threshold values of the CHL. Details of the CHL standard threshold values and their obtaining procedures are presented in Table 1 and Section 2.8, respectively. It can be defined as follows:

$$ATSI = (NF_h - NF_l) - \left[\frac{\left(CHL_c - CHL_{t_l}\right)}{\left(CHL_{t_u}\right)}\right] \times NF_h \; \ldots\ldots\ldots\ldots (9.3)$$

where NF_h is the higher value (100) of normalization factor, NF_l lower value (0) of normalization factor, CHL_c is the chlorophyll a concentration level whereas c refers to the measured or predicted concentration, CHL_{t_l} is the threshold lower value, and CHL_{t_u} is the threshold upper value, respectively, for the guidelines value of CHL that are obtained based on the median value of salinity. The details of the procedure for obtaining the WQ indicator's criteria are discussed in Section 9.8.

9.4.4.3 ATSI model score translation

Most index models have the ultimate goal of converting the numerical value (well known as the index score) into qualitative measures like "excellent", "good", "bad" etc. Like other index models, the ATSI model's ultimate goal is to translate the ATSI score into categorical measures using a particular classification scheme. Most indexes commonly use a 0 to 100 score for translating the scores, where 0 indicates the "worst" and 100 is the "good" state of trophic. For the purposes of interpreting the ATSI score, the present study proposed a brand new classification scheme for assessing the trophic state in TrC waters. Table 9.2 provides the detailed classification scheme for TrC waters. The classification scheme developed (modified) based on the ATSEBI system. Details of the ASTEBI system can be found in Toner et al., (2005).

Table 9.2 Proposed a new classification scheme for the assessment of trophic status using ASTI model.

Classes	Threshold of ASTI score	Definition
(i) Unpolluted	≥ 80	Recommended water quality indicators meet the guidelines' values, and water bodies are lowly productive due to the lowest levels of nutrients.
(ii) Moderate	50 – 79	Water bodies are moderately productive, and at least one or two indicators have breached the guidelines.
(iii) Eutrophic	30 - 49	The majority of indicators fail to meet the guidelines' values, and waterbodies are highly productive.
(iv) Hypertrophic	≤ 29	All the recommended indicators are breached the guidelines' values; enrichment of nutrient components significantly increases the growth of algae, and undesirable water quality disturbances occur simultaneously.

9.5 Model sensitivity analysis

A "model sensitivity study" refers to the study of the relationship between model input and output (Chen et al., 2020; Chicco et al., 2021). It can be determined how much the input influences the model's output (Chicco et al., 2021; Hamby, 1995; Uddin et al., 2022a; 2022b; 2022d; 2023a). There are a range of tools and techniques used to determine the model's sensitivity, and the coefficient of determination (R^2) is one of the most effective measures to assess the effects of model input on output (Chen et al., 2020; Hamby, 1995, 1994; Suvarna et al., 2022; W. Zhang et al., 2022). Recently, many water research studies have utilized this technique for evaluating the model's sensitivity (Singh and Rashmi, 2014; Uddin et al., 2022a; 2022b; 2023a; W. Zhang et al., 2022). Usually, its values range from 0 to 1, where 1 indicates "excellent" agreement between model input and output and 0 refers to "worst" (Uddin et al., 2022a). For the purposes of sensitivity analysis, the present study utilized this technique according to the methodology of Uddin et al., (2022a). Details of the methodology are described in Uddin et al., (2022a).

9.6 Model uncertainty analysis

For the purposes of estimating model uncertainty, a number of tools and techniques are used, but Monte Carlo simulation (MCS) is the most widely used technique (Pasquier et al., 2016; Seifi et al., 2020a; Shaw, 2017; Uddin et al., 2023a). Recently, several studies have utilized this method for estimating uncertainties. A few studies have used machine learning (ML) approaches to calculate the model uncertainty by incorporating the MCS (Abdar et al., 2021; Tavazza et al., 2021; Uddin et al., 2023a). In this research, for quantification of model uncertainty, the Gaussian process regression (GPR) ML technique was applied, incorporating the MCS technique. Because, this technique can predict measured values with a 95% confidence interval (CI). Recently, a number of studies have performed this novel approach for quantification of water quality model uncertainty. In order to calculate the ATSI model uncertainty with 95% of CI, the present study utilized the improved methodology of Uddin et al., (2023a). Details of the methodology can be found in Uddin et al., (2023a). To obtain better performance from the GPR-ML model, 10,000 random samples were generated for predictors (CHL) and responses (ASTI scores) and utilized to develop the GPR prediction model using the MCS technique. The GPR model's best optimal parameters, parameterization technique, and details of the MCS methodology for generating random samples can be found in (Uddin et al., 2023a). After obtaining the predicted CI and ATSI scores, the ATSI model uncertainty was modelled using the inferential error technique using the approach of (Cumming et al., 2007), because a number of studies have utilized this technique (Commowick and Warfield, 2010; Cumming et al., 2007; Cumming and Finch, 2005; Jolliffe, 2007; Krueger, 2017; Seifi et al., 2020). The inferential CI can be defined as:

$$Inferential\ CI = M_o \pm t_{(n-1)} \times SE \quad \dots\dots\dots\dots\dots\dots..(9.4)$$

Where M_o is the observation mean, $t_{(n-1)}$ is a critical values of t, and SE is the standard error.

9.7 Model efficiency analysis

For the purposes of the model efficiency analysis, a number of tools and techniques have utilized in literature. Recently, several studies have widely used various performance metrics, including mean square error, ones are bias, correlation coefficient , etc., for measuring the model's efficacy in water modelling and research. The Nash-Sutcliffe efficiency (NSE) is one of the most commonly used techniques (Baloch et al., 2015; McCuen et al., 2006; Şen et al., 2022; Uddin et al., 2022a; 2022d). Its value ranges from -∞ to 1, whereas close to 1 indicate the “excellent” performance and 0 is “poor” (Camera et al., 2020; Guo et al., 2019; Moriasi et al., 2015; Uddin et al., 2022d). A few studies have utilized an improved metric, the model efficiency factor (MEF), in order to assess model efficiency in terms of predicting errors (Sharif et al., 2022; Uddin et al., 2022d, 2022e). Unlike the NSE score, the MEF score ranges from 0 to 1, where 0 indicates "excellent" efficacy of the model and 1 refers to "worst". Therefore, the present study utilized NSE and MEF metrics for measuring the ATSI model efficiency in terms of XGBoost prediction errors in assessing the trophic status across four coastal and transitional waterbodies using the methodology of Uddin et al., (2022d). (Uddin 2022d). Details of the methodology for assessing water quality model efficiency can be found in Uddin et al., (2022d).

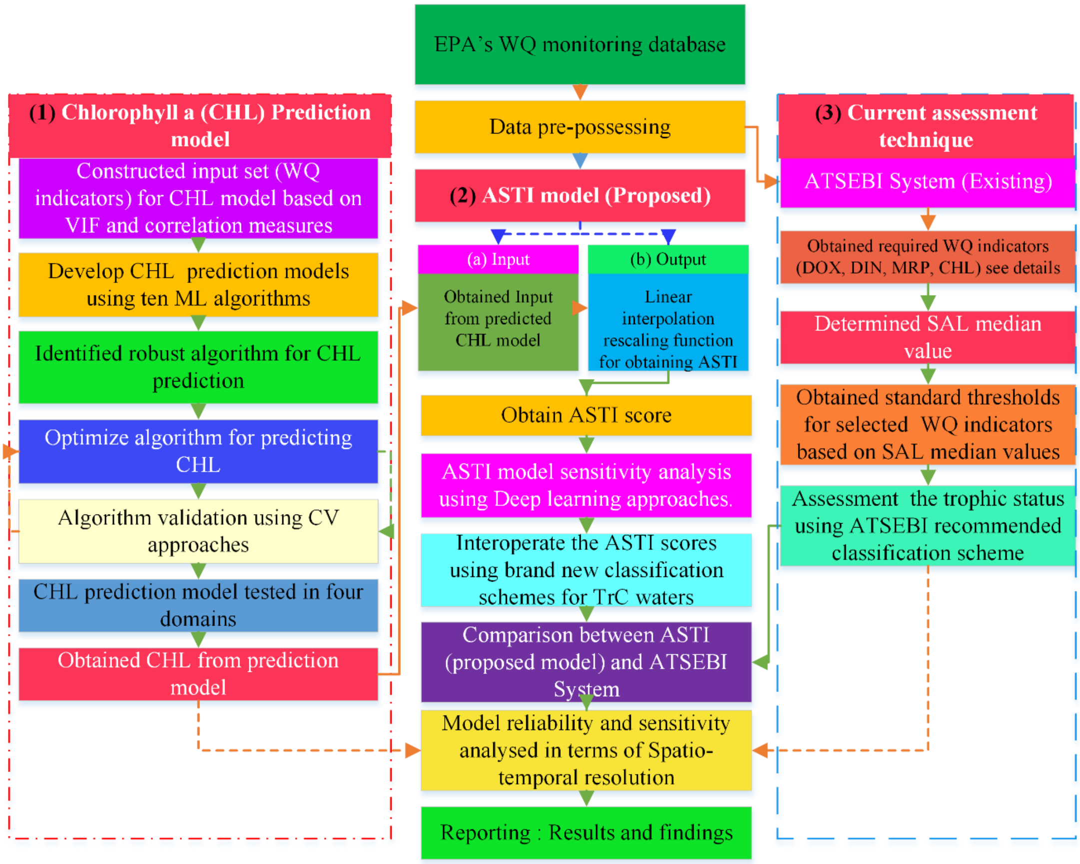


Figure 9.2. A schematic methodological framework of this research.

9.8 Assessment of Trophic Status of Estuaries and Bays in Ireland (ATSEBI) System

In order to assess the performance of the new ATSI approach, the present study was compared the results between the ATSI model and existing ATSEBI system. The Environmental Protection Agency (EPA), Ireland in 2001, has developed the ATSEBI System. Mainly, this technique developed based on the OSPAR (Oslo and Paris) guidelines for protecting the marine environment. The primary purposes of this technique is to the assessment of trophic status in coastal and transitional waters. To the best of the author's knowledge, up to now, this approach is widely used by the EPA, Ireland for assessing the trophic status in coastal and transitional waters. Details of the ATSEBI system development history, architecture and its components can be found in Toner et al., (2005). The ATSEBI system composes of three typical components including (i) Particular water quality indicators (input), (ii) Obtaining criteria of indicators and (iii) determining the trophic status.

(i) Particular water quality indicators

The ATSEBI system recommended four identical water quality indicators including (i) saturated dissolved oxygen (DOX), (ii) dissolved inorganic nitrogen (DIN), (iii) molybdate reactive phosphorus of total phosphorus (MRP), and (iv) chlorophyll a (CHL). Details of the indicators selection procedures are discussed in Toner et al., (2005).

(ii) Obtaining criteria of indicators

For the purposes of the determination of trophic status, it is required to obtain the standard threshold values of water quality indicators. Recently, several studies have revealed that transitional and coastal water quality characteristics are primarily controlled by the variation in the degree of mixing of fresh and marine waters, as reflected by salinity. Consequently, it is essential to scale the criteria for water quality indicators based on the characteristics of salinity (SAL). In order to obtain the criteria values for four indicators (DOX, DIN, MRP, and CHL), the present study utilized the SAL median value for the determination of the threshold value of the criteria according to the approach of Toner et al., (2005). Details of the procedures for obtaining criteria for indicators can be found in Toner et al., (2005). Table 9.S2 provides the full range of the SAL median values and their corresponding criteria values for various indicators.

(iii) Determining the trophic status.

The ultimate goal of the ATSEBI system is to assess trophic status. For the assessment of trophic status, the ATSEBI system adopted a range of criteria for the determination of trophic status. Table 9.3 provides the classification scheme and their definition. Commonly, the ATSEBI system determined the trophic status by comparing between indicators measured and criteria values (see Table 9.1). Commonly, the ATSEBI system determined the trophic status by manually comparing the indicator values to the criteria values (see Table 9.1). The determination processes can be clarified by an example as below-

For example, the MRP criterion is scaled from 0.0 mg/l as P to 0.044 mg/l as P at the 31 SAL median value in Cork Harbour (Table 9.1). As assumed, the present study found 0.21 mg/l as P at x monitoring site; if the measured MRP does not fall within the criteria range, the MRP has breached the criteria.

Table 9.3 Criteria for determining the trophic status of TrC waters according to ATSEBI system of Toner et al., (2005).

Trophic state	Definition
(i) Unpolluted	Unpolluted of water are those that do not exceed any of the requirements.
(ii) Intermediate	Waterbodies are those that do not fall into the groups of Eutrophic or Potentially Eutrophic, but in which one or two of the requirements are breached;
(iii) Potentially eutrophic	Waterbodies are those that breach two of the indicators and fall within 15% of the applicable threshold value / values in the third.
(iv) Eutrophic	Waterbodies are those in which one of the requirements is exceeded, i.e. where simultaneously elevated nutrient concentrations, rapid plant growth, and unacceptable disruptions of water quality occur.

9.9. Results and discussion

9.9.1 Physico-chemical assessment of water quality indicators

For the assessment of the trophic status, the present study selected ten WQ indicators, including DOX, MRP, DIN, TON, BOD_5, pH, TEMP, CHL, SAL, and TRAN. Details of the indicator concentration at each monitoring site can be found in Tables 9.S1 (Appendix 9). Figure 9.4 shows the z-statistics of various WQ indicators across the four TrC waterbodies in Ireland. As regards Cork Harbour and Dublin Bay, most indicators were found between the guidelines' values, except the TON, TRAN, DIN, and MRP. These indicators exceeded the permissible limit during the study period (Figure 9.3a; Figure 9.3b). In contrast to those domains, in Galway Bay, a slight data difference was found for water quality indicators throughout the year, whereas the majority of indicators were found within the permissible limit, with the exception of MRP, whereas this indicator breached the guidelines for indicators in Galway Bay (Figure 9.3c). Compared to other waterbodies, all WQ indicators were found within the permissible limit at each monitoring site in Mulroy Bay through the study period (Figure 9.3d). However, the z statistics of WQ indicators reveal that a significant data deviation was found for the nutrients elements in both domains (Cork Harbour and Dublin Bay). Recent research has revealed that various anthropogenic pressures like agricultural wastewater; domestic wastewater; industrial wastewater, etc. have a significant detrimental effect on WQ in both domains (EPA, 2016; 2018; O’Boyle et al., 2013 ; Toner et al., 2005; Uddin et al., 2020a; 2022a; Uddin et al., 2022a; 2023b).

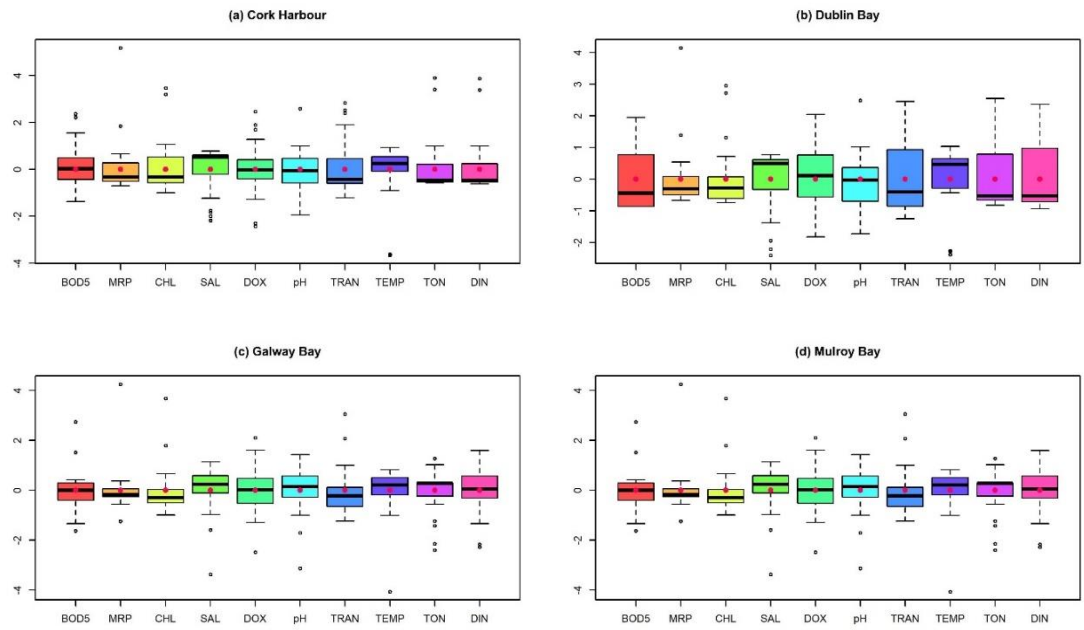


Figure 9.3. Statistical summary of various water quality indicators in Cork Harbour over the study period.

9.9.2 Results of ATSI model development

9.9.2.1 Selection of model inputs

9.9.2.1.1 Multicollinearity analysis of WQ indicators

For the purposes of selecting the optimal input for developing the ATSI model, the present study utilized the VIS and Pearson correlation analysis. Figure 9.4 presents the VIF and correlation results of various WQ indicators. Commonly, VIF scores greater than three are considered indicators of higher inflation of variables in a regression model (Daoud, 2018; Dormann et al., 2013; Filstrup and Downing, 2017; Mansfield and Helms, 1982; Yoo and Cho, 2019; Yu et al., 2015). In this research, input indicators were selected to be less than or equal to three VIF scores because a number of studies have recommended this threshold for avoiding model complexity in order to minimize the uncertainty model (Daoud, 2018; Dormann et al., 2013; Shi et al., 2020; Yoo et al., 2014). As shown in figure 9.4, it can be seen from the results of VIF that the DIN (2199), TON (2199), SAL (6.02), pH (3.50), and MRP (3.19) have larger VIF scores (Figure 9.4a). In the case of Pearson's correlation results, higher correlation values were found for these WQ indicators (Figure 9.4b).

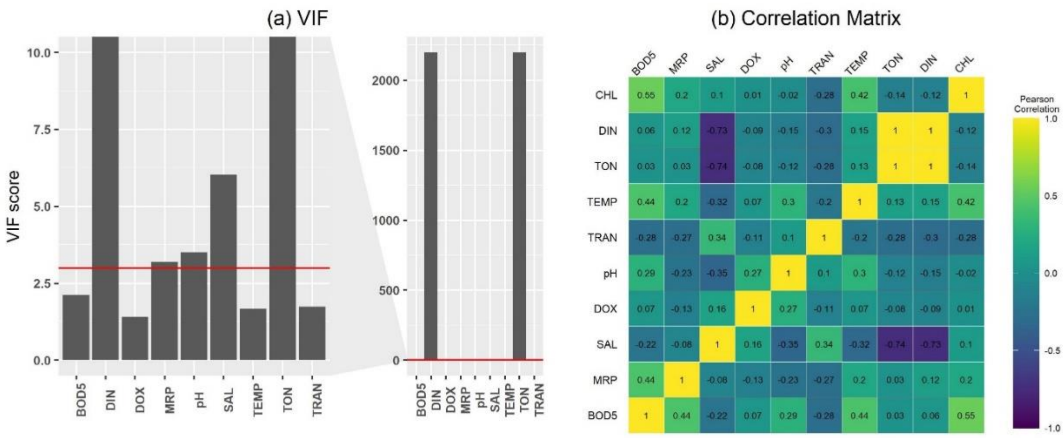


Figure 9.4. Results of VIFs and Pearson correlation analysis.

9.9.2.1.2 MLR results

For the purposes of selecting the optimal input for the ATSI model, initially seven MLR models were developed for predicting CHL using various input combinations. Based on the VIF and correlation results, seven input combinations were constructed using different thresholds of the VIF scores. Details of the various input combinations and their built-up criteria are given in Table 9.4.

Table 9.4 MLR regression model for different inputs; these were constructed based on VIFs and correlation results for developing Chlorophyll a prediction model.

Models	model predictors	Criteria for input	number of predictors	model response
Model-1	BOD_5, DIN, MRP, TEMP, pH, DOX, TON, TRAN, SAL	Initial input	9	
Model-2	**BOD_5, TEMP, DOX, TRAN**	**VIFs ≤ 3**	**4**	
Model-3	DIN, MRP, pH, TON, SAL	VIFs ≥ 3	5	
Model-4	DIN, TON, MRP	Nutrients	3	CHL
Model-5	BOD_5, MRP, TEMP, pH, DOX, TRAN	VIFs ≤ 5	6	
Model-6	TON, DIN	VIFs > 100	2	
Model-7	TEMP, DOX, TRAN	VIFs ≤ 2	3	

In order to identify the best-input combination, the primary assessment of various input combinations was evaluated using the MLR model. For determining, the MLR performance, the present study utilized three identical evaluation metrics, including RMSE, MSE, and R^2. Table 9.5 provides the MLR performance results. It can be seen from the data in Table 9.5 that the Model-2 performed better than other models. Relatively, the smallest prediction error (RMSE = 5.46, MSE = 29.81, and R^2 = 0.30) was found for the Model-2 (Table 9.5). Based on the MLR results, four WQ indicators, including BOD_5, TEMP, DOX, and TRAN, were selected for the input of the ATSI model.

Table 9.5 Determination of robust set of model predictors (input) using MLR technique for developing a CHL prediction model.

Constructed models	Model evaluation metrics		
	RMSE	MSE	R^2
Model-1	13.28	176.36	0.00
Model-2	**5.46**	**29.81**	**0.30**
Model-3	19.35	374.42	0.01
Model-4	19.28	371.72	0.02
Model-5	10.35	107.12	0.00
Model-6	20.05	402.00	0.02
Model-7	6.15	37.82	0.11

9.9.3 Prediction results of the CHL model

Prior to developing the CHL prediction model; initialize the model predictors (BOD_5, TEMP, DOX, and TRAN) and response (CHL) Ten machine learning algorithms were used to develop the prediction of CHL after the model's attributes were established, with the goal of comparing the results to determine which algorithm(s) was/were the most reliable.

9.9.3.1 Performance of prediction models

In this research, four widely used ML model evaluation metrics including RMSE, MSE, MAE and R^2 were utilized. Table 9.6 provides the 10-fold cross-validation results of various ML models. According to the cross-validation results, XGBoost showed the highest prediction performance during both training (RMSE = 0, MSE = 0, and MAE = 0.01) and testing (RMSE =0, MSE = 0, and MAE = 0.01) among ten algorithms (Table 9.6). Relatively, smaller error also calculated for the DNN and ExT models during both (RMSE = 1.47, MSE = 2.15, and MAE = 0.93 and RMSE = 3.02, MSE = 9.11, and MAE = 2.37, respectively) and testing (RMSE =0.09, MSE = 0.01, and MAE = 0.00 and RMSE =0.0, MSE = 0.0, and MAE = 0.00, respectively) (Table 9.6). The cross-validation results indicate that the XGBoost model is effective for predicting CHL in terms of minimizing model error during both training and testing phases.

In addition, the present study utilized the R^2 for the assessment of the relationship between model predictors and response according to the methodology of Uddin et al., (2022a; 2022b). Figure 9.5 presents the R^2 results of various ML algorithms. As can be seen from Figure 9.5, the XGBoost (R^2 = 1.0), ExT (R^2 = 1.0), and DT (R^2 = 1.0) were associated with good agreement between model predictions and response.

Table 9.6 Cross-validation results and ranking the algorithms based on the performance during both training and testing period of various CHL prediction models.

	Training error				Testing error				Cumulative score	Rank
ML models	RMSE	MSE	MAE	Score	RMSE	MSE	MAE	Score		
XGBoost	**0.0**	**0.0**	**0.01**	**1**	**0.0**	**0.0**	**0.01**	**2**	**3**	**1**
MLR	3.15	9.90	2.57	6	2.07	4.27	1.72	5	11	6
RF	2.90	8.40	1.80	3	1.73	2.98	1.08	3	6	4
DNN	1.47	2.15	0.93	2	0.09	0.01	0.0	2	4	2
SVM	3.35	11.25	2.62	10	2.13	4.53	1.46	6	16	8
ExT	3.02	9.11	2.37	4	0.0	0.0	0.0	1	5	3
GNB	3.11	9.67	2.52	5	2.10	4.40	1.72	7	12	7
KNN	3.17	10.03	2.48	8	2.26	5.13	1.93	8	16	8
CatBoost	3.16	9.98	2.40	7	1.77	3.15	0.83	4	11	6
DT	3.36	11.31	2.60	9	0.0	0.0	0.0	1	10	5

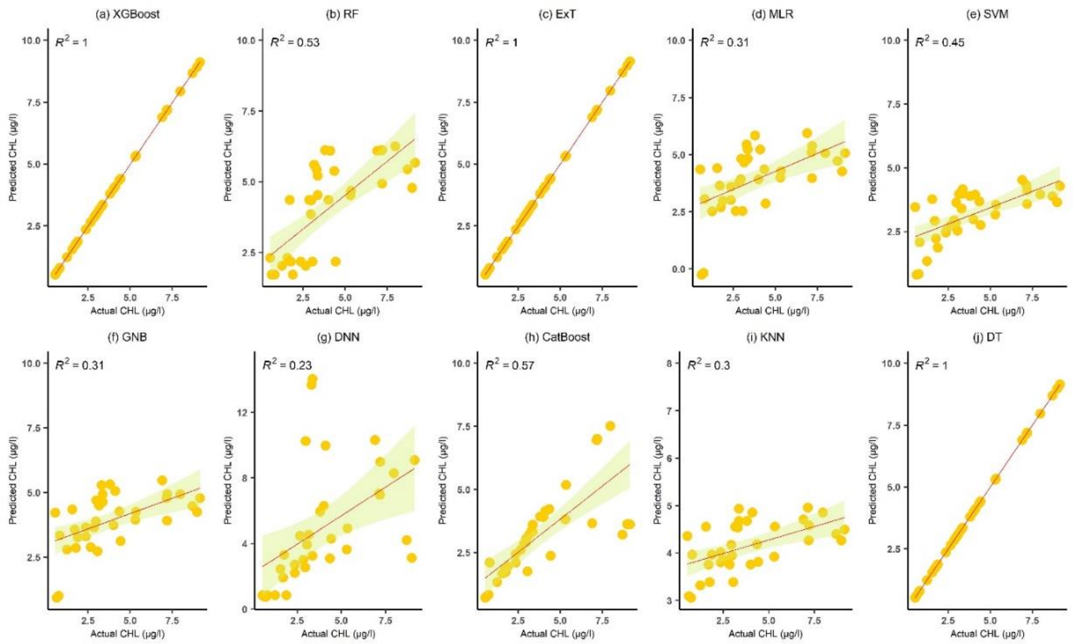


Figure 9.5. Scatter plots of actual and predicted CHL based on the testing datasets for various ML regression models for the validation of prediction results.

The results of the coefficient of determination also reveal that the XGBoost model could be effective for predicting CHL in order to reduce the model's prediction errors. After identifying the robust algorithm (XGBoost) for predicting CHL, the algorithm was tested across four waterbodies in Ireland for predicting CHL. Figure 6 shows the point based comparison between actual and predicted CHL across four application domains. As can be seen in Figure 9.6, the XGBoost model predicted CHL accurately at each monitoring site across all domains.

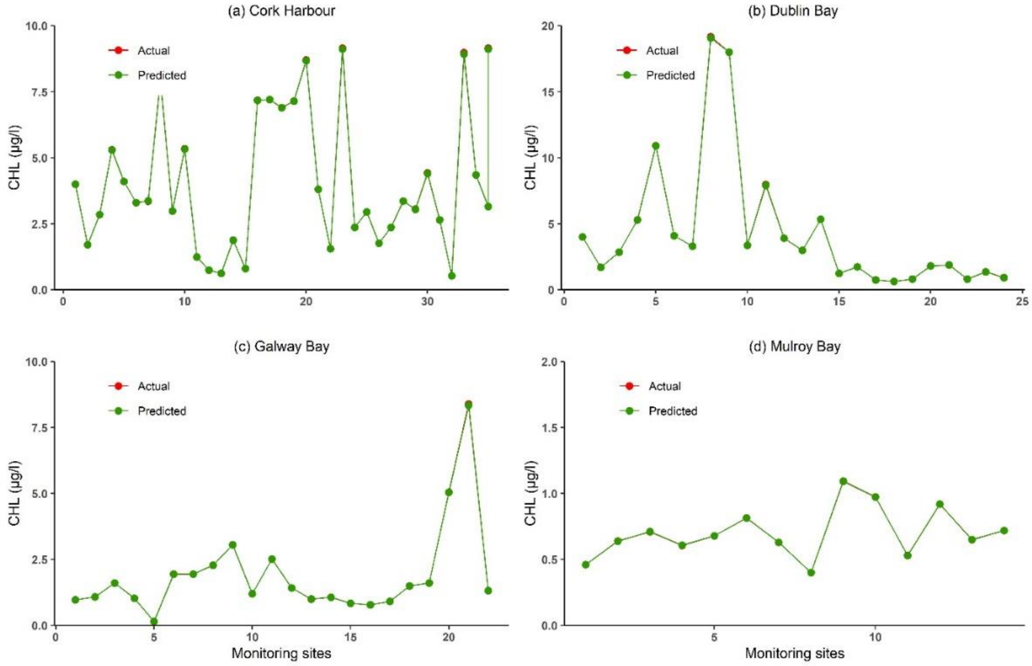


Figure 9.6. Point based comparison between actual and predicted ATSI scores in various domains.

9.9.4 Model development for the assessment of trophic status index (ASTI)

9.9.4.1 Input selection results

For the selection of crucial WQ indicators, the present study was utilized MLR model incorporating ML and AI approaches. Based on the multicollinearity results and MLR performance, suggested BOD5, TEMP, DOX and TRAN were significant for the assessment of trophic status in TrC waterbodies by predicting the CHL (Table 9.4; Table 9.5). Details of the MLR performance results and indicators subsets are provided in Table 9.4 and Table 9.5, respectively. Similar metrics have been used by several studies to evaluate trophic status (Carlson, 1984; Cotovicz Junior et al., 2013; Gupta, 2014; Liu et al., 2022; Malek et al., 2011; Matus-Hernández et al., 2018; O'Boyle et al., 2013; Parparov, 2010; Vollenweider et al., 1998; Wei et al., 2019). Therefore, the present study was used the predicted CHL values for the assessment trophic status in Irish TrC water bodies. Due to the higher correlation between the CHL and other WQ indicators recently, several studies have only used the CHL to determine the trophic status in coastal waters in an effort to reduce data redundancy from the assessment

(Lake et al., 2013; Mamun et al., 2021b; Salem et al., 2017; Watanabe et al., 2015; Zhou et al., 2021).

9.9.4.2 Results of ATSI functions

The present study used the linear rescaling interpolation function for converting the CHL value into the unitless ATSI score. Higher ATSI scores indicate an "unpolluted" state, while a lower score refers to an "eutrophic" state of ecosystems (see Table 9.2). Figure 9.7 shows the calculated (actual) and predicted ASTI scores across four application domains over the study period. Compared to the ATSI score in four waterbodies, higher ASTI scores were calculated for all domains except Cork Harbour (Figure 9.7). As shown in Figure 9.7, a relatively higher ATSI score deviation was found in Cork Harbour for both actual and predicted scores. In addition, as can be seen from the data in Figure 9.7, there were no significant differences between actual and predicted ATSI scores across all domains with the exception of Cork Harbour.

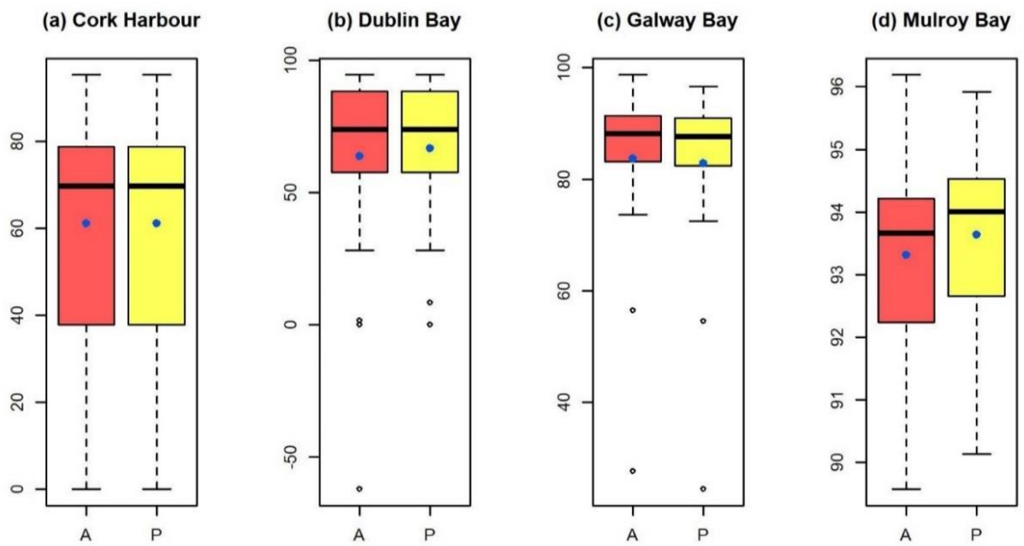


Figure 9.7. Statistical summary of actual and predicted ATSI scores across four waterbodies. Note A and P on x-axes represent actual and predicted ATSI score, respectively.

Figure 9.8 presents the point based ATSI scores at each monitoring site across four application domains. Details of the monitoring sites and their attributes can be found in Table 7.S1 and a graphical presentation in Figure 9.1, respectively. It can be seen from Figure 9.8 that lower ATSI scores were calculated at the majority of monitoring sites in the River Lee and North Channel in Cork Harbour (Figure 9.8a; Figure 9.14a), because the upper part of the Harbour receives a significant amount of waste water from the various sources (EPA, 2018; O'Boyle et al., 2013 ; Toner et al., 2005; Uddin et al., 2022a;2022b; 2020a; 2020b). The results of the ATSI scores in Cork Harbour were found to be in line with the previous studies (O'Boyle et al., 2013; Toner et al., 2005).

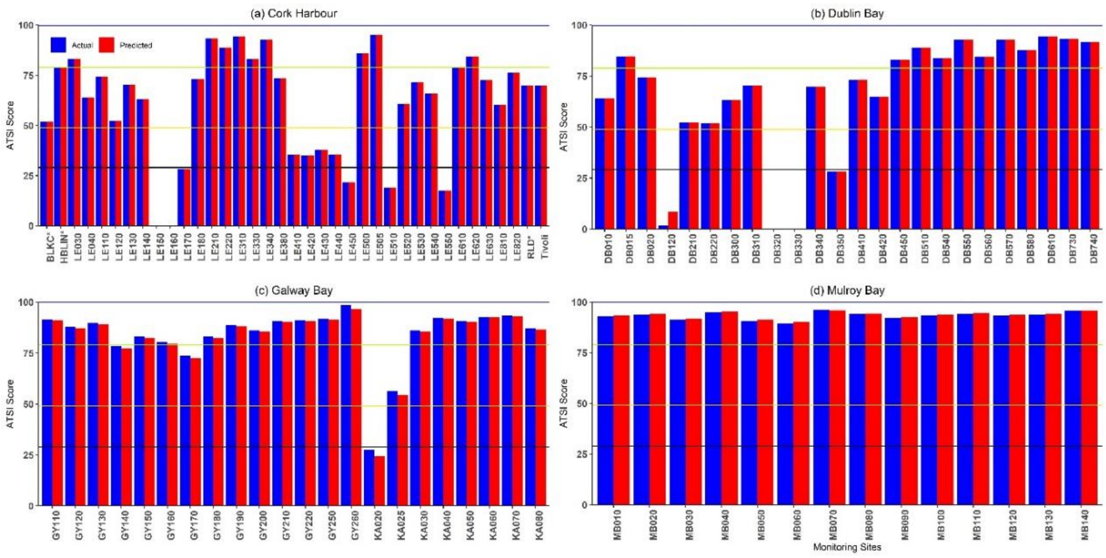


Figure 9.8. Comparison of spatial distribution of ATSI scores between actual and predicted at each monitoring site in four waterbodies in Ireland.

Like Cork Harbour, smaller ASTI scores were calculated at most monitoring sites nearby the urban functional zone in Dublin Bay (Figure 9.8b; Figure 9.14b). The quality of the Bay's water decreases due to a variety of pressures, such as raw wastewater pressure, domestic waste pressure, agricultural pressure, nutrient loads, etc. (Barr and Mcelroy, 2019; Environmental Protection Agency, 2021). Recently, the EPA revealed that the closer part of the Bay from the urban area received a significant amount of wastewater from the different sources (EPA, 2017; Wall et al., 2020).

On the other hand, higher ASTI scores were obtained at most monitoring sites in Galway Bay except KA020 and KA025 (Figure 9.8c; Figure 9.14c). Like other waterbodies, the Galway Bay experiences significant pressure from domestic wastewater (EPA, 2017; 2020). Contrary to expectations, higher scores were estimated at all monitoring sites in Mulroy Bay (Figure 9.8d; Figure 9.14d). The results of the spatial distribution of ATSI scores are consistent with the earlier studies (O'Boyle et al., 2013;Toner et al., 2005; Uddin et al., 2020a; 2020b; 2022a; 2022b;2023b).

9.9.4.3 Model sensitivity results

For the purposes of determining the ATSI model sensitivity, many studies have utilized the coefficient determination (R^2) techniques for understanding the relationship between actual and predicted ASTI scores in water research (Chen et al., 2020; Chicco et al., 2021; Hamby, 1995; Uddin et al., 2022a; 2022b; 2022e; W. Zhang et al., 2022). In order to determine the model sensitivity, the present study utilized this approach according to the methodology of Uddin et al., (2022a). The R^2 value(s) was obtained from the XGBoost prediction model for four application domains.

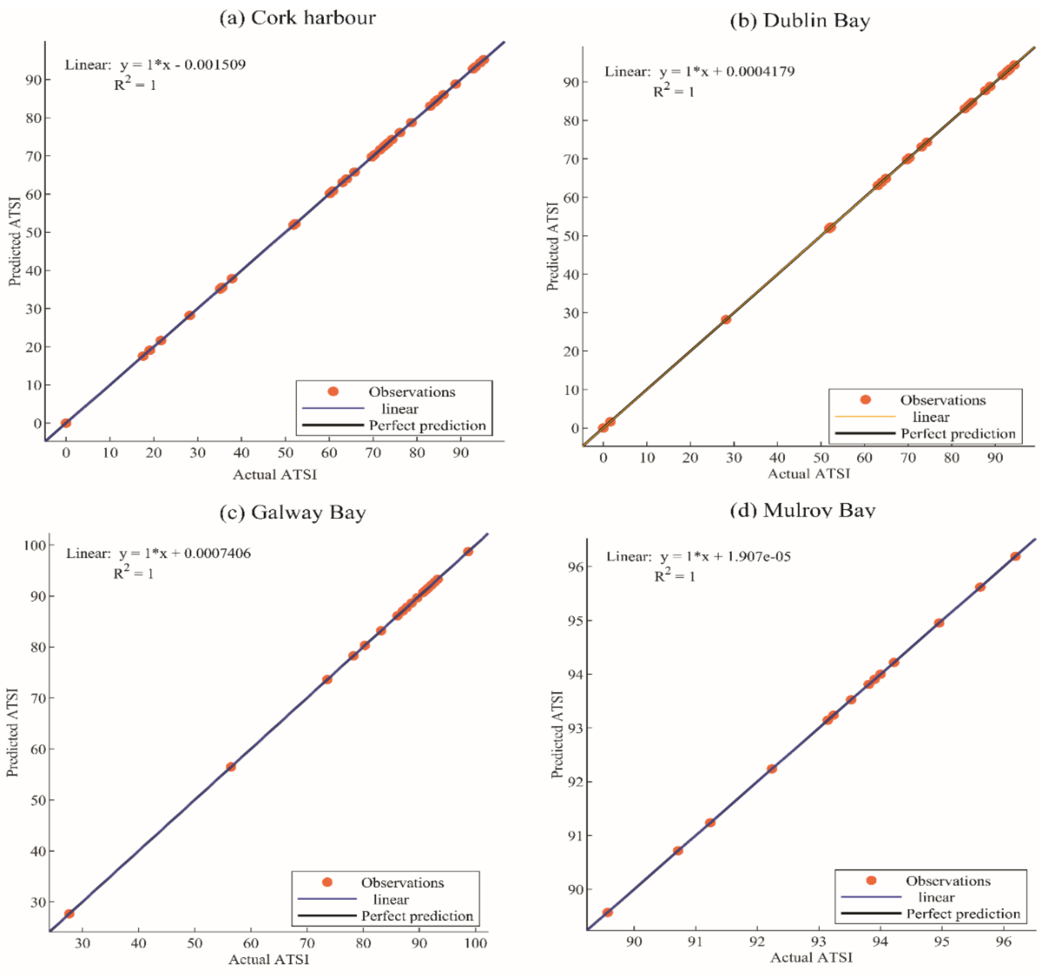


Figure 9.9. Comparison between actual and predicted ATSI scores across four application domains.

Figure 9 shows the R^2 between actual and predicted ASTI scores. As can be seen from the figure below, the ATSI model's sensitivity was excellent ($R^2 = 1$) across the four waterbodies in Ireland. Moreover, Figure 9.10 presents the ASTI model response for various CHL input levels at the particular monitoring site across four domains. From

Figure 9.10, it can be seen that higher ATSI scores (unpolluted) were calculated for lower concentrations of CHL, while the lowest score (hypereutrophic) was estimated for a higher level of CHL concentration. The results of R^2 and point based assessments of model response reveal that the ATSI model could be effective for the assessment of trophic state in terms of the spatio-temporal resolution of application domains.

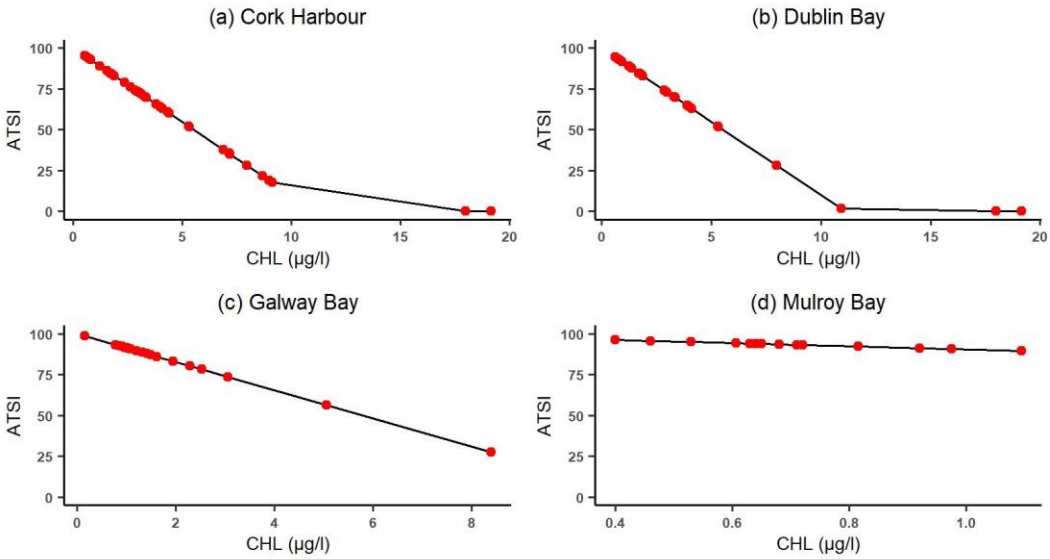


Figure 9.10. Model responses for different level of CHL concentration at particular monitoring site over the various application domains.

9.9.4.4 Model efficiency analysis

Commonly, "Model efficiency" refers to a model's strength and capacity to produce higher productivity with fewer resources (Şen et al., 2022). The present study utilized the NSE and MEF for determining the ATSI model efficiency in the assessment of trophic status, because many studies have used these metrics for the purposes of evaluating model efficiency in water resource research (Guo et al., 2019; Izhar Shah et al., 2021; Minh et al., 2022; Moriasi et al., 2015; Sharif et al., 2022; Uddin et al., 2022d, 2022e). NSE values near 1 typically denote "excellent" efficiency, while the reversal value denotes "poor" efficiency (close to 0). On the other hand, the MEF value is advised to be as low as possible; lower values indicate "excellent" performance, while 1 refers “poor" performance. Results for model effectiveness across four waterbodies are shown in Figure 9.11. Figure 9.11 demonstrates that the ATSI model performs "excellently" across all domains. Compared to other areas during the study period, Cork Harbour and Dublin Bay had higher MEF values (Figure 9.11).

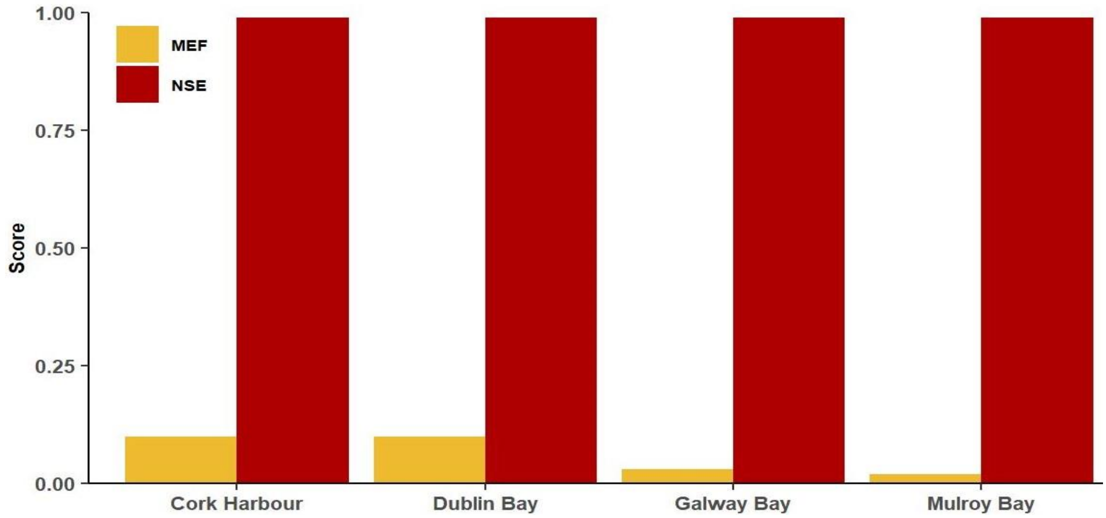


Figure 9.11. ATSI model efficiency across four waterbodies over the study period.

9.9.4.5 Model uncertainty results

In this research, PDF and error bar analysis were utilized to estimate the model uncertainty. Figure 9.12 presents the CDFs and error bars statistics with a 95% CI value of the ATSI score. Over the four domains, the ATSI score was found to be normally distributed for both actual and predicted simulated scores (Figure 9.12a). As can be seen from the figure below, there were no significant statistical differences between the actual simulated and predicted simulated ATSI score (Figure 9.12a). Unlike to the PDFs results, the CI error bar analysis indicates that a small difference was found between the actual simulated and predicted simulated ATSI score across four application domains. As shown in figure 12b, there was a small but significant ($p < 0.001$) ATSI score difference between the actual simulated and predicted simulated ATSI mean, SE (uncertainty intervals). The results of the uncertainty analysis indicate that the ATSI model could be effective in assessing trophic states more accurately in terms of its reliability and accuracy.

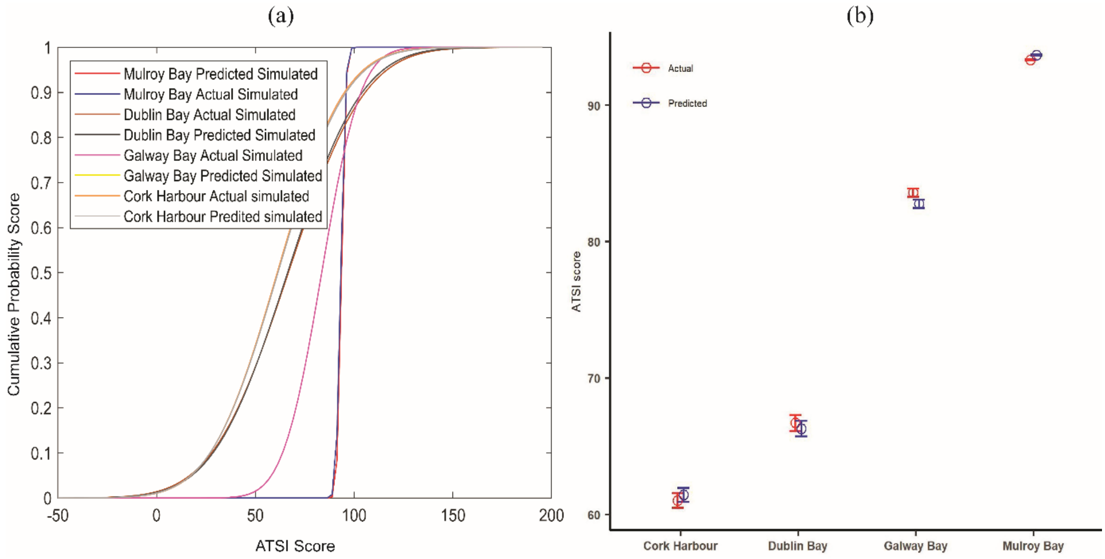


Figure 9.12. Graphical and statistical summary of the ATSI model uncertainty: (a) PDF comparison between actual simulated and predicted simulated of ATSI scores across four domains; (b) ATSI score mean value with 95% CI error bars for four waterbodies, when n = 10000, $p < 0.001$.

9.10. Assessment of ecological status using ATSI and ATSEBI system

The ultimate goal of the ATSI is to assess the trophic status by translating the ATSI score using the particular classification scheme. The present study utilized a brand new classification scheme (see table 9.2) for determining trophic state. Details of the classification scheme can be found in table 9.2 (above). For the purposes of the comparison between the proposed approach (ATSI) and the ATSEBI system, trophic state is also determined using the ATSEBI system classification scheme. Details of the classification scheme and procedures can be found in Table 9.S3 (Appendix 9). Figure 9.13 shows the trophic status across four application domains in Ireland using the ATSI model and ATSEBI system, respectively.

The ASTI model classified four types of trophic status, including "unpolluted (24%)," "moderate (49%)," "eutrophic (11%)," and "hypertrophic (16%)," whereas the ATSEBI system recommended two types of trophic status ["unpolluted (59%)" and "intermediate (41%)"] in Cork Harbour through the study period. In Dublin Bay, the ATSI model determined three trophic states, including "unpolluted" (46%), "moderate" (38%)" and "hypertrophic" (17%)", while the ATSEBI system classified the trophic states into two classes, "unpolluted" (67%)", and "intermediate" (33%). In the case of Galway Bay, the ATSI model categorized the trophic states into three types: "unpolluted," "moderate," and "eutrophic," respectively, at 82% (16), 13% (3), and 5% (1), whereas the ATSEBI system suggested the trophic state was "unpolluted" during the study period. Contrary to their expectations, both techniques (ATSI and ATSEBI) recommended that Mulroy Bay's trophic status was "unpolluted" throughout this research (Figure 9.13).

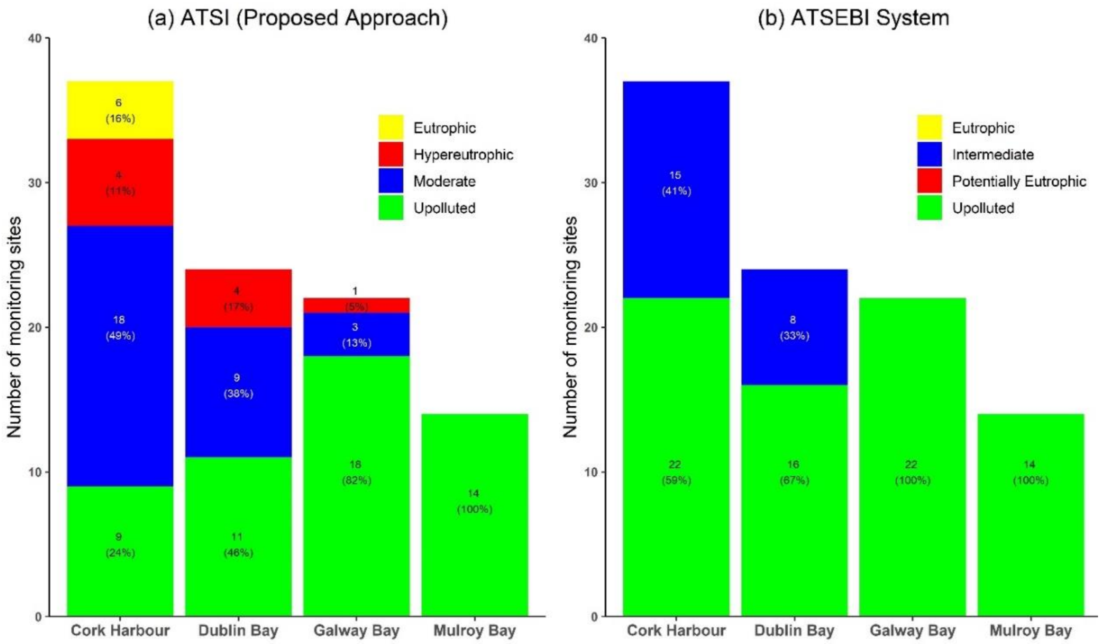


Figure 9.13. Comparison of trophic assessment results between the ATSI model and ATSEBI system across four waterbodies.

Figures 9.14 and Figure 9.15 present the trophic status at each monitoring site across four waterbodies for the ATSI model and the ATSEBI system, respectively, during the study period. In the case of the ATSI model, most monitoring sites in the upper were dominated by the "hypertrophic," "eutrophic," and "moderate" trophic status in Cork Harbour. As can be seen in Figure 9.14a, the worst status was found in a nutrient sensitive area in Cork Harbour, whereas, relatively good status was determined in the lower and outer Harbour during the study period. Unlike the ATSI model, the ATSEBI system provided surprising results, most monitoring sites' trophic status was found to be "unpolluted" in the upper and lower Harbour, whereas "moderate" quality was observed in the river Lee (upper Harbour) and outer Harbour during the study period (Figure 9.15a). In terms of spatial attributes in Cork Harbour, the ATSEBI system produces completely unexpected results because Cork Harbour is a complex hydrodynamic system and the most functional Harbour in Ireland. It could be the overestimation problem of the ATSEBI system. Contrary, the ATSI model results indicate that it could be effective for assessing the trophic status using the new approach in terms of the geospatial settings of the domain. In addition, several studies have reported that the quality of the Cork Harbour water has degraded over the years due to various anthropogenic pressures like domestic wastewaters, agricultural activities, aquaculture, etc. (Hartnett et al., 2012; O'Boyle et al., 2013; Toner et al., 2005; G. Uddin et al., 202a; 202ab; 2022a; 2022b;2022c, 2022d; 2023b, 2023b).

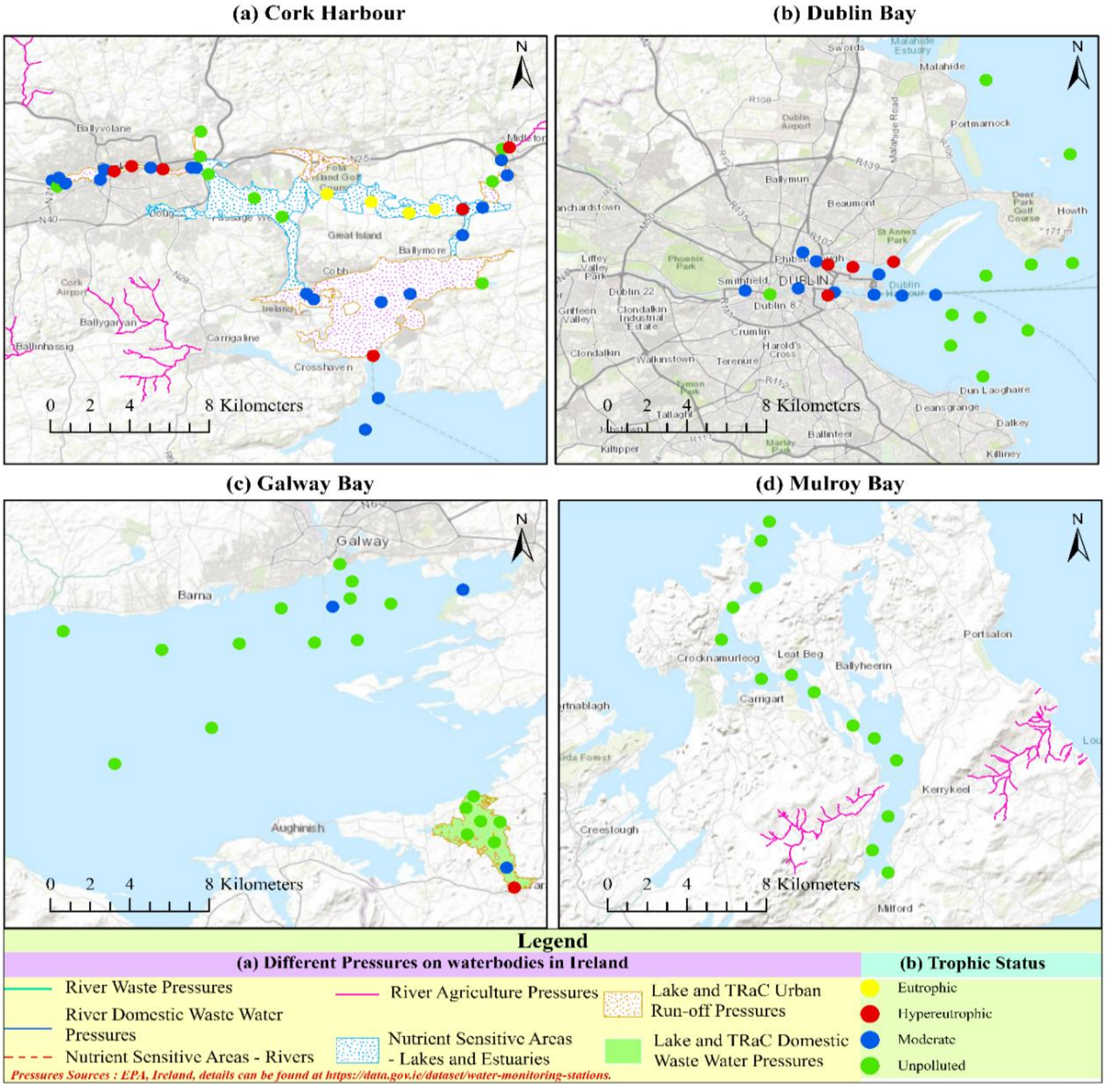


Figure 9.14. Point based trophic status assessment results using the ATSI model across four waterbodies in Ireland.

Similarly, in Dublin Bay, the ATSI model ranked "moderate" to "eutrophic" status at monitoring sites in the upper part of the bay, whereas, relatively, "unpolluted" status was found in the outer part of the Bay (Figure 9.14b). On the other hand, the ATSEBI system was investigated for "unpolluted" to "moderate" water quality in Dublin Bay through the research period (Figure 9.15b).

In Galway Bay, the ATSI model found hypertrophic status at a monitoring site that was located in the area of domestic wastewater pressures, whereas most monitoring sites were classified as "unpolluted" to "moderate" quality (Figure 9.14c). Although, the ATSEBI system suggested "unpolluted" quality at all monitoring sites in Galway Bay over the study period (Figure 9.15c).

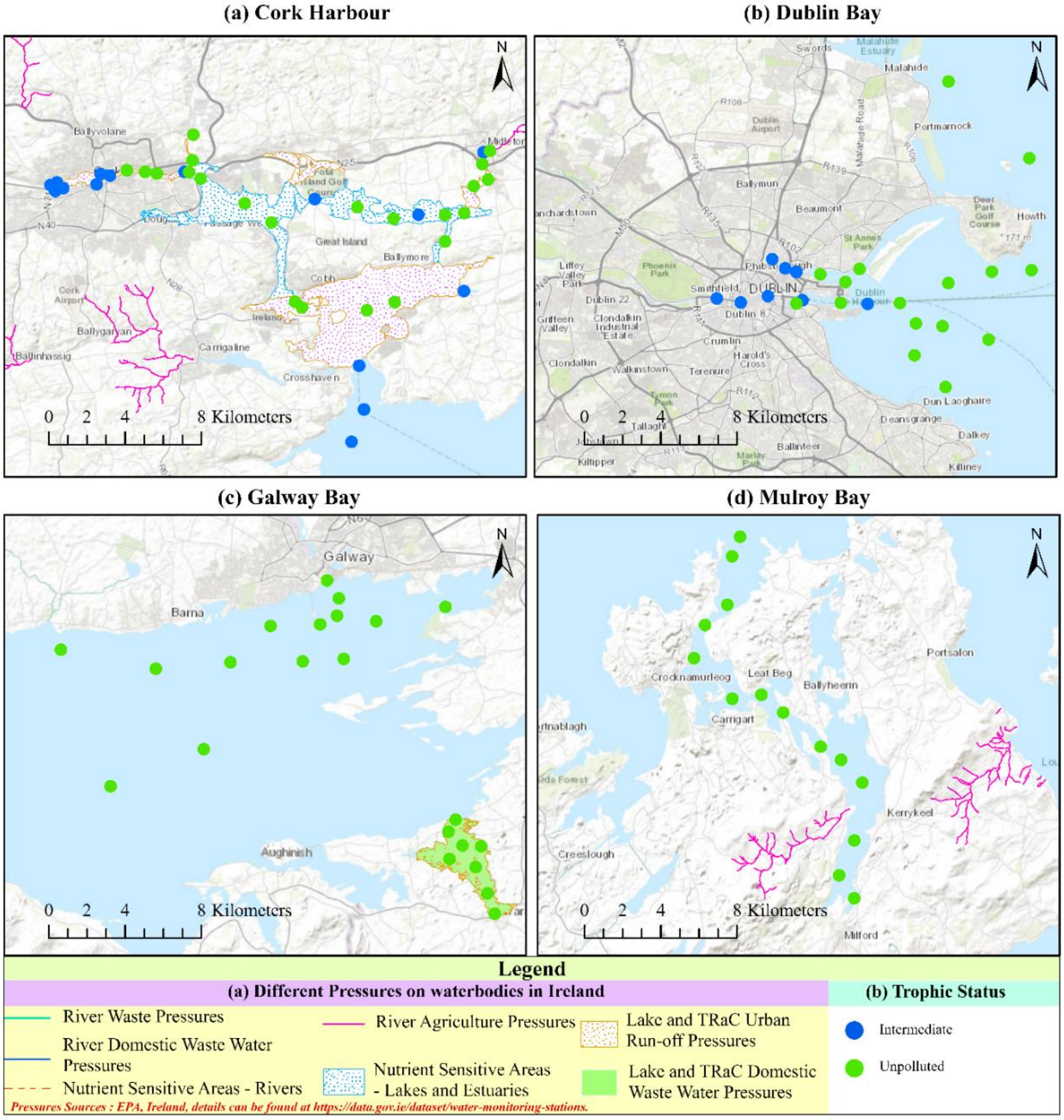


Figure 9.15. Point based trophic status assessment results using the existing ATSEBI system across four waterbodies in Ireland.

Unlike the other domains, both techniques were classified as having "unpolluted" trophic status at all monitoring sites across Mulroy Bay (Figure 9.14d; Figure 9.15d). Based on the point assessment of trophic status, relatively, good agreements were found in the ATSI model because the results were in line with the literature. Moreover, the ATSI model is sensitive to the domain functional attributes (like domestic wastewater pressures, nutrient loading pressures, urban runoff pressures etc.) and can reflect the impact of various pressures in waterbodies. Different types of pressures are presented in Figures 9.14 and 9.15. In the case of the ATSEBI system, in contrast to earlier findings, the ATSEBI results do not support the previous findings in the literature in terms of the application domains' physical and functional attributes.

However, in comparison between methods, a significant difference was found in assessment results between the ATSI model and the ATSEBI system. According to the assessment results, the ATSEBI system was found to have an overestimation issue in comparison to both techniques, whereas the ATSI model exhibits good agreement (R^2 = 1.0) between model inputs and outputs (Figure 9.9).

9.11 Conclusion

The aims of this research were to develop an improved method for assessing the trophic state in TrC waterbodies. With a few common prerequisites, a variety of tools and techniques have been used to assess trophic status in the literature. To the best of the author's knowledge, this study was the first initiative to develop the ATSI model that was conducted using extensive application of ML and AI techniques for avoiding the limitations of the existing trophic assessment techniques. The key contributions and major findings from the research are as follows:

(i) In order to minimize the model input redundancy, indicators were selected using the ML and AI approach incorporating VIF and correlation techniques.

(ii) Four identical water quality indicators, including BOD_5, TEMP, DOX, and TRAN, were found to be essential inputs for the ATSI model and these could be useful for monitoring the trophic state of TrC ecosystems and aquatic health.

(iii) The results of the CHL prediction models reveals that the XGBoost algorithm could be efficient for predicting CHL in TrC waters.

(iv) The results of the ATSI model are in line with those earlier studies. The ASTI results reveal that the newly developed ATSI model could be effective in transferring the various WQ indicators' information into a numerical value,

(v) Results of the trophic state indicate that the ATSI score may be effectively decoded using the new trophic classification system.

(vi) Multicollinearity test reveal that the input redundant problem has had a significant impact on the present ATSEBI system.

(vii) A significant difference was found between models (ATSI and ATSEBI) in terms of spatial resolution of application domain.

Moreover, the model sensitivity and efficiency results also indicate that the ATSI model could be effective for assessing trophic status in any geographical extent in terms of model uncertainty because the model showed excellent agreement (R^2 = 1) between the model input and response across four domains in Ireland. Although the present study only considered the average concentration of WQ indicators, the model's performance should be evaluated and validated by further investigation. However, the present study provided comprehensive statistical and ML-AI-incorporated approaches for the assessment of trophic state in TrC waters. Therefore, the finding of this study could helpful a number of stakeholders including researchers, decision-makers, and agencies/organizations those responsible for water resources monitoring, and management.

9.12 Declaration of competing interest

The authors confirm that they did not experience competing financial interests or personal interactions that could have had potential influences on this paper.

9.13 Acknowledgement

The authors gratefully acknowledge the editor's and anonymous reviewers' contributions to the improvement of this paper. This research was funded by the Hardiman Research Scholarship of the National University of Ireland Galway, which funded the first author as part of his PhD program. The authors would like to thank the Environmental Protection Agency of Ireland for providing water quality data. The authors would like to acknowledge support from MaREI, the SFI Research Centre for Energy, Climate, and Marine research. The authors also sincerely acknowledge Charles Sturt University for providing all necessary supports to this PhD

project through the international co-supervision.

9.14 References

Abdar, M., Pourpanah, F., Hussain, S., Rezazadegan, D., Liu, L., Ghavamzadeh, M., Fieguth, P., Cao, X., Khosravi, A., Acharya, U.R., Makarenkov, V., Nahavandi, S., 2021. A review of uncertainty quantification in deep learning: Techniques, applications and challenges. Information Fusion 76, 243–297. https://doi.org/10.1016/j.inffus.2021.05.008

Abdi, B., Bozorg-Haddad, O., Loáiciga, H.A., 2020. Analysis of the effect of inputs uncertainty on riverine water temperature predictions with a Markov chain Monte Carlo (MCMC) algorithm. Environ Monit Assess 192. https://doi.org/10.1007/s10661-020-8062-3

Ahmad, Z., Rahim, N.A., Bahadori, A., Zhang, J., 2017. Improving water quality index prediction in Perak River basin Malaysia through a combination of multiple neural networks. International Journal of River Basin Management 15, 79–87. https://doi.org/10.1080/15715124.2016.1256297

Aldhyani, T.H.H., Al-Yaari, M., Alkahtani, H., Maashi, M., 2020. Water Quality Prediction Using Artificial Intelligence Algorithms. Appl Bionics Biomech 2020. https://doi.org/10.1155/2020/6659314

Almeida, C., Branco, P., Segurado, P., Ramos, T.B., Ferreira, T., Neves, R., de Oliveira, R.P., 2021. Evaluation of the trophic status in a mediterranean reservoir under climate change: An integrated modelling approach. Journal of Water and Climate Change 12, 817–832. https://doi.org/10.2166/wcc.2020.247

Andricevic, R., Kekez, T., Vojkovic, M., 2021. Trophic status assessment of Central Eastern Adriatic Sea using water quality variables and loading capacity concept for estuaries. Mar Pollut Bull 173. https://doi.org/10.1016/j.marpolbul.2021.113126

Angel, Y., McCabe, M.F., 2022. Machine Learning Strategies for the Retrieval of Leaf-Chlorophyll Dynamics: Model Choice, Sequential Versus Retraining Learning, and Hyperspectral Predictors. Front Plant Sci 13. https://doi.org/10.3389/fpls.2022.722442

Baloch, M.A., Ames, D.P., Tanik, A., 2015. Hydrologic impacts of climate and land-use change on Namnam Stream in Koycegiz Watershed, Turkey. International Journal of Environmental Science and Technology 12, 1481–1494. https://doi.org/10.1007/s13762-014-0527-x

Band, S.S., Janizadeh, S., Pal, S.C., Chowdhuri, I., Siabi, Z., Norouzi, A., Melesse, A.M., Shokri, M., Mosavi, A., 2020. Comparative analysis of artificial intelligence models for accurate estimation of groundwater nitrate concentration. Sensors (Switzerland) 20, 1–23. https://doi.org/10.3390/s20205763

Bennett, M.G., Schofield, K.A., Lee, S.S., Norton, S.B., 2017. Response of chlorophyll a to total nitrogen and total phosphorus concentrations in lotic ecosystems: A systematic review protocol. Environ Evid. https://doi.org/10.1186/s13750-017-0097-8

Best, N., Richardson, S., Clarke, P., 2008. A Comparison of model-based methods for Small Area Estimation. ESRC National Centre for Research Methods 1–26.

Bonansea, M., Rodriguez, M.C., Pinotti, L., Ferrero, S., 2015. Using multi-temporal Landsat imagery and linear mixed models for assessing water quality parameters in Río Tercero reservoir (Argentina). Remote Sens Environ 158, 28–41. https://doi.org/10.1016/j.rse.2014.10.032

Bricker, S.B., Ferreira, J.G., Simas, T., 2003. An integrated methodology for assessment of estuarine trophic status. Ecol Modell 169, 39–60. https://doi.org/10.1016/S0304-3800(03)00199-6

Bui, D.T., Khosravi, K., Tiefenbacher, J., Nguyen, H., Kazakis, N., 2020. Improving prediction of water quality indices using novel hybrid machine-learning algorithms. Science of the Total Environment 721, 137612. https://doi.org/10.1016/j.scitotenv.2020.137612

Camera, C., Bruggeman, A., Zittis, G., Sofokleous, I., Arnault, J., 2020. Simulation of extreme rainfall and streamflow events in small Mediterranean watersheds with a one-way-coupled atmospheric–hydrologic modelling system. Natural Hazards and Earth System Sciences 20, 2791–2810. https://doi.org/10.5194/nhess-20-2791-2020

Carlson, R.E., 1984. The trophic state concept: A lake management perspective. Lake Reserv Manag 1, 427–430. https://doi.org/10.1080/07438148409354550

Carsten Von Der Ohe, P., Prüß, A., Schäfer, R.B., Liess, M., de Deckere, E., Brack, W., 2007. Water quality indices across Europe - A comparison of the good ecological status of five river basins. Journal of Environmental Monitoring 9, 970–978. https://doi.org/10.1039/b704699p

Chen, S., Ren, Y., Friedrich, D., Yu, Z., Yu, J., 2020. Sensitivity analysis to reduce duplicated features in ANN training for district heat demand prediction. Energy and AI 2, 100028. https://doi.org/10.1016/j.egyai.2020.100028

Chicco, D., Warrens, M.J., Jurman, G., 2021. The coefficient of determination R-squared is more informative than SMAPE, MAE, MAPE, MSE and RMSE in regression analysis evaluation. PeerJ Comput Sci 7, e623. https://doi.org/10.7717/peerj-cs.623

Cho, J.H., Lee, J.H., 2018. Multiple linear regression models for predicting nonpoint-source pollutant discharge from a highland agricultural region. Water (Switzerland) 10. https://doi.org/10.3390/w10091156

Clarke, R.A., Stanley, C.D., MacLeod, B.W., McNeal, B.L., 1997. Relationship of seasonal water quality to chlorophyll a concentration in Lake Manatee, Florida. Lake Reserv Manag 13, 253–258. https://doi.org/10.1080/07438149709354316

Commowick, O., Warfield, S.K., 2010. Estimation of inferential uncertainty in assessing expert segmentation performance from STAPLE. IEEE Trans Med Imaging 29, 771–780. https://doi.org/10.1109/TMI.2009.2036011

Cotovicz Junior, L.C., Brandini, N., Knoppers, B.A., Mizerkowski, B.D., Sterza, J.M., Ovalle, A.R.C., Medeiros, P.R.P., 2013. Assessment of the trophic status of four coastal lagoons and one estuarine delta, eastern Brazil. Environ Monit Assess 185, 3297–3311. https://doi.org/10.1007/s10661-012-2791-x

Cumming, G., Fidler, F., Vaux, D.L., 2007. Error bars in experimental biology. Journal of Cell Biology 177, 7–11. https://doi.org/10.1083/jcb.200611141

Cumming, G., Finch, S., 2005. Inference by eye confidence intervals and how to read pictures of data. American Psychologist 60, 170–180. https://doi.org/10.1037/0003-066X.60.2.170

Danasingh, A.A.G.S., Subramanian, A. alias B., Epiphany, J.L., 2020. Identifying redundant features using unsupervised learning for high-dimensional data. SN Appl Sci 2. https://doi.org/10.1007/s42452-020-3157-6

Daoud, J.I., 2018. Multicollinearity and Regression Analysis, in: Journal of Physics: Conference Series. Institute of Physics Publishing. https://doi.org/10.1088/1742-6596/949/1/012009

Degenhardt, F., Seifert, S., Szymczak, S., 2019. Evaluation of variable selection methods for random forests and omics data sets. Brief Bioinform 20, 492–503. https://doi.org/10.1093/bib/bbx124

Devlin, M., Bricker, S., Painting, S., 2011. Comparison of five methods for assessing impacts of nutrient enrichment using estuarine case studies. Biogeochemistry 106, 177–205. https://doi.org/10.1007/s10533-011-9588-9

Dias Curto, J., Castro Pinto, J., 2007. New Multicollinearity Indicators in Linear Regression Models.

Dormann, C.F., Elith, J., Bacher, S., Buchmann, C., Carl, G., Carré, G., Marquéz, J.R.G., Gruber, B., Lafourcade, B., Leitão, P.J., Münkemüller, T., Mcclean, C., Osborne, P.E., Reineking, B., Schröder, B., Skidmore, A.K., Zurell, D., Lautenbach, S., 2013. Collinearity: A review of methods to deal with it and a simulation study evaluating their performance. Ecography 36, 27–46. https://doi.org/10.1111/j.1600-0587.2012.07348.x

Duan, H., Zhang, Y., Zhang, B., Song, K., Wang, Z., 2007. Assessment of chlorophyll-a concentration and trophic state for lake chagan using landsat TM and field spectral data. Environ Monit Assess 129, 295–308. https://doi.org/10.1007/s10661-006-9362-y

Elgeldawi, E., Sayed, A., Galal, A.R., Zaki, A.M., 2021. Hyperparameter tuning for machine learning algorithms used for arabic sentiment analysis. Informatics 8, 1–21. https://doi.org/10.3390/informatics8040079

El-Serehy, H.A., Abdallah, H.S., Al-Misned, F.A., Al-Farraj, S.A., Al-Rasheid, K.A., 2018. Assessing water quality and classifying trophic status for scientifically based managing the water resources of the Lake Timsah, the lake with salinity stratification along the Suez Canal. Saudi J Biol Sci 25, 1247–1256. https://doi.org/10.1016/j.sjbs.2018.05.022

EPA, 2016. Urban Waste Water Treatment in 2015. EPA.

EPA, 2017. Urban waste water treatment in 2017. Off. J. Eur. Union 40–52.

EPA, 2018. Lee-Cork Harbour Catchment Assessment 2015. EPA.

EPA, 2021. Ireland's National Water Framework Directive Monitoring Programme 2019-2021.

Farnaz Nojavan, A., Kreakie, B.J., Hollister, J.W., Qian, S.S., 2019. Rethinking the lake trophic state index. PeerJ 2019. https://doi.org/10.7717/peerj.7936

Fergus, C.E., Brooks, J.R., Kaufmann, P.R., Pollard, A.I., Herlihy, A.T., Paulsen, S.G., Weber, M.H., 2021. National framework for ranking lakes by potential for anthropogenic hydro-alteration. Ecol Indic 122. https://doi.org/10.1016/j.ecolind.2020.107241

Ferreira, J.G., Bricker, S.B., Simas, T.C., 2007. Application and sensitivity testing of a eutrophication assessment method on coastal systems in the United States and European Union. J Environ Manage 82, 433–445. https://doi.org/10.1016/j.jenvman.2006.01.003

Filstrup, C.T., Downing, J.A., 2017. Relationship of chlorophyll to phosphorus and nitrogen in nutrient-rich lakes. Inland Waters 7, 385–400. https://doi.org/10.1080/20442041.2017.1375176

Fiori, E., Zavatarelli, M., Pinardi, N., Mazziotti, C., Ferrari, C.R., 2016. Observed and simulated trophic index (TRIX) values for the Adriatic Sea basin. Natural Hazards and Earth System Sciences 16, 2043–2054. https://doi.org/10.5194/nhess-16-2043-2016

Frolov, S., Kudela, R.M., Bellingham, J.G., 2013. Monitoring of harmful algal blooms in the era of diminishing resources: A case study of the U.S. West Coast. Harmful Algae 21–22, 1–12. https://doi.org/10.1016/j.hal.2012.11.001

Fu, Y., Xu, S., Liu, J., 2016. Temporal-spatial variations and developing trends of Chlorophyll-a in the Bohai Sea, China. Estuar Coast Shelf Sci 173, 49–56. https://doi.org/10.1016/j.ecss.2016.02.016

Ghawi, R., Pfeffer, J., 2019. Efficient Hyperparameter Tuning with Grid Search for Text Categorization using kNN Approach with BM25 Similarity. Open Computer Science 9, 160–180. https://doi.org/10.1515/comp-2019-0011

gibbs, n.d. Factors influencing chlorophyll a concentrations in the Waikato River Retention time and thermal stratification in the hydro lakes.

Gillett, D.J., Weisberg, S.B., Grayson, T., Hamilton, A., Hansen, V., Leppo, E.W., Pelletier, M.C., Borja, A., Cadien, D., Dauer, D., Diaz, R., Dutch, M., Hyland, J.L., Kellogg, M., Larsen, P.F., Levinton, J.S., Llansó, R., Lovell, L.L., Montagna, P.A., Pasko, D., Phillips, C.A., Rakocinski, C., Ranasinghe, J.A., Sanger, D.M., Teixeira, H., van Dolah, R.F., Velarde, R.G., Welch, K.I., 2015. Effect of ecological group classification schemes on performance of the AMBI benthic index in US coastal waters. Ecol Indic 50, 99–107. https://doi.org/10.1016/j.ecolind.2014.11.005

Giordani, G., Zaldívar, J.M., Viaroli, P., 2009. Simple tools for assessing water quality and trophic status in transitional water ecosystems. Ecol Indic 9, 982–991. https://doi.org/10.1016/j.ecolind.2008.11.007

Giovanardi, F., Vollenweider, R.A., 2004. Trophic conditions of marine coastal waters: experience in applying the Trophic Index TRIX to two areas of the A... Trophic conditions of marine coastal waters: experience in applying the Trophic Index TRIX to two areas of the Adriatic and Tyrrhenian seas, J. Limnol.

Glibert, P.M., 2017. Eutrophication, harmful algae and biodiversity — Challenging paradigms in a world of complex nutrient changes. Mar Pollut Bull 124, 591–606. https://doi.org/10.1016/j.marpolbul.2017.04.027

Guo, D., Lintern, A., Webb, J.A., Ryu, D., Liu, S., Bende-Michl, U., Leahy, P., Wilson, P., Western, A.W., 2019. Key Factors Affecting Temporal Variability in Stream Water Quality. Water Resour Res 55, 112–129. https://doi.org/10.1029/2018WR023370

Gupta, M., 2014. A New Trophic State Index for Lagoons. Journal of Ecosystems 2014, 1–8. https://doi.org/10.1155/2014/152473

Hagy, J.D., Kreakie, B.J., Pelletier, M.C., Nojavan, F., Kiddon, J.A., Oczkowski, A.J., 2022. Quantifying coastal ecosystem trophic state at a macroscale using a Bayesian analytical framework. Ecol Indic 142. https://doi.org/10.1016/j.ecolind.2022.109267

Hale, S.S., Cicchetti, G., Deacutis, C.F., 2016. Eutrophication and hypoxia diminish ecosystem functions of benthic communities in a New England Estuary. Front Mar Sci 3. https://doi.org/10.3389/fmars.2016.00249

Hamby, D.M., 1995. A comparison of sensitivity analysis techniques. Health Phys 68, 195–204. https://doi.org/10.1097/00004032-199502000-00005

Hamby, D.M., 1994. a Review of Techniques for Parameter Sensitivity. Environmental Monitoring and Assessment 32, 135–154.

Hartnett, M., Nash, S., 2015. An integrated measurement and modeling methodology for estuarine water quality management. Water Science and Engineering 8, 9–19. https://doi.org/10.1016/j.wse.2014.10.001

Hartnett, M., Nash, S., Olbert, I., 2012. An integrated approach to trophic assessment of coastal waters incorporating measurement, modelling and water quality classification. Estuar Coast Shelf Sci 112, 126–138. https://doi.org/10.1016/j.ecss.2011.08.012

Heisler, J., Glibert, P.M., Burkholder, J.M., Anderson, D.M., Cochlan, W., Dennison, W.C., Dortch, Q., Gobler, C.J., Heil, C.A., Humphries, E., Lewitus, A., Magnien, R., Marshall, H.G., Sellner, K., Stockwell, D.A., Stoecker, D.K., Suddleson, M., 2008. Eutrophication and harmful algal blooms: A scientific consensus. Harmful Algae 8, 3–13. https://doi.org/10.1016/j.hal.2008.08.006

Hollister, J.W., Milstead, W.B., Kreakie, B.J., 2016. Modeling lake trophic state: A random forest approach. Ecosphere 7, 1–14. https://doi.org/10.1002/ecs2.1321

Izhar Shah, M., Alaloul, W.S., Alqahtani, A., Aldrees, A., Ali Musarat, M., Javed, M.F., 2021. Predictive modeling approach for surface water quality: Development and comparison of machine learning models. Sustainability (Switzerland) 13. https://doi.org/10.3390/su13147515
Jamshidi, S., Bin, N., Bakar, A., 2011. A study on distribution of chlorophyll-a in the coastal waters of Anzali Port, south Caspian Sea. Ocean Sci. Discuss 8, 435–451. https://doi.org/10.5194/osd-8-435-2011
Jiang, X., Xu, C., 2022. Deep Learning and Machine Learning with Grid Search to Predict Later Occurrence of Breast Cancer Metastasis Using Clinical Data. J Clin Med 11. https://doi.org/10.3390/jcm11195772
Jolliffe, I.T., 2007. Uncertainty and inference for verification measures. Weather Forecast. https://doi.org/10.1175/WAF989.1
Kärcher, O., Filstrup, C.T., Brauns, M., Tasevska, O., Patceva, S., Hellwig, N., Walz, A., Frank, K., Markovic, D., 2020. Chlorophyll a relationships with nutrients and temperature, and predictions for lakes across perialpine and Balkan mountain regions. Inland Waters 10, 29–41. https://doi.org/10.1080/20442041.2019.1689768
Khatri, P., Gupta, K.K., Gupta, R.K., 2021. A review of partial least squares modeling (PLSM) for water quality analysis. Model Earth Syst Environ. https://doi.org/10.1007/s40808-020-00995-4
Kim, J.H., 2019. Multicollinearity and misleading statistical results. Korean J Anesthesiol 72, 558–569. https://doi.org/10.4097/kja.19087
Kim, K.M., Ahn, J.H., 2022. Machine learning predictions of chlorophyll-a in the Han river basin, Korea. J Environ Manage 318. https://doi.org/10.1016/j.jenvman.2022.115636
Kothari, V., Vij, S., Sharma, S.K., Gupta, N., 2021. Correlation of various water quality parameters and water quality index of districts of Uttarakhand. Environmental and Sustainability Indicators 9. https://doi.org/10.1016/j.indic.2020.100093
Kouadri, S., Elbeltagi, A., Islam, A.R.M.T., Kateb, S., 2021. Performance of machine learning methods in predicting water quality index based on irregular data set: application on Illizi region (Algerian southeast). Appl Water Sci 11. https://doi.org/10.1007/s13201-021-01528-9
Koussouris, T.S., Diapoulis, A.C., Balopoulos, E.T., 1989. Assessing the trophic status of Lake Mikri Prespa, Greece. Ann Limnol 25, 17–24. https://doi.org/10.1051/limn/1989001
Kraha, A., Turner, H., Nimon, K., Zientek, L.R., Henson, R.K., 2012. Tools to support interpreting multiple regression in the face of multicollinearity. Front Psychol 3. https://doi.org/10.3389/fpsyg.2012.00044
Krueger, T., 2017. Bayesian inference of uncertainty in freshwater quality caused by low-resolution monitoring. Water Res 115, 138–148. https://doi.org/10.1016/j.watres.2017.02.061
Kulshreshtha, A., Shanmugam, P., 2018. Assessment of trophic state and water quality of coastal-inland lakes based on Fuzzy Inference System. J Great Lakes Res 44, 1010–1025. https://doi.org/10.1016/j.jglr.2018.07.015
Kumar, P., Mahajan, A.K., 2020. Trophic status and its regulating factor determination at the Rewalsar Lake, northwest Himalaya (HP), India, based on selected parameters and multivariate statistical analysis. SN Appl Sci 2. https://doi.org/10.1007/s42452-020-3082-8
Lake, Jarvis, Res, J., Lake, Jessie, Lake Kehiwin Lake, J., 2013. TROPHIC STATE OF ALBERTA LAKES Based On Average (May-October) Chlorophyll-a Concentrations.
Li, Hongzhi, Li, W., Pan, X., Huang, J., Gao, T., Hu, L.H., Li, Hui, Lu, Y., 2018. Correlation and redundancy on machine learning performance for chemical databases. J Chemom 32. https://doi.org/10.1002/cem.3023
Li, M., Sun, Y., Li, X., Cui, M., Huang, C., 2021. An improved eutrophication assessment algorithm of estuaries and coastal waters in liaodong bay. Remote Sens (Basel) 13. https://doi.org/10.3390/rs13193867
Liu, H., He, B., Zhou, Y., Kutser, T., Toming, K., Feng, Q., Yang, X., Fu, C., Yang, F., Li, W., Peng, F., 2022. Trophic state assessment of optically diverse lakes using Sentinel-3-derived trophic level index. International Journal of Applied Earth Observation and Geoinformation 114, 103026. https://doi.org/10.1016/j.jag.2022.103026
Li, X., Sha, J., Wang, Z.L., 2017. Chlorophyll-A Prediction of lakes with different water quality patterns in China based on hybrid neural networks. Water (Switzerland) 9. https://doi.org/10.3390/w9070524
Malek, S., Syed Ahmad, S.M., Singh, S.K.K., Milow, P., Salleh, A., 2011. Assessment of predictive models for chlorophyll-a concentration of a tropical lake. BMC Bioinformatics 12. https://doi.org/10.1186/1471-2105-12-S13-S12

Mamun, M., An, K.G., 2017. Major nutrients and chlorophyll dynamics in Korean agricultural reservoirs along with an analysis of trophic state index deviation. J Asia Pac Biodivers 10, 183–191. https://doi.org/10.1016/j.japb.2017.04.001

Mamun, M., Atique, U., An, K.G., 2021. Assessment of water quality based on trophic status and nutrients-chlorophyll empirical models of different elevation reservoirs. Water (Switzerland) 13. https://doi.org/10.3390/w13243640

Mansfield, E.R., Helms, B.P., 1982. Detecting Multicollinearity. Am Stat 36, 158–160. https://doi.org/10.1080/00031305.1982.10482818

Markad, A.T., Landge, A.T., Nayak, B.B., Inamdar, A.B., Mishra, A.K., 2019. Trophic state modeling for shallow freshwater reservoir: a new approach. Environ Monit Assess 191. https://doi.org/10.1007/s10661-019-7740-5

Matus-Hernández, M.Á., Hernández-Saavedra, N.Y., Octavio Martínez-Rincón, R., 2018. Predictive performance of regression models to estimate Chlorophyll - A concentration based on Landsat imagery. PLoS One 13. https://doi.org/10.1371/journal.pone.0205682

McCuen, R.H., Knight, Z., Cutter, A.G., 2006. Evaluation of the Nash–Sutcliffe Efficiency Index. J Hydrol Eng 11, 597–602. https://doi.org/10.1061/(asce)1084-0699(2006)11:6(597)

Minh, H.V.T., Tri, V.P.D., Ut, V.N., Avtar, R., Kumar, P., Dang, T.T.T., Hoa, A. van, Ty, T. van, Downes, N.K., 2022. A Model-Based Approach for Improving Surface Water Quality Management in Aquaculture using MIKE 11: A Case of the Long Xuyen Quadangle, Mekong Delta, Vietnam. Water (Switzerland) 14. https://doi.org/10.3390/w14030412

Mnyango, S.S., Thwala, M., Oberholster, P.J., Truter, C.J., 2022. Using Multiple Indices for the Water Resource Management of a Monomictic Man-Made Dam in Southern Africa. Water (Basel) 14, 3366. https://doi.org/10.3390/w14213366

Mohd Zebaral Hoque, J., Nor, N.A., Alelyani, S., Mohana, M., Hosain, M., 2022. Improving Water Quality Index Prediction Using Regression Learning Models. Int J Environ Res Public Health 19. https://doi.org/10.3390/ijerph192013702

Morgan, A.M., Royer, T. v., David, M.B., Gentry, L.E., 2006. Relationships among Nutrients, Chlorophyll- a , and Dissolved Oxygen in Agricultural Streams in Illinois . J Environ Qual 35, 1110–1117. https://doi.org/10.2134/jeq2005.0433

Moriasi, D.N., Gitau, M.W., Pai, N., Daggupati, P., 2015. Hydrologic and water quality models: Performance measures and evaluation criteria. Trans ASABE 58, 1763–1785. https://doi.org/10.13031/trans.58.10715

Mozo, A., Morón-López, J., Vakaruk, S., Pompa-Pernía, Á.G., González-Prieto, Á., Aguilar, J.A.P., Gómez-Canaval, S., Ortiz, J.M., 2022. Chlorophyll soft-sensor based on machine learning models for algal bloom predictions. Sci Rep 12. https://doi.org/10.1038/s41598-022-17299-5

Nash, S., Hartnett, M., Dabrowski, T., 2011. Modelling phytoplankton dynamics in a complex estuarine system. Proceedings of the Institution of Civil Engineers: Water Management 164, 35–54. https://doi.org/10.1680/wama.800087

Nguyen, T., Nemery, J., Gratiot, N., Strady, E., Quoc Tran, V., Nguyen, A., Aimé, J., Peyne, A., Nu, al, 2019. Nutrient dynamics and eutrophication assessment in the tropical river system of Saigon-Dongnai (southern Vietnam). Science of the Total Environment 653, 370–383. https://doi.org/10.1016/j.scitotenv.2018.10.319ï

O'Boyle, S., McDermott, G., Noklegaard, T., Wilkes, R., 2013. A Simple Index of Trophic Status in Estuaries and Coastal Bays Based on Measurements of pH and Dissolved Oxygen. Estuaries and Coasts 36, 158–173. https://doi.org/10.1007/s12237-012-9553-4

Ogorodnyk, O., Lyngstad, O.V., Larsen, M., Martinsen, K., 2019. Application of feature selection methods for defining critical parameters in thermoplastics injection molding, in: Procedia CIRP. Elsevier B.V., pp. 110–114. https://doi.org/10.1016/j.procir.2019.03.020

Park, J., Lee, W.H., Kim, K.T., Park, C.Y., Lee, S., Heo, T.Y., 2022. Interpretation of ensemble learning to predict water quality using explainable artificial intelligence. Science of the Total Environment 832. https://doi.org/10.1016/j.scitotenv.2022.155070

Parparov, A., 2010. Water Quality Assessment, Trophic Classification and Water Resources Management. J Water Resour Prot 02, 907–915. https://doi.org/10.4236/jwarp.2010.210108

Parween, S., Siddique, N.A., Mahammad Diganta, M.T., Olbert, A.I., Uddin, Md.G., 2022. Assessment of urban river water quality using modified NSF water quality index model at Siliguri city, West Bengal, India. Environmental and Sustainability Indicators 16, 100202. https://doi.org/10.1016/j.indic.2022.100202

Pasquier, R., D'Angelo, L., Goulet, J.-A., Acevedo, C., Nussbaumer, A., Smith, I.F.C., 2016. Measurement, Data Interpretation, and Uncertainty Propagation for Fatigue Assessments of

Structures. Journal of Bridge Engineering 21, 04015087. https://doi.org/10.1061/(asce)be.1943-5592.0000861

Pérez-Ruzafa, A., Campillo, S., Fernández-Palacios, J.M., García-Lacunza, A., García-Oliva, M., Ibañez, H., Navarro-Martínez, P.C., Pérez-Marcos, M., Pérez-Ruzafa, I.M., Quispe-Becerra, J.I., Sala-Mirete, A., Sánchez, O., Marcos, C., 2019. Long-term dynamic in nutrients, chlorophyll a, and water quality parameters in a coastal lagoon during a process of eutrophication for decades, a sudden break and a relatively rapid recovery. Front Mar Sci 6. https://doi.org/10.3389/fmars.2019.00026

Pettine, M., Casentini, B., Fazi, S., Giovanardi, F., Pagnotta, R., 2007. A revisitation of TRIX for trophic status assessment in the light of the European Water Framework Directive: Application to Italian coastal waters. Mar Pollut Bull 54, 1413–1426. https://doi.org/10.1016/j.marpolbul.2007.05.013

P. Obite, C., P. Olewuezi, N., U. Ugwuanyim, G., C. Bartholomew, D., 2020. Multicollinearity Effect in Regression Analysis: A Feed Forward Artificial Neural Network Approach. Asian Journal of Probability and Statistics 22–33. https://doi.org/10.9734/ajpas/2020/v6i130151

Primpas, I., Karydis, M., 2011. Scaling the trophic index (TRIX) in oligotrophic marine environments. Environ Monit Assess 178, 257–269. https://doi.org/10.1007/s10661-010-1687-x

Rahman, A., 2020. Statistics for Data Science and Policy Analysis, Statistics for Data Science and Policy Analysis. Springer Singapore. https://doi.org/10.1007/978-981-15-1735-8

Rahman, A., 2019. Statistics-Based Data Preprocessing Methods and Machine Learning Algorithms for Big Data Analysis | Rahman | International Journal of Artificial Intelligence™. International Journal of Artificial Intelligence 17, 44–65.

Rahman, A., Harding, A., 2016. Small area estimation and microsimulation modeling, 1st ed, Small Area Estimation and Microsimulation Modeling. CRC Press. https://doi.org/10.1201/9781315372143/SMALL-AREA-ESTIMATION-MICROSIMULATION-MODELING-AZIZUR-RAHMAN-ANN-HARDING

Rahman, A., Harding, A., Tanton, R., Liu, S., 2013. Simulating the characteristics of populations at the small area level: New validation techniques for a spatial microsimulation model in Australia. Comput Stat Data Anal 57, 149–165. https://doi.org/10.1016/J.CSDA.2012.06.018

Rueda, F.J., Fleenor, W.E., de Vicente, I., 2007. Pathways of river nutrients towards the euphotic zone in a deep-reservoir of small size: Uncertainty analysis. Ecol Modell 202, 345–361. https://doi.org/10.1016/j.ecolmodel.2006.11.006

Salem, S.I., Higa, H., Kim, H., Kobayashi, H., Oki, K., Oki, T., 2017. Assessment of chlorophyll-a algorithms considering different trophic statuses and optimal bands. Sensors (Switzerland) 17. https://doi.org/10.3390/S17081746

Saluja, R., Garg, J.K., 2017. Trophic state assessment of Bhindawas Lake, Haryana, India. Environ Monit Assess 189. https://doi.org/10.1007/s10661-016-5735-z

Sathishkumar, R.S., Sundaramanickam, A., Mohanty, A.K., Sahu, G., Ramesh, T., Balachandar, K., Nithin, A., Surya, P., Silambarasan, K., 2022. Seasonal assessment of the trophic status in the coastal waters adjoining Tuticorin harbor in relation to water quality and plankton community in the Gulf of Mannar, India. Oceanologia 64, 749–768. https://doi.org/10.1016/j.oceano.2022.07.002

Schober, P., Schwarte, L.A., 2018. Correlation coefficients: Appropriate use and interpretation. Anesth Analg 126, 1763–1768. https://doi.org/10.1213/ANE.0000000000002864

Seifi, A., Dehghani, M., Singh, V.P., 2020. Uncertainty analysis of water quality index (WQI) for groundwater quality evaluation: Application of Monte-Carlo method for weight allocation. Ecol Indic 117, 106653. https://doi.org/10.1016/j.ecolind.2020.106653

Şen, Z., Şişman, E., Kizilöz, B., 2022. A new innovative method for model efficiency performance. Water Supply 22, 589–601. https://doi.org/10.2166/ws.2021.245

Sharif, O., Hasan, M.Z., Rahman, A., 2022. Determining an effective short term COVID-19 prediction model in ASEAN countries. Sci Rep 12, 1–11. https://doi.org/10.1038/s41598-022-08486-5

Shaw, B.D., 2017. Uncertainty Analysis of Experimental Data with R. Chapman and Hall/CRC, Boca Raton : CRC Press, 2017. https://doi.org/10.1201/9781315366715

Shekar, B.H., Dagnew, G., 2019. Grid search-based hyperparameter tuning and classification of microarray cancer data. 2019 2nd International Conference on Advanced Computational and Communication Paradigms, ICACCP 2019. https://doi.org/10.1109/ICACCP.2019.8882943

Shi, J., Zhang, J., Shen, C., 2020. Construct and evaluate the classification models of six types of geological hazards in Bijie city, Guizhou province,China. https://doi.org/https://doi.org/10.5194/nhess-2020-124

Shin, Y., Kim, T., Hong, S., Lee, S., Lee, E., Hong, S.W., Lee, C.S., Kim, T.Y., Park, M.S., Park, J., Heo, T.Y., 2020. Prediction of chlorophyll-a concentrations in the Nakdong river using machine learning methods. Water (Switzerland) 12. https://doi.org/10.3390/w12061822

Shrestha, N., 2020. Detecting Multicollinearity in Regression Analysis. Am J Appl Math Stat 8, 39–42. https://doi.org/10.12691/ajams-8-2-1

Siddik, M.A.Z., 2022. Application of machine learning approaches in predicting estuarine dissolved oxygen (DO) under a limited data environment. Water Quality Research Journal 57, 140–151. https://doi.org/10.2166/wqrj.2022.002

Singh, K., Rashmi, P., 2014. Water quality management using statistical analysis and time-series prediction model 425–434. https://doi.org/10.1007/s13201-014-0159-9

Sokolova, E., Ivarsson, O., Lillieström, A., Speicher, N.K., Rydberg, H., Bondelind, M., 2022. Data-driven models for predicting microbial water quality in the drinking water source using E. coli monitoring and hydrometeorological data. Science of the Total Environment 802. https://doi.org/10.1016/j.scitotenv.2021.149798

Speiser, J.L., Miller, M.E., Tooze, J., Ip, E., 2019. A comparison of random forest variable selection methods for classification prediction modeling. Expert Syst Appl 134, 93–101. https://doi.org/10.1016/j.eswa.2019.05.028

Suvarna, M., Araújo, T.P., Pérez-Ramírez, J., 2022. A generalized machine learning framework to predict the space-time yield of methanol from thermocatalytic CO2 hydrogenation. Appl Catal B 315. https://doi.org/10.1016/j.apcatb.2022.121530

Tavazza, F., Decost, B., Choudhary, K., 2021. Uncertainty prediction for machine learning models of material properties. ACS Omega 6, 32431–32440. https://doi.org/10.1021/acsomega.1c03752

Toner, P., Bowman, J., Clabby, K., Lucey, J., Mc, McGarrigle, M., Concannon, C., Clenaghan, C., Cunningham, P., J., D., O'Boyle, S., MacCárthaigh, M., Craig, M., Quinn, R., 2005. Water Quality in Ireland 2001-2003.

Tugrul, S., Ozhan, K., Akcay, I., 2019. Assessment of trophic status of the northeastern Mediterranean coastal waters: eutrophication classification tools revisited. Environmental Science and Pollution Research 26, 14742–14754. https://doi.org/10.1007/s11356-018-2529-6

Uddin, Md. G., Moniruzzaman, Md., & Khan, M. 2017. Evaluation of Groundwater Quality Using CCME Water Quality Index in the Rooppur Nuclear Power Plant Area, Ishwardi, Pabna, Bangladesh. American Journal of Environmental Protection. https://doi.org/10.12691/env-5-2-2

Uddin, M. G., Moniruzzaman, M., Quader, M. A., & Hasan, M. A. 2018. Spatial variability in the distribution of trace metals in groundwater around the Rooppur nuclear power plant in Ishwardi, Bangladesh. Groundwater for Sustainable Development, 7. https://doi.org/10.1016/j.gsd.2018.06.002

Uddin, M.G., Stephen Nash, Olbert, A.I., 2020a. Application of Water Quality Index Models to an Irish Estuary, in: Civil and Environmental Research. Civil Engineering Research Association of Ireland (CERAI), pp. 576–581.

Uddin, M. G., Olbert, A. I., & Nash, S. 2020b. Assessment of water quality using Water Quality Index (WQI) models and advanced geostatistical technique. Civil Engineering Research Association of Ireland (CERAI), 32(Special Issue), 594–599. http://hdl.handle.net/10379/16427

Uddin, G., Nash, S., Olbert, A.I., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol Indic 122, 107218. https://doi.org/10.1016/j.ecolind.2020.107218

Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022a. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment. Water Res 219, 118532. https://doi.org/10.1016/j.watres.2022.118532

Uddin, M.G., Nash, S., Mahammad Diganta, M.T., Rahman, A., Olbert, A.I., 2022b. Robust machine learning algorithms for predicting coastal water quality index. J Environ Manage 321. https://doi.org/10.1016/j.jenvman.2022.115923

Uddin, Md.G., Nash, S., Diganta, M.T.M., Rahman, A., Olbert, A.I., 2022c. A comparison of geocomputational models for validating geospatial distribution of water quality index, in: Priyanka, H., Rahman, A., Basant agarwal, Binita Tiwari (Eds.), Computational Statistical Methodologies and Modeling for Artificial Intelligence. CRC Press, Taylor & Francis Publisher, USA.

Uddin, G., Nash, S., Rahman, A., Olbert, A.I., 2022d. Assessing optimization techniques for improving water quality model.

Uddin, G., Nash, S., Rahman, A., Olbert, A.I., 2022e. A sophisticated model for rating water quality.

Uddin, Md.G., Nash, S., Rahman, A., Olbert, A.I., 2023a. A novel approach for estimating and predicting uncertainty in water quality index model using machine learning approaches. Water Res 119422. https://doi.org/10.1016/J.WATRES.2022.119422

Uddin, G., Nash, S., Rahman, A., Olbert, A.I., 2023b. Performance analysis of the water quality index model for predicting water state using machine learning techniques. Process Safety and Environmental Protection 169. https://doi.org/10.1016/j.psep.2022.11.073

Villalobos-Arias, L., Quesada-López, C., Guevara-Coto, J., Martínez, A., Jenkins, M., 2020. Evaluating hyper-parameter tuning using random search in support vector machines for software effort estimation. PROMISE 2020 - Proceedings of the 16th ACM International Conference on Predictive Models and Data Analytics in Software Engineering, Co-located with ESEC/FSE 2020 31–40. https://doi.org/10.1145/3416508.3417121

Vollenweider, R.A., Giovanardi, F., Montanari, G., Rinaldi, A., 1998. Characterization of the trophic conditions of marine coastal waters with special reference to the NW Adriatic Sea: proposal for a trophic scale, turbidity and generalized water quality index. Environmetrics 9, 329–357. https://doi.org/10.1002/(SICI)1099-095X(199805/06)9:3<329::AID-ENV308>3.0.CO;2-9

Wall, B., Cahalane, A., Derham, J., 2020. Ireland's Environment - An Integrated Assessment.

Wasmund, N., Andrushaitis, A., Łysiak-Pastuszak, E., Müller-Karulis, B., Nausch, G., Neumann, T., Ojaveer, H., Olenina, I., Postel, L., Witek, Z., 2001. Trophic status of the south-eastern Baltic Sea: A comparison of coastal and open areas. Estuar Coast Shelf Sci 53, 849–864. https://doi.org/10.1006/ecss.2001.0828

Watanabe, F.S.Y., Alcântara, E., Rodrigues, T.W.P., Imai, N.N., Barbosa, C.C.F., Rotta, L.H. da S., 2015. Estimation of chlorophyll-a concentration and the trophic state of the barra bonita hydroelectric reservoir using OLI/landsat-8 images. Int J Environ Res Public Health 12, 10391–10417. https://doi.org/10.3390/ijerph120910391

Wei, Y., Huang, H., Chen, B., Zheng, B., Wang, Y., 2019. Application of Extreme Learning Machine for Predicting Chlorophyll-A Concentration Inartificial Upwelling Processes. Math Probl Eng 2019. https://doi.org/10.1155/2019/8719387

Westad, F., Marini, F., 2022. Variable Selection and Redundancy in Multivariate Regression Models. Frontiers in Analytical Science 2. https://doi.org/10.3389/frans.2022.897605

Wurtsbaugh, W.A., Paerl, H.W., Dodds, W.K., 2019. Nutrients, eutrophication and harmful algal blooms along the freshwater to marine continuum. Wiley Interdisciplinary Reviews: Water 6. https://doi.org/10.1002/WAT2.1373

Xiao, Y., Ferreira, J.G., Bricker, S.B., Nunes, J.P., Zhu, M., Zhang, X., 2007. Trophic Assessment in Chinese coastal systems-review of methods and application to the Changjiang (Yangtze) Estuary and Jiaozhou Bay. Estuaries and Coasts 30, 901–918. https://doi.org/10.1007/BF02841384

Xu, F.L., Jiao, Y., 2018. Trophic classification for lakes. Encyclopedia of Ecology 487–494. https://doi.org/10.1016/B978-0-12-409548-9.11176-5

Yao, Y., Hu, Q., Yu, H., Grzymala-Busse, J.W., 2015. Rough Sets, Fuzzy Sets, Data Mining, and Granular Computing, Proceedings.

Yoo, C., Cho, E., 2019. Effect of multicollinearity on the bivariate frequency analysis of annual maximum rainfall events. Water (Switzerland) 11. https://doi.org/10.3390/w11050905

Yoo, W., Mayberry, R., Bae, S., Singh, K., Lillard, J.W., 2014. A Study of Effects of MultiCollinearity in the Multivariable Analysis, Int J Appl Sci Technol.

Yucel-Gier, G., Pazi, I., Kucuksezgin, F., Kocak, F., 2011. The composite trophic status index (TRIX) as a potential tool for the regulation of Turkish marine aquaculture as applied to the eastern Aegean coast (Izmir Bay). Journal of Applied Ichthyology 27, 39–45. https://doi.org/10.1111/j.1439-0426.2010.01576.x

Yu, H., Jiang, S., Land, K.C., 2015. Multicollinearity in hierarchical linear models. Soc Sci Res 53, 118–136. https://doi.org/10.1016/j.ssresearch.2015.04.008

Yurista, P.M., Kelly, J.R., Scharold, J. v., 2016. Great Lakes nearshore-offshore: Distinct water quality regions. J Great Lakes Res 42, 375–385. https://doi.org/10.1016/j.jglr.2015.12.002

Zhang, J., Fu, P., Meng, F., Yang, X., Xu, J., Cui, Y., 2022. Estimation algorithm for chlorophyll-a concentrations in water from hyperspectral images based on feature derivation and ensemble learning. Ecol Inform 71. https://doi.org/10.1016/j.ecoinf.2022.101783

Zhang, W., Huang, W., Tan, J., Guo, Q., Wu, B., 2022. Heterogeneous catalysis mediated by light, electricity and enzyme via machine learning: Paradigms, applications and prospects. Chemosphere. https://doi.org/10.1016/j.chemosphere.2022.136447

Zhou, Y., He, B., Fu, C., Giardino, C., Bresciani, M., Liu, H., Feng, Q., Xiao, F., Zhou, X., Liang, S., 2021. Assessments of trophic state in lakes and reservoirs of Wuhan using Sentinel-2 satellite data. Eur J Remote Sens 54, 461–475. https://doi.org/10.1080/22797254.2021.1960201

10. Conclusion and recommendations

10.1 Conclusion

The conclusions that have been drawn from the research are as follows:

- To the best of the author's knowledge, the research is the first comprehensive methodology for developing a WQI model in a systematic manner.
- In developing the WQI model, important indicator selection is a crucial component. The research used eighteen different FS techniques, including (i) nine filter methods, (ii) two wrapper methods, and (iii) seven embedded methods, to analyse the effects of various input sets (combinations of various WQ indicators) on the WQI model. The results indicate that the embedded based random forest (RF) algorithm is an effective technique for selecting the crucial water quality indicators for the development a WQI model. The research suggests that eight water quality indicators (BOD_5, DIN, MRP, TEMP, pH, DOX, TON, and TRAN) are important for monitoring and assessing coastal water quality using the new approach.
- WQI models are subject to significant uncertainty due to the selection of inappropriate indicators, according to the literature. The values of the selected water quality indicators generated by the improved method less than 1% of the total model uncertainty. The research also shows that the number of input indicators has a significant effect on the input uncertainties of the model.
- The sub-index (SI) function(s) is/are another vital source of model uncertainty (due to the eclipsing issue) in WQI model. The research developed three linear interpolation rescaling functions, including a few binary rules. In terms of reducing the eclipsing problem, the developed SI functions outperformed other approaches. The SI functions were tested using different datasets across four domains in terms of spatio-temporal resolution. During the study period, there were no eclipsing issues with SI functions. The SI functions' sensitivity results show that the developed functions are effective at transferring various water quality indicator information into the SI score without hiding or losing any of the indicator's actual attributes.

- Sub-index functions were found to contribute significantly (< 13%) to the WQI model uncertainties, and hence affect the model reliability. Therefore, the determination of sub-index functions needs to be taken with care.
- The estimation of indicator weights is one of the sources of uncertainty in the WQI model. In order to estimate weight values, four mathematical approaches were compared: (i) rank sum, (ii) rank reciprocal, (iii) rank order centroid, and (iv) equivalent incorporating the random forest machine learning technique. In comparison to the other methods, the rank sum method significantly reduces uncertainty and produces relatively low levels of uncertainty (1%).
- The aggregation function is a great concern in the WQI model in terms of producing uncertainty. The research compared eight functions (five are most widely used in the existing system, and three are newly tested, including one weighted and two unweighted) in order to compute the WQI scores for similar attributes of water quality. There were significant statistical differences found between the eight aggregation functions. The weighted quadratic mean (WQM) function was found to provide a plausible assessment of the WQ of coastal waters at reduced uncertainty levels. The findings of this study also suggest that the unweighted root mean squared (RMS) aggregation function could also be potentially used for the assessment of coastal WQ. Both techniques produced less than 2% uncertainty, whereas higher uncertainty was associated with other models.
- In addition, relatively, the lowest rate of ambiguity problem (< 5%) was found both aggregation functions for assessing TrC waters.
- Ultimate goal of the WQI approach is to rank water quality using classification scheme (score translation method). Another drawback of the existing WQI approaches, several WQI models are provided different rank of water quality for similar water quality attribute. Consequently, it is hard to determine the actual state of the water quality. In this circumstance, the present research was developed a brand new classification scheme for assessing TrC waters in order to the generalized uses.
- For the purposes of the performance analysis of the new classification scheme in order to assess TrC waters incorporating the eight WQI models using most widely used four classifier algorithms. The results of from the research shows

that the model could be effective for the proper rating of water quality using the new classification scheme.

- It should be noted that the author developed the methodology for estimating and predicting WQI model uncertainty at each step of the WQI model in order to determine a composite scenario of model uncertainty, which was the first attempt in improving the WQI model.
- Moreover, to the Author’s knowledge, the present research is the first attempt to define in detail the eclipsing and ambiguity problems, sources, nature, their impact on the WQI model, and determination procedures for them.
- The model was tested across four Irish waterbodies: (i) Dublin Bay, (ii) Cork harbour, (iii) Galway Bay, and (iii) Mulroy Bay in order to assess the model sensitivity in terms of Spatio-temporal resolution using summer and winter water quality data. The sensitivity results of model indicate that the model outputs could be explained by more than 95% of the input entities, including less than 2% uncertainty with a 95% confidence interval at $p < 0.0001$.
- The model performance validation results of NSE and MEF show that the developed model is superior for computing WQI scores at most monitoring sites across four application domains through the summer and winter periods.
- All statistical measures of performance metrics also indicate that the model is more effective for the prediction of WQI, whereas the lowest prediction errors were found during the testing phase for predicting WQI scores across four waterbodies for both seasons.
- The assessment results of water quality proved that the model could be reliable for optimizing the model ambiguity and eclipsing problems in order to assess TrC waters in any geographical extent.
- Moreover, the performance of model applications reveals that suggested indicators might be adequate and reliable to monitor the TrC waters with the improved model.

However, to the best of the Author's knowledge, the model is the first improved WQI approach that was developed focused on the TrC water, whereas the model is widely tested, validated in terms of spatio-temporal resolution. Also, the research has widely analysed the model's sensitivity, efficiency, and uncertainty, including eclipsing, and ambiguity, that could be helpful for further improvement of the model. Although the research proposed the model for transitional and coastal water quality, it is likely that the method could be used to measure water quality in other waterbodies, especially rivers, lakes, etc. It should be noted that, even though the model was developed using water quality indicators for Cork Harbour, results from applications show that the model could be adapted at any geospatial scale.

10.2 Recommendation for further research

The research developed a comprehensive IEWQI model for assessing marine waters, including trophic state, that provides an accurate, cost-effective, and universal solution that will be applicable to any marine waterbody. The developed model could be an effective WQI model for monitoring marine waters in terms of reducing model uncertainty as well as avoiding eclipsing, ambiguity, and metaphoring problems in the final assessment. For the purposes of global application, the IEWQI model was tested and validated across four Irish waterbodies in order to assess the model's sensitivity. The research suggested that the model could aid surface water monitoring and resource management as directed by the European Union Water Framework Directives (EU-WFD) as well as EPA, Ireland. The model could be used for monitoring and assessing lakes, rivers, etc. at low computational costs in order to minimize the cost of the typical monitoring program. In order to apply the model at the global scale, further scientific research is required for validating the model's performance using different Spatio-temporal scales. The recommendations can be divided into two scopes in terms of enhancing model functionality and applications. The following are recommendations for future research that could be carried out to enhance the model's functionality:

10.2.1 Model architectural improvement

Model elements, particularly sub-index functions, should be further revised and tested using various sets of water quality data in order to ascertain the sub-index functions' spatio-temporal sensitivity in order to increase the model's efficacy. This might help to reduce model uncertainty and increase model reliability.

10.2.2 Global sensitivity analysis

The research developed the IEWQI model based on the Irish coastal water quality attributes. The goal of this project was to provide a universal solution for assessing

TrC waters. Prior to applying the model globally, it is required to assess the model sensitivity in terms of the spatio-temporal resolution of various waterbodies around the world. Therefore, the model sensitivity should be analysed by applying the IEWQI model to both developing countries like Bangladesh, India, Malaysia, Indonesia, China, Egypt, Iran etc., and developed countries such as Northern Ireland, the UK, Turkey, Poland, Greece, Netherland, Portugal, France, Australia, New Zealand etc.. After determining the model sensitivity, water quality indicators should be revised and updated for forwarding to global application of the IEWQI model.

10.2.3 Hydrodynamic impact assessment on the IEWQI model

The research only utilized the physicochemical characteristics of waters based on the WFD guidelines for monitoring and assessment of the general state of marine waters in order to develop the IEWQI model. Hydrodynamic characteristics like water depth, tidal regime, water surface elevation, current velocity, waves, or flushing characteristics like residence time were not taken into account. Several studies have revealed that hydrodynamic properties significantly influence the various water quality attributes, for example DOX, COD, BOD, pH, turbidity, and various nutrient components of water. In addition, a few studies have reported that the hydrodynamics components *plays an important role in* the spatial distribution of various water quality indicators. Along with the hydrodynamic characteristics, residence time can have an impact on the flushing characteristics, which in turn can influence the water quality attributes and reveal estuary dynamics.

Therefore, further research should be carried out to assess the impact of hydrodynamic features on the IEWQI model. In order to assess the impact, it is proposed to develop a coupled DIVAST-IEWQI model for marine waters and then compare the results between the integrated DIVAST-IEWQI and independent IEWQI models. Figure 10.1 presents the complex architecture of the integrated DIVAST-IEWQI model. The DIVAST-IEWQI model should be developed to enable the following goals:

- Calculate IEWQI indices at each timestep of the model so as to estimate IEWQI values at particular locations
- Produce time series output locations at the same locations to generate water quality at specific locations
- Calculate IEWQI values manually in Excel using DIVAST timeseries data

based on water quality module output

- Compare the IEWQI values produced by the integrated DIVAST-IEWQI model with the Excel WQI values could be used to validate DIVAST-WQI model
- Apply the integrated DIVAST-IEWQI model to various acse study waterbodies in Ireland.

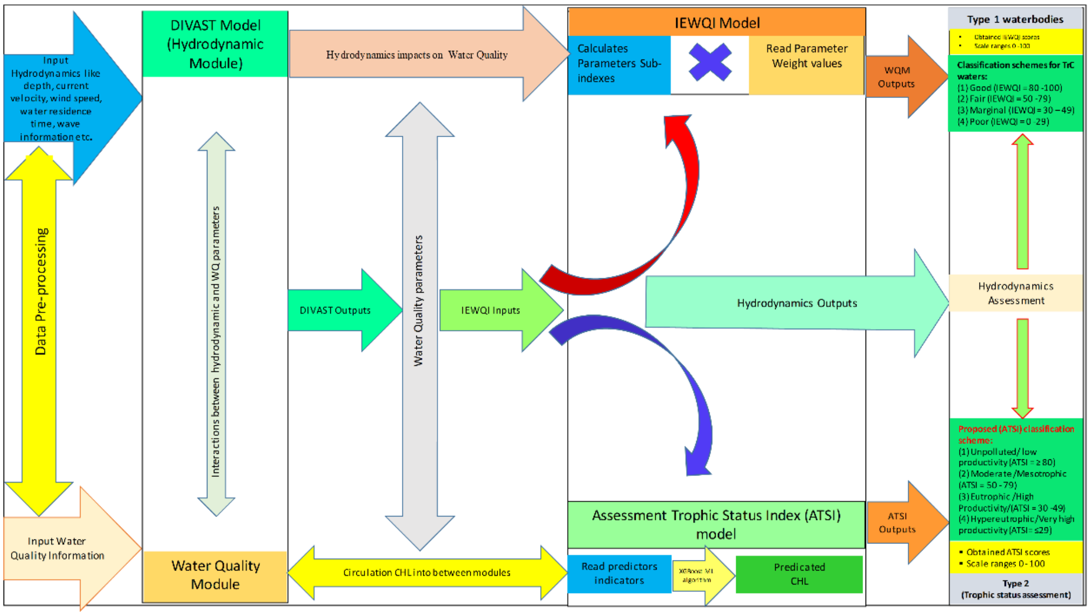


Figure 10.1. Proposed framework for the integrated the DIVAST-IEWQI model for assessing and monitoring marine waters.

The findings of this research would be useful for determining the impacts of various hydrodynamic components on water quality in marine ecosystems. Also, the integrated DIVAST-IEWQI model could be an effective tool for supporting the WFD in order to monitor marine waters more accurately and cost-effectively. Additionally, the research would be useful for improving the IEWQI model further in terms of optimizing and upgrading the model inputs that can be converted into attributes for both hydrodynamics and water quality for the IEWQI score.

10.2.4 Model validation using remote sensing data

The IEWQI model was developed based on conventional monitoring data. Due to the limitations of existing monitoring systems, many countries/organizations/researchers have recently paid much more attention to monitoring water quality using cutting-edge remote sensing (RS) techniques. A number of studies may be carried out to validate the IEWQI model using RS data in terms of investigating model sensitivity, uncertainty, etc. Although several studies have revealed that there are a few constraints to the RS technique when it comes to monitoring water quality, prior to the study, the probability of an RS application for monitoring Irish waterbodies should be explored. This study might be helpful to improve the existing monitoring program by incorporating the new IEWQI approach.

10.2.5 Generalized model application

Although the IEWQI model was developed for marine waters, there is a high possibility that the IEWQI approach could be utilized to assess the water quality of other waterbodies, particularly rivers, lakes, and other bodies of water where fresh water predominates. Therefore, a few studies may be carried out to assess river and lake water quality using the model, which would enhance the current monitoring program as well as increase the suitability of the model for general application.

10.2.6 The IEWQI-ATSI model as a tool of the WFD

Further research could be carried out to investigate the use of WQI models as a tool for the implementation of the EU Water Framework Directive (WFD) and the improvement of typical monitoring programs. A water quality-monitoring program is an effective tool for routinely assessing the water quality, whereas the WFD is a useful tool for implementing the monitoring and evaluating the program for managing "good" water quality in EU regions. It contains detailed guidelines for developing a monitoring program to determine water quality for various purposes. The WFD advises three different types of waterbodies in Europe so that regular monitoring can be done to ensure that all stats are "good." Table 10.1 (above) provides in detail the WFD’s different types of water bodies and the implementation of the IEWQI-ATSI model. The developed IEWQI model is currently only suitable to assess type I waterbodies, and the developed ATSI model is enabled to assess type II waterbodies, whereas the proposed comprehensive model is not suitable for assessing type III (bathing water quality) waterbodies because it is a mandatory requirement to consider biological indicators like fecal coliform or other bacteriological indicators must be added into the model. Using the suggested strategy, it might be possible to address type III waterbodies as well. Further investigation could be done to evaluate the type III waterbodies using the IEWQI approach, taking into account the biological indicators in addition to the model's suggested inputs, which could be used for evaluating the entire range of water quality in the EU region. Therefore, other EU members could implement and use the IEWQI model as a universal tool for evaluating surface water quality. It could be a powerful tool for fully implementing the WFD across the EU.

10.2.7 Develop automation architecture for improving monitoring program

Most countries or organizations use the manual approach for assessing the state of water quality, including EU member states. In the traditional WQ monitoring program, the WQ state is determined by comparing selected indicators with their respective guideline values and applying a certain methodology for an assessment of the WQ category. This manual approach is time consuming and costly. More recently, the water quality index (WQI) models for have been successfully applied for surface water (e.g., rivers, lakes) quality assessment and gained popularity among various countries/organizations/agencies. Compared to other water quality models, the WQI model is a simple yet accurate technique that uses standard WQ indicators to assign WQ status. While WQI models are typically used for freshwater systems, the research developed an Irish WQI model (IEWQI) that focused on TraC waters. For the implementation of the IEWQI-ATSI model application at a global scale, an automation architecture for water quality monitoring and assessment across the EU can be developed, incorporating cloud computing systems using ML and AI techniques. Figure 10.2 shows a conceptual framework for the proposed automation architecture using IEWQI-ATSI model. That could be useful to improve the monitoring program and assess water quality most accurately using an automated process in a cost-effective and rapid manner.

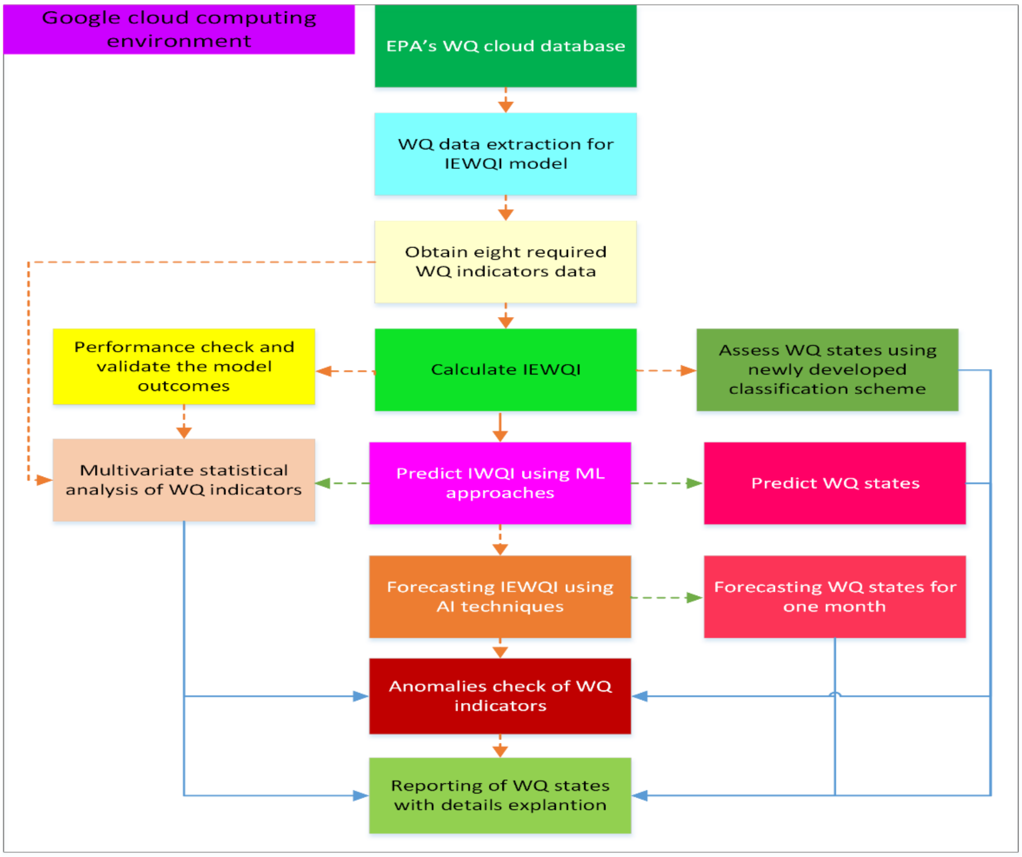


Figure 10.2. A conceptual framework for the proposed automation architecture using IEWQI-ATSI model.

List of supporting studies: Conference proceeding, Book chapter and abstracts

Study 1: Application of Water Quality Index Models to an Irish Estuary

1.1 Abstract

The paper investigates the application of different Water Quality Index (WQI) models for to estuarine waters. WQI models are aggregation based mathematical models that convert extensive water quality data into a single value. They typically contain four crucial components with the functions of (1) selecting parameters, (2) developing sub-index rules, (3) generating weighting values, and (4) aggregating the sub-indices. They are attractive because of their relative simplicity and ease of application. However, there is a level of uncertainty in the final aggregated indices due to the potentially large spatial and temporal variations in the input water parameter values. Here we apply seven different WQI models to Cork Harbour, an estuary on the southwest coast of Ireland. The water quality data input data included measurements of nine water quality monitoring parameters from 31 monitoring sites in Cork Harbour. The spatial uncertainty of the WQI models was estimated based on the standard deviation of the computed indices. The spatial uncertainty of the input water quality data was also determined and compared with that of the WQIs for any correlation.

Keywords: Water Quality Index; WQI model; estuary; uncertainty

1.2 Introduction

Water is a crucial component of the biosphere since it is essential for living organisms. Surface water quality has gradually been deteriorated by both natural and anthropogenic processes in the last number of decades. In recent times, the global community has been faced with a significant challenge to maintain good water quality status. Management of water quality requires effective water quality assessment tools and techniques. The Water Quality Index (WQI) model has become a popular method for assessing water quality since it was first developed by Horton in 1965. It is a relatively simple tool which allows one to convert extensive water quality data into a single numerical value which describes the water quality. Since it is relatively easy to use by professionals and the output is easy to understand, particularly for non-professionals, it is widely used around the world.

Many countries/agencies have developed different WQI models to evaluate different types of waterbodies (Fig. 1). A review of 107 studies of WQI applications determined more than 35 different WQI models with 80% of the applications to rivers, 10% to lakes and 10% to estuaries. Of the 35 different WQIs, many are variations of earlier models. Due to the many variations between models and the nature of their basic function (i.e. converting large amounts of temporally- and spatially-varying data into single values), the resulting WQI model index values have differing levels of uncertainty. This uncertainty is mainly associated with the formulations of the WQI model components [1]. Most WQI models have four components including: (1) selection of parameters to be included in the model, (2) development of sub-indices for each water quality parameter, (3) generation of weightings for each parameter and (4) aggregation of the sub-indices.

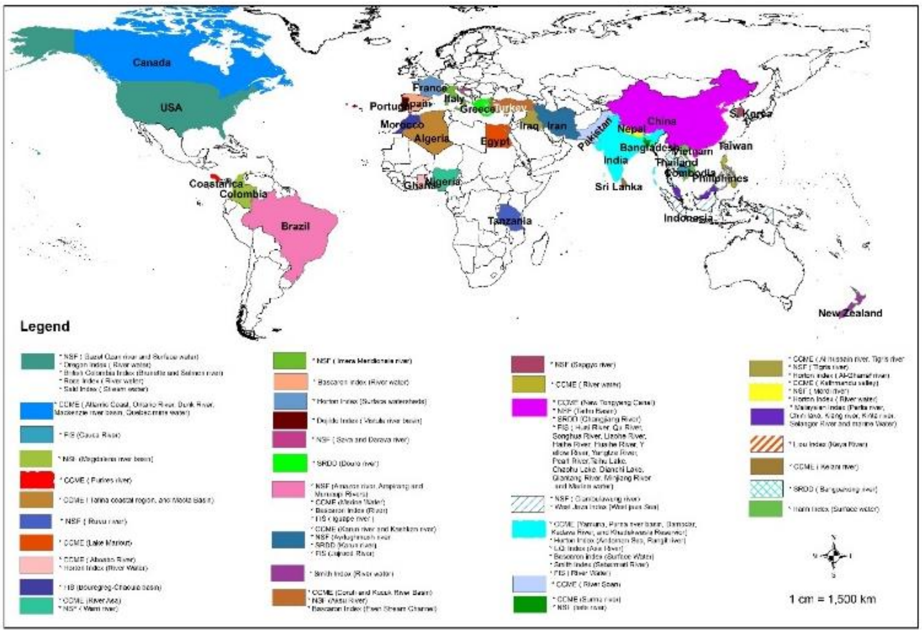


Figure 1: Global applications of WQI models.

Some researchers have shown that most of the model uncertainty is contributed by the sub-indexing and parameter weighting components [2, 3] but, more recently, other researchers have reported that the aggregation function is the primary source of the uncertainty [4]. The present research applies seven of the most commonly used WQI models to an Irish estuary – Cork Harbour – and assesses the levels of uncertainty in the computed water quality indices. Cork Harbour was chosen for the study as a broader research aim is to explore the viability of using WQI models for assessment of water quality in estuaries; there is currently a dearth of literature in this area.

Section 1.3 of this paper presents a description of Cork Harbour and the monitoring stations. Section 3 describes the materials and methods and Section 4 presents the results of the WQI applications and the uncertainty assessment. Section 5 presents some conclusions based on the research.

1.3 The study area – Cork Harbour

Cork Harbour is a macro-tidal estuary on the southwest coast of Ireland. It has a typical spring tide range of 4.2 m at the entrance to the harbour [5]. Water depths are generally relatively shallow with much of the estuary having a depth of less than 5 meters on spring tides. At low water, a major portion of the harbour area is exposed with mud-flats and sand-flats (Fig 2). The harbor deepens towards the mouth in the main Channel to depths of about 30 m.

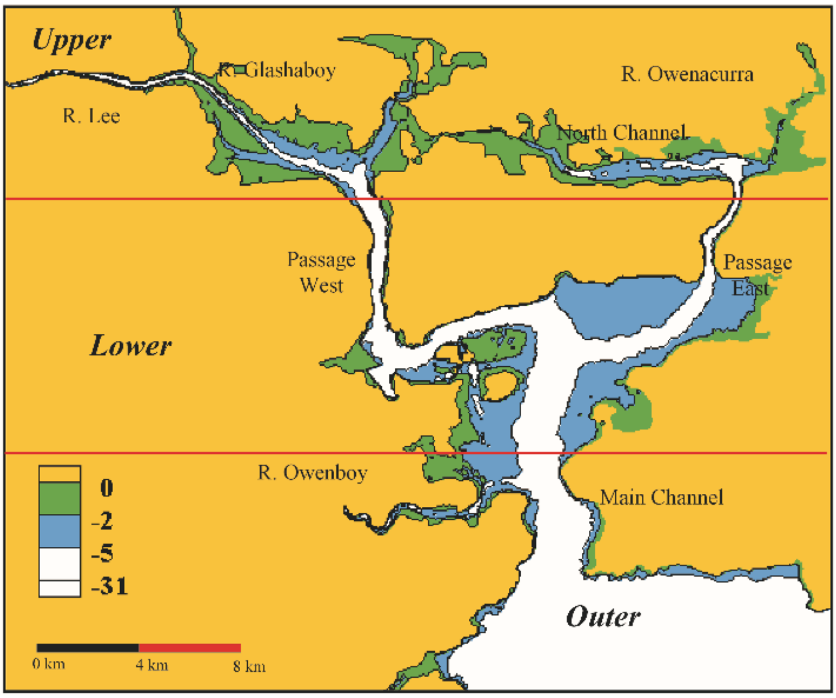


Figure 2: Plan view of Cork Harbour showing mean water depths. Green areas are inter-tidal.

Cork Harbour is the largest natural harbor in Ireland and it is heavily populated and industrialised. A number of rivers flow into the estuary, the largest being the River Lee which flows through Cork City and accounts for approximately 75% of the freshwater delivered to the estuary [5]. Cork city on the River Lee is home to a population of approximately 125,000. When its immediate suburbs are included, the population rises to approximately 200,000. The city is the industrial centre of the Irish southwest region. It is home to a number of large multinationals in the pharmaceutical (e.g. Boston Scientific and Pfeizzer) and ICT (e.g. Apple and Logitec) sectors as well as having a strong domestic industry base. In addition, the surrounding hinterland is subject to relatively intense agricultural activity. As part of the water quality framework, water quality is monitored by the Irish Environmental Protection Agency at 31 monitoring stations in the harbour (Fig 3).

1.4 Materials and methods

Seven WQI models were applied to Cork Harbour for the study area extents shown in Fig 3. Brief descriptions of the WQIs and the input water quality data follow.

1.4.1 Water Quality Index (WQI) Models

A review of WQI models used in the literature, identified seven basic models which are evaluated in this research [6]. These are:

- The Horton Index model
- The National Sanitation Foundation (NSF) model
- The Scottish Research Development Department (SRDD) model
- The Canadian Council of Ministers of the Environment (CCME) model
- The West-Java (WJ) model
- The Bascaron model
- The Hanh model.

Details of the model structures, mathematical approaches and their applications can be found in [6].

1.4.1.1 Water quality Input Data

In total, nine water quality parameters were used in the WQI models, namely:

- Salinity
- Temperature (0 c)
- pH
- Dissolved oxygen (DO)
- Total organic nitrogen (TON)
- Ammoniacal nitrogen (NH_3^+)
- Nitrate (NO_3^-)
- Orthophosphate (PO_4^{3-})
- Chlorophyll-a (Chl-a) (as a measure of algae)

Water quality parameters were selected based on the WQI model's requirements and monitoring guidelines of surface water quality. Data from the 31 EPA monitoring locations in Cork Harbour shown in Fig 3 were used. 2007 was selected as the test year as the data were available from another research project. EPA generally take measurements at each location at approximately high and low tide on the same day in winter and summer conditions, although the months of collection vary from year to year.

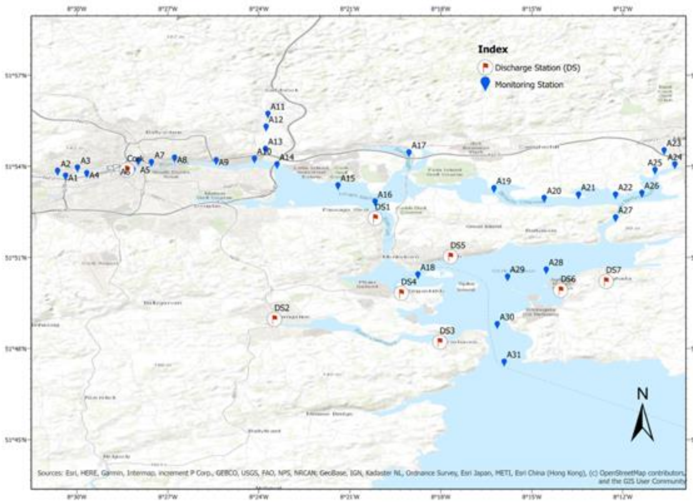


Figure 3: Water quality monitoring locations used in study.

1.4.1.2 WQI Application Procedure

The water quality data at each location were depth- and time-averaged at to give an average annual value. The same input water quality data were then supplied to all seven WQI models. The parameter weighting values for the models were produced by applying the Analytical Hierarchy Process (AHP) technique. Final WQI scores were obtained according to the aggregation functions of each WQI model. The different WQI model aggregation functions are defined in equations (1)-(7).

$$\text{Horton index} = \left[\frac{W_1S_1+W_2S_2+W_3S_3+\cdots.+W_nS_n}{W_1+W_2+W_3\ldots\ldots+W_n}\right] m_1m_2 \qquad (1)$$

where s_i and w_i are the sub-index and weight values of water quality parameter i, n is the number of parameters, and m_1 correction factors of temperature and m_2 is the correction factor for pollution respectively; both are ranges between 0.5 to 1.0.

$$NSF\ index = \sum_{i=1}^{n} w_i s_i \qquad (2)$$

$$SRDD\ index = \frac{1}{100}\left(\sum_{i=1}^{n} S_i W_i\right)^2 \quad (3)$$

$$CCME = \frac{\sqrt{F_1{}^2 + F_2{}^2 + F_3{}^2}}{1.732} \quad (4)$$

where F_1 is the percentage of failed parameters that do not meet with regarding their guideline value; F_2 is the percentage of individual test cases these do not meet with the guideline value and F_3 is the variation percentage of the failed test parameters that do not meet their objectives; and 1.732 is a divisor that is applied for normalization [7].

$$West\ Java\ Index = \prod_{i=1}^{n} S_i{}^{w_i} \quad (5)$$

$$Bascaron\ Index = \frac{\sum C_i P_i}{\sum P_i} \quad (6)$$

$$Hanh\ Index = \left[\frac{1}{6}\sum_{i=1}^{6} q_i \times \frac{1}{2}\sum_{i=1}^{2} q_j \times q_k\right]^{1/3} \quad (7)$$

where q_i is the sub-index value of the organic and nutrients group including pH, DO, NH_4^+ NO_3^-, PO_4^{3-}, TON; q_j is the sub-index value of the particulates group, including temperature and salinity; and q_k is the sub-index value of the biological group containing only *Chlorophyll-a*.

1.4.1.3 Uncertainty analysis

Each WQI model produced 31 index values, one for each monitoring station. For each WQI model, the standard deviation of the 31 indices was used as the measure of spatial uncertainty. The spatial uncertainty of the water quality input data was also determined in the same way for each water quality parameter. All statistical parameters were calculated using SPSS.

1.5 Results and discussion

1.5.1 WQI Index Values

The model indices computed at each monitoring location are presented in figure (4) – (10) for each of the WQI models. Each station is attributed a ranking using the model ranking scales. The ranking systems used are shown in Table 1.

Unlike the other models, for the Horton model a lower score indicates better water quality. The lowest index obtained was 18 while the highest index was 24 (Fig. 4).

According to the ranking system, excellent water quality was observed at all stations. The NSF indices ranged from 68 to 98 and 15 of the 31 stations (48%) in Cork harbour were attributed excellent water quality status. Around 23 % of monitoring locations water quality was evaluated with good status, while the remaining locations were attributed medium quality status (Fig. 5). The SRDD model indices ranged from 55 to 98 and gave excellent water quality in 15 of the 31 stations (Fig. 6). For the CCME model, indices ranged from 93-100 and excellent water quality was therefore observed at 17 locations (Fig. 7).

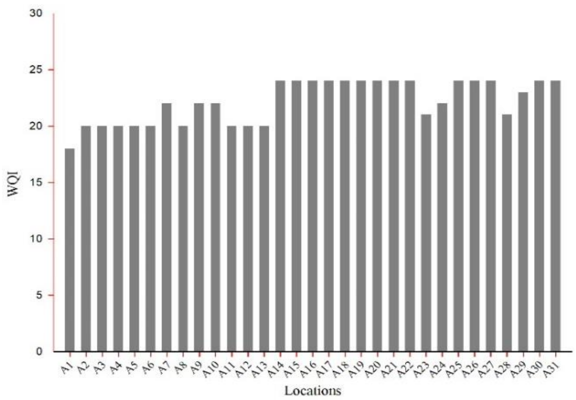


Figure 4: Horton WQI scores

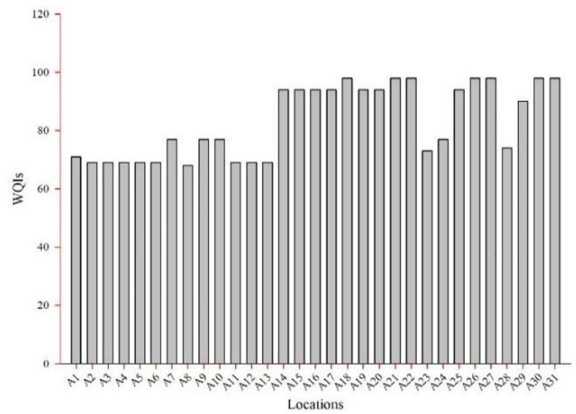


Figure 5: NSF WQI scores

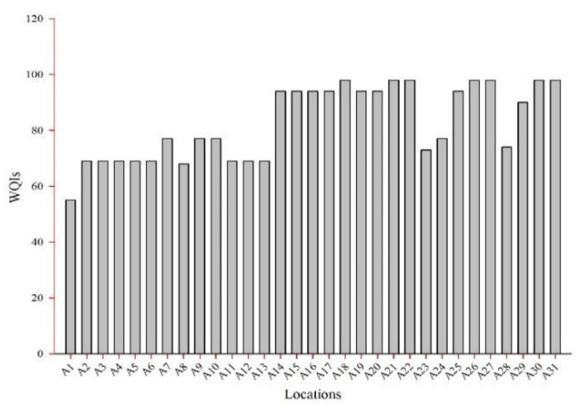


Figure 6: SRDD WQI scores

Approximately 41% of monitoring locations were ranked excellent quality by the West Java model for which indices ranged from 0-55 (Fig. 8). The other locations water quality was determined “good” to “fair”. Comparatively, the poorest water quality status was estimated by the Hanh model. Approximately, 16 locations water quality were ranked in the marginal category that ranges between 26 – 50 (Fig. 10).

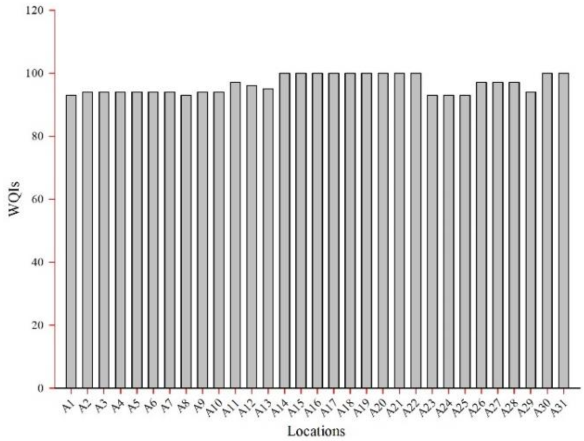


Figure 7: CCME WQI scores

Table 2. Analysis of the spatial uncertainty of measured WQI models.

WQI Models	Minimum	Maximum	Mean	SD	CoV
Horton	18	24	22.16	1.92	0.09
NSF	68	98	83.23	12.56	0.15
SRDD	55	98	82.71	13.38	0.16
CCME	93	100	96.45	2.92	0.03
WJ	54	100	82.68	15.81	0.19
Bascaron	74	99	90.71	7.45	0.08
Hanh	0	55	47.87	9.99	0.21

In general, looking across all the models, with the exception of the Horton model water quality status was poorer in stations A1-A13 relative to the rest of the harbour. These stations lie in the River Lee and are thus subject to agricultural run-off from the Lee catchment and combined sewer overflow discharges from Cork city which straddles the river.

1.5.2 Uncertainty analysis of WQI Indices

Uncertainty is a fundamental inherent feature in any hydrological model that is associated with different components of the model [1]. Its quantification is crucial for assessing the model reliability [8]. A number of studies have used SD to evaluate uncertainty of WQI models. [3] and [4] used the SD for estimating the model uncertainty of the sustainability index model and the West-Java WQI model, respectively. The smallest SD value indicates the final outputs does not propagate by the model input components [7]. However, the standard deviation must be assessed in relation to the mean value. The spatial uncertainty of the WQI models was therefore apprised using the coefficient of variation (CoV) calculated as the ratio of the standard deviation (SD) of the indices to the mean across all 31 stations. These values are given in Table 2 along with the maximum and minimum values recorded across all stations. The CoV was lowest for the CCME model (0.03) followed by the Bascaron and Horton models (0.08, 0.09) respectively. The spatial uncertainties of the other models were significantly higher with CoV values ranging from 0.15 to 0.21.

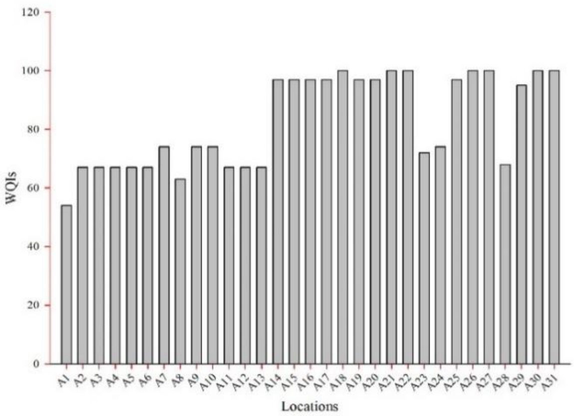


Figure 8: West Java WQI scores

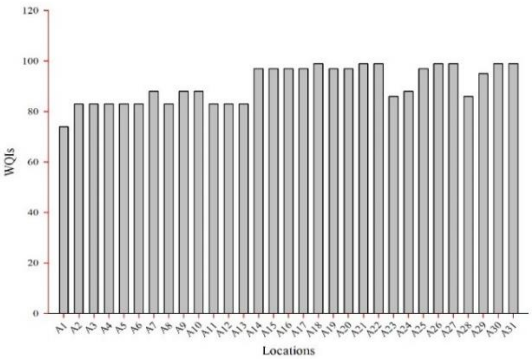


Figure 9: Bascaron WQI scores

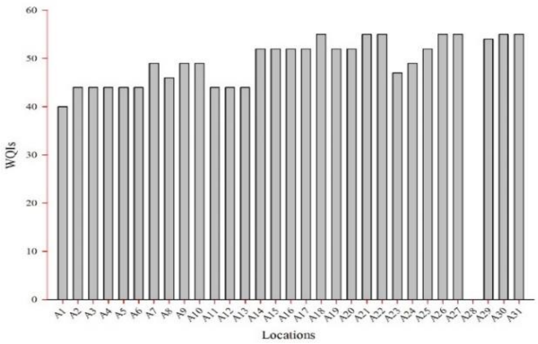


Figure 10: Hanh WQI scores

Table 1 Water quality ranking scales of different WQI model

WQI model	Ranking scales	WQ status
Horton	0 – 25	Excellent
	25 – 50	Good
	51 – 75	Fair
	101 – 150	Very poor
NSF	90 – 100	Excellent
	70 – 89	Good
	50 – 69	Medium
	25 – 49	Bad
	0 – 24	Very bad
SRDD	90 – 100	Excellent
	70 – 89	Good
	40 – 69	Tolerable
	30 – 39	Polluted
	0 – 29	Severely polluted
CCME	95 – 100	Excellent
	80 – 94	Good
	65 – 79	Fair
	45 – 64	Marginal
	0 – 44	Poor
West Java	90 – 100	Excellent
	75 – 89	Good
	50 – 74	Fair
	25 – 49	Marginal
	0 – 24	Poor
Bascarón	91 – 100	Good
	61 – 90	Acceptable
	31 – 60	Regular
	16 – 30	Bad
	0 – 15	Very bad
Hanh	91 – 100	Excellent
	76 – 90	Good
	51 – 75	Fair
	26 – 50	Marginal
	<25	Poor

1.5.2.1 Uncertainty analysis of WQI Input Data

Some of the spatial uncertainty of the indices calculated by the various model undoubtedly comes from the spatial variation of the input water quality parameters. Many researchers have determined input entities are one of the main sources of uncertainty in WQI models [1, 8]. The uncertainty of the model input parameters was also evaluated using CoV values of the measured time-averaged water quality data at each station. Water quality parameters statistics are presented in Table 2. The highest levels of spatial uncertainty were recorded for TON, NO_3^- and Chl-a where CoV was greater than 1. Significant levels of spatial uncertainty were also observed for salinity, NH_3^+ and PO_4^{3-} ; while the lowest CoV was calculated for DO, pH and water temperature, respectively (Table 3).

In the WQI models, weightings are attributed to the various water quality parameters when the parameter sub-indices are combined into the overall index using the aggregation functions in equations (1)-(7). The same parameter weight values were used in each model. One of the highest weight values is attributed to Chl a given that is a result of eutrophication and thus an indicator of heavily polluted waters. Since Chl-a also had the highest CoV of all the input parameters, it is likely that spatial variations in chlorophyll-a are one of the main sources of the spatial uncertainty in the computed water quality indices.

Table 3. Spatial uncertainty analysis of WQI models inputs.

WQ Parameters	Min	Max	Mean	SD	CoV
Salinity (g/Kg)	.25	34.68	19.45	13.69	0.70
Temp (0 C)	12.45	16.46	14.83	0.99	0.07
pH	7.66	8.21	8.01	0.17	0.02
DO (mg/l)	5.05	10.55	8.59	1.07	0.12
TON (mg/l)	.02	8.05	1.73	1.99	1.15
NH_3^+(mg/l)	.02	.32	0.08	0.07	0.88
NO_3^-(mg/l)	.02	8.05	1.73	1.99	1.15
PO_4^{3-} (μg/l)	9.90	68.50	25.75	13.03	0.51
Chl a (μg/l)	.65	76.90	6.13	13.27	2.16

1.6 Conclusion

Water Quality Index (WQI) models are a useful method to assess water quality. Worldwide it has become a popular tool due to its simplicity, ease-of-use and low computational cost. However, there have been relatively few applications of WQIs to estuarine waters. The present study was conducted firstly to determine the ease of application of a number of WQI index models to an estuarine system. Seven WQI models were successfully adapted for application to estuaries and indices were successfully calculated. Water quality was assessed mostly in the “fair” to “excellent” classes in Cork harbour but water quality in the River Lee was consistently assessed as poorer quality than the rest of the harbour. A second objective was to assess the level of spatial uncertainty in the computed indices across the 31 monitoring stations used in the study. The lowest uncertainty was found in the CCME, Bascaron and Horton models while the highest uncertainty was found in the Hanh model. Given that chl-a had the highest spatial variation of all of the input water quality parameters and one of the highest parameter weight values, it therefore contributes strongly to some of the observed model uncertainty.

1.7 Acknowledgements

This research was funded by the Department of Civil Engineering, NUI Galway. The authors would like to thank the Environmental Protection Agency for water quality data.

1.8 References

[1] Abbasi, T., Abbasi, S.A., 2012. Water Quality Indices, Statistical Accounting of Water Resources. Elsevier publications.

[2] Juwana, I., Muttil, N., Perera, B.J.C., 2016a. Application of west Java water sustainability index to three water catchments in west Java, Indonesia. Ecol. Indic. 70, 401–408. https://doi.org/10.1016/j.ecolind.2016.06.017

[3] Juwana, I., Muttil, N., Perera, B.J.C., 2016b. Uncertainty and sensitivity analysis of West Java Water Sustainability Index - A case study on Citarum catchment in Indonesia. Ecol. Indic. 61, 170–178. https://doi.org/10.1016/j.ecolind.2015.08.034

[4] Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2018. Development of a water quality index for rivers in West Java Province, Indonesia. Ecol. Indic. 85, 966–982. https://doi.org/10.1016/j.ecolind.2017.11.049

[5] Hartnett, M., Nash, S., 2015. An integrated measurement and modeling methodology for estuarine water quality management. Water Sci. Eng. 8, 9–19. https://doi.org/10.1016/j.wse.2014.10.001

[6] Uddin, M.G., Nash, S., Olbert, A.I., 2020b. A review study of water quality index models and their use for assessing surface water quality. Manuscript submitted for publication.

[7] Canadian Council of Ministers of the Environment, 2001. Canadian Sediment Quality Guidelines for the Protection of Aquatic Life: Summary tables. Can. Counc. Minist. Environ.

[8] Mishra, S., 2009. Uncertainty and sensitivity analysis techniques for hydrologic modeling. J. Hydroinformatics 11, 282–296. https://doi.org/10.2166/hydro.2009.048

Study 2. Assessment of Water Quality Using Water Quality Index (WQI) Models and Advanced Geostatistical technique

2.1 Abstract

Water quality index (WQI) models are popular tools to evaluate the quality of water; as such they have been developed and used by many agencies worldwide. However, the WQI model may generate excessive uncertainties in the aggregation process. This research is focused on the performance of various WQI modes. In this study, seven WQI models (Horton, CCME, NSF, West-Java, SRDD, Baccarin and Hanh) were applied in order to intercompare their performances and results generated by them. The Cork Harbour in the south of Ireland is used as a study case. Six years (2007 - 2012) of water quality monitoring data across the Harbour is used to conduct the analysis. Development of a WQI model involves four consecutive steps: (1) parameters selection, generation of (2) sub-indices, (3) weight values and (4) aggregation function; these were applied in the study. In total, nine crucial water quality parameters from 31 monitoring locations were selected in step (1) of the analysis. The EU Water Framework Directive (WFD) guidelines were applied to create the parameter sub-index rules (step 2). In step (3) the parameters weight values were generated by applying the Analytic Hierarchy Process (AHP). Finally, in step (4) the WQI model aggregation functions were applied to estimate the final WQI score for each of the seven models. Ultimately, the advanced geostatistical Empirical Bayesian Kriging (EBK) technique was used to spatially interpolate WQI calculated at the monitoring stations onto the whole domain of Cork Harbour. A comparison of the cross-validation parameters (ASE, MSE, RMSE, RMSSE and CRPS) was used to select the WQI model for the least uncertainty interpolation. The results show that the lowest uncertainty was generated by the EBK model for WQI generated by the CCME model, while the highest uncertainty obtained for the Hanh and West Java WQIs. Based on the EBK result, a ranked water quality map was proposed to be used for an assessment of surface water quality and its classification. The water quality ranked map proposed in this research can help not only to assess water quality but also to enhance understanding of water quality spatial variability in any waterbody. Based on the analysis of WQI models, it was concluded that the Cork Harbour water quality was of ‘good’ to ‘excellent’ status during the period of analysis 2007-2012.

Keywords: Modified WQI architecture; Empirical Bayesian Kriging (EBK) technique; model prediction uncertainty; Cork Harbour water quality; water quality ranked map

2.2. Introduction

Environmental concerns are central to sustainable water resource management and planning. Over many decades, freshwater consumption has been increasing worldwide due to population growth, industrialisation and urbanisation [1]. The surface water quality deteriorates in many basins due to pollution of anthropogenic sources [2, 3]. In this context, a water resources conservation and sustainable management are critically important for achieving at least good surface water quality status.

In recent years, a range of tools and techniques has been developed to evaluate surface water quality and diagnose the health of aquatic ecosystem. The water quality index (WQI) model is one of such tools. It assesses the status of water quality based on a characteristics of water quality parameters [4, 5, 6] by converting extensive water quality data into a single number. This number as the WQI model output can be associated with a simple description of water quality status using a simple terminology such as “excellent”, “good”, “medium”, “bad or acceptable”, “very bad or unfit” [6, 7] . This allows the non-expert communities to easily understood the status of the water quality without an expert knowledge of underlying conditions and processes [2].

Due to its simple structure and application process, the WQI models have gained popularity in recent years. As the number of models and their application increases, more sensitivity and uncertainty analyses have been conducted to reveal shortcomings of the WQI models. A significant contribution of the model uncertainty has been associated with the model aggregation function [4, 8]. The parameter sub-indexing and weighting process are known to generate uncertainty in the WQI models too [9].

The aim of this study is to assess surface water quality in Cork Harbour by apply various WQI models. The assessment is initially made for the monitoring stations and later extended to the whole domain of Cork Harbour using a sophisticated interpolation technique. Also in this study, a comparative analysis of the various WQI models is performed.

2.3 Materials and methods

2.3.1 Water quality data

Cork Harbour is designated as the Special Protection Area. Water quality in the harbour is assessed by the Environmental Protection Agency (EPA), Ireland through their monitoring programme which comprises of 31 sampling stations (Fig 1). In total, nine water quality parameters listed in Table 1 are routinely analysed as part of the programme. From this dataset, water quality data for the period 2007-2012 was used to calculate WQI for each year and each station.

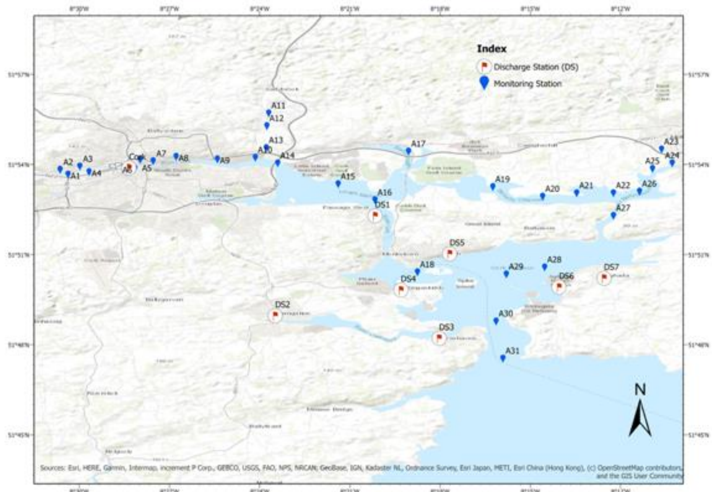


Fig 1. Map of EPA monitoring stations and effluent discharges in Cork Harbour (from EPA report 2016, pp. 135).

2.3.2 Analytical procedures

2.3.2.1 WQI models

For the purpose of this research, the existing WQI models have been extensively reviewed and their suitability to the current study preliminarily assessed. In total, seven WQI models were ultimately selected for in-depth analysis of their performance. They are (1) the National Sanitation Foundation (NSF WQI), (2) Canadian Council of Ministers of the Environment (CCME WQI), (3) Scottish Research Development Department (SRDD), (4) West Java (WJ WQI), (5) Horton Index, (6) Hanh Index, and (7) Bascaron Index.

2.3.2.2 WQI model architecture

Commonly, the WQI calculations comprise of four consecutive steps: (1) parameter selection, (2) parameter sub-index selection, (3) parameter weighting, and (4) application of the aggregation function [4, 6]. The WQI model architecture and parameters used are discussed in [2].

The following steps were applied to calculate WQI and to estimate uncertainty for each WQI model:

(a) Acquisition of water quality data for Cork Harbour
(b) Selection of water quality parameters based on the EU water quality monitoring guidelines, WQI model requirements and data availability
(c) Transformation of WQ parameter units and dimensions to a common dimensionless scale using sub-indexing process
(d) Determination of weight values for each WQ parameter using the Analytic Hierarchy Process
(e) Aggregation of sub-indices for each of the WQI model to obtain final WQI scores for each model and dataset.
(f) Implementation of the Empirical Bayesian Kriging (EBK) advanced geostatistical interpolation technique to produce spatial variability maps of WQI and WQ ranks in Cork Harbour, and finally
(g) Assessment of the EBK model uncertainties by utilizing the cross-validation statistical methods.

In this study, a range of WQI models is reviewed and best performance model is utilized to evaluate the surface water quality and its classification in Cork Harbour.

2.3.2.3 Parameter selection

The parameter selection is based on screening of the water quality parameters in respect of their environmental significance [5]. As such the process is subjective, site specific and lacks universality. Table 1 lists these parameters along with recommended and optional parameters for each WQI model.

Table 1: Developed WQI model parameters

WQ Parameters	WQI models						
	Horton	NSF	CCME	SRDD	WJ	Hanh	Bascaron
Temperature	×[b]	✓[a]	✓	✓[a]	✓[a]	×[b]	✓[a]
Salinity	×[b]	×[b]	✓	×[b]	×[b]	×[b]	×[b]
pH	✓[a]	✓[a]	✓	✓[a]	×[b]	×[b]	✓[a]
DO	✓[a]	✓[a]	✓	✓[a]	✓[a]	✓[a]	✓[a]
T. Ammonia	×[b]	×[b]	✓	✓[a]	✓[a]	✓[a]	✓[a]
T. Phosphate	×[b]	✓[a]	✓	✓[a]	×[b]	✓[a]	✓[a]
Nitrates	×[b]	✓[a]	✓	×[b]	×[b]	×[b]	✓[a]
TON	×[b]	×[b]	✓	✓[a]	✓[a]	×[b]	×[b]
Chl a	×[b]	×[b]	✓	×[b]	×[b]	×[b]	×[b]

✓[a] WQI Model recommended; ✓ optional parameters; ×[b] used in this study;

2.3.2.4 Parameter sub-indexing

The parameters sub-indexes are established to transform dimensions and units of each parameter to a common scale [5]. Typically, the conversion rates are adopted from legislated water quality standards guidelines for the water quality classification operated in a given country [e.g. 5, 10, 11]. Similarly here, the sub-index rules were developed based on the EPA guidelines for surface water quality assessment [12] with is an implementation of the European Communities regulations for 'Quality of surface water intended for the abstraction of drinking water (1989)'[20], 'Quality of Shellfish waters (2006)' and OECD classification scheme for lake waters (1982). Depending on their values, each parameter is assigned to one of the three categories A1 – A3. Table 2 describes classification criteria for each water quality category.

The conversion of a parameter value to sub-index is based on a reference value for a parameter and rules for each category. Sub-index score normalizes a parameter value into 0-100 range with the value of 100 assigned to A1 class and value of 0 to A3 class. The exception for this rule is West-Java WQI model where for the for computational reasons the lowest sub-index value assigned to 5.

Table 2. Classification of the surface water quality and required actions proposed by the European Communities regulations.

Category	Definitions and required actions
A1	Need to modest physical treatment and disinfection, e.g. rapid filtration and disinfection.
A2	Typical physical treatment, chemical treatment and disinfection, e.g. prechlorination, coagulation, flocculation, decantation, filtration, disinfection (final chlorination).
A3	Required to intensive physical and chemical treatment, extended treatment and disinfection, e.g. chlorination to break-point, coagulation, flocculation, decantation, filtration, adsorption (activated carbon), disinfection (ozone, final chlorination).

2.3.2.5 Parameters weighting process

The third step in the determination of WQI involves an assignment of weight values to each parameter to produce a hierarchy of all parameters with respect to their environmental significance and impact on water quality. The Analytic Hierarchy Process (AHP) proposed by [18] was adopted to develop a rank of parameters (or their weight values) based on a multi-criteria analysis of their importance respectively to other parameters. A ranged of water quality guidelines issued by EPA Ireland, EPA USA, the UK as well as the personal experience of the research team and environmental conditions in Cork Harbour were used to establish importance of each parameter on water quality. The AHP ranking scale ranges from 1 – equal importance to 9 – extreme importance, and their assigned values for parameters selected in step 1 are shown in Table 4. The normalized AHP values were used to develop paired comparison of criteria in a pair-wise all-parameter matrix [9x9] to ultimately generate weight values for each parameter (Table 4). Such methodology was previously successfully applied for a range of water quality studies [5].

The second step of the weighting process is to calculate consistency ratio (CR) to evaluate consistency of the set of judgments made in relation to AHP ranking and weights. A true Consistency Ratio (CR) is calculated by dividing the Consistency Index (CI) for the set of judgments by the Random Index (RI) for the corresponding random matrix as follows

$$\text{Consistency Ratio (CR)} = \frac{\text{Consistency Index (CI)}}{\text{Random Index (RI)}} \qquad (1)$$

The RI value is set to 1.45 for 9 as recommended in [24] while the CI value was calculated using the following equation

$$\text{CI} = \frac{\lambda_{max} - n}{\text{n}-1} \qquad (2)$$

where λ_{max} is the largest eigenvalue of the matrix and n represents the total associate of the matrix [13]. If the CR exceeds 0.1 the set of judgments may be too inconsistent to be reliable and as such the set of judgments needs to be revised [14]. The CR was found to be close to 0 and as such the consistency of subjective judgment in relation to the derived AHP ranking is satisfied.

2.3.2.6 The aggregation process

Final step in calculation of WQI scores employs aggregation functions of each WQI model. The different WQI model aggregation functions are defined in equations (1)-(7).

$$\text{Horton index} = \sum_{i=1}^{n} w_i s_i \qquad (1)$$

where s_i and w_i are the sub-index and weight values of water quality parameter i, *n* is the number of parameters.

$$NSF\ index = \sum_{i=1}^{n} w_i s_i \qquad (2)$$

$$SRDD\ index = \frac{1}{100}\left(\sum_{i=1}^{n} S_i W_i\right)^2 \qquad (3)$$

$$CCME = \frac{\sqrt{{F_1}^2 + {F_2}^2 + {F_3}^2}}{1.732} \quad (4)$$

where F_1 is the percentage of failed parameters that do not meet with regarding their guideline value; F_2 is the percentage of individual test cases these do not meet with the guideline value and F_3 is the variation percentage of the failed test parameters that do not meet their objectives; and 1.732 is a divisor that is applied for normalization [15].

$$West\ Java\ Index = \prod_{i=1}^{n} {S_i}^{w_i} \quad (5)$$

$$Bascaron\ Index = \frac{\sum C_i P_i}{\sum P_i} \quad (6)$$

$$Hanh\ Index = \left[\frac{1}{6}\sum_{i=1}^{6} q_i \times \frac{1}{2}\sum_{i=1}^{2} q_j \ \times q_k\right]^{1/3} \quad (7)$$

where q_i is the sub-index value of the organic and nutrients group including pH, DO, NH_4^+ NO_3^-, PO_4^{3-}, TON; q_j is the sub-index value of the particulates group, including temperature and salinity; and q_k is the sub-index value of the biological group containing only *Chlorophyll-a*.

2.4 Empirical Bayesian kriging (EBK) technique

In this study, the water quality indices are produced for geographical locations in Cork Harbour where WQ data are available. In order to better understand horizontal distributions of water quality within the Harbour, WQI were spatially interpolated. *From a arrange of interpolation techniques, the* Empirical Bayesian Kriging (EBK) was selected to predict WQI at points not included in the monitoring programme. EBK is a geostatistical interpolation method that automatically calculates the kriging model parameters through a process of sub-setting and simulations. Also, the model, when calculates the samivariogram, takes into account the uncertainty of semivariogram estimation and by that reduce underestimation of standard errors of predictions [21]. These are the significant advantages of the method over the other kriging models [16]. The empirical semivariogram was calculated using the following equation

$$\gamma\ (h \pm \delta) = \frac{1}{2|N(h \pm \delta|} \sum_{(i,j)\in N(h\pm\delta)} \left|z_i - \ z_j\right|^2 \quad (8)$$

where h is the distance between sampling points, δ is the tolerance range between points, N(h $\pm$ δ) is a set of points N(h $\pm$ δ) $\equiv \{(S_{i,}\ S_j): |S_i S_j| = h \pm \delta; i, j = 1,2, \ldots, N\}$. $|z_i - z_j|^2$ are the squared variances between observations. The squared variances are added and normalized by the natural number N(h $\pm$ δ). The empirical transformation function was employed to predict the probability distribution of the aggregation value of WQI model.

Table 3. Water quality parameters, standard values, classes, sub-index rules and their S_i values.

Selected parameters	Units	[a]References values	[b]Water categories	Rules	Sub-index values (S_i)
pH			A1	5.5 – 8.5	100
		6.5 – 9.0	A2 -A3	> 8.5	0 or 5[e]
Temperature	(^{0}C)	25	A1 – A2	= <25	100
			A3	>25	0 or 5[e]
DO	(mg/L)		A1	equal or >6	100
		> 6	A2	> 5	75 <Si ≤ 50
			A3	>3	50 < Si ≤ 25 or 5[e]
NO3	(mg/L)	50	A1 -A2	equal or <50	100
			A3	>50	0 or 5[e]
[c]Salinity	(g/Kg)		A1	equal or <35	100
			A2	> 10	75 < Si ≤ 50
		35	A3	< 10	50 < Si ≤ 25
			A4	0 or >35	0 or 5[e]
[d]Chlorophyll a	(μg/L)		A1	equal or <8	100
		8	A2 -A3	> 8	0 or 5[e]
NH3	mg/L as N)		A1	equal or < 0.2	100
		0.2	A2	equal or < 1.5	50
			A3	equal or > 4	0 or 5[e]
TON	(mg/L)	1	A1	equal or <1	100
			A2	equal or >2	75 < Si ≤ 50
			A3	equal or >3	0 or 5[e]
PO4	(μg/L as P)	500	A1	equal or <500	100
			A2 -A3	equal or > 700	0 or 5[e]

[a]EPA, Ireland (2001), recommended values for the surface water/freshwater/river water/aquatic life.
[b] water categories were defined as per guidelines of the European Communities (Quality of surface water intended for the abstraction of drinking water) regulations, 1989 (S.I. No. 294/1989).
[c] the European communities (Quality of Shellfish waters) regulations, 2006 (S.I. No. 268/2006).
[d]the Organisation for Economic Cooperation and Development (OECD) classification scheme for lake waters, 1982, adopted by (with modifications) EPA, Ireland.
[e]this scale only applied for West Java WQI model when criteria do not meet to the objective values.

2.4.1 EBK validation process

The cross-validation of the interpolated data was used to assess the accuracy and uncertainty of the EBK interpolation model [17]. The EBK model uncertainty was estimated using the prediction standard errors parameters. When the average standard error (ASE) is close in value to the root mean squared error (RMSE), then the EBK output exhibits the lowest uncertainty for a given WQI model. ASE values smaller than RMSE indicate an underestimation of variability in interpolated data. Also, the root mean squared standardised errors (RMSSE) close to one suggests that the model prediction standard errors are valid. The RMSSE value larger (smaller) than 1 indicates underestimation (overestimation) of variability in model predictions.

$$ASE = \frac{1}{n}\sum_{i=1}^{n}(p_i - \left(\sum_{i=1}^{n} p_i\right)/n)^2 \qquad (4)$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(p_i - m_i) \qquad (5)$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(p_i - m_i)^2} \qquad (6)$$

$$RMSSE = \sqrt{\frac{1}{n}[\sum_{i=1}^{n}(ps_i - ms_i)\Big/\sigma s_i]^2} \qquad (7)$$

where n is the number of measured sampling locations; p is the predicted value at i^{th} sampling locations (I = 1, 2,.. …n); m is the calculated value; ps is the standardized predicted value; ms is the standardized measured value and σs standardized deviation.

The average Continuous Ranked Probability Score (CRPS) is used to estimate uncertainty of EBK predictions [5]. CRPS measures the deviation of cumulative distribution function [9].

$$CRPS = \frac{1}{n-1}\sum_{j=1}^{n}\left(\sum_{j=1}^{n}p_j - \sum_{j=1}^{n}m_j\right)^2 \qquad (8)$$

where n is the number of outputs, p_j is the predicted probability of output j^{th} location, and m_j is the measured probability of output j^{th} location. Usually, the CRPS score lies between 0 to 1. The smaller CRPS score is the better the fit of EBK model to data.

2.5 Results

In this study the accuracy and usability of existing water quality index models were evaluated. In total 7 WQI models were used to generate WQIs. Cork Harbour, a hydrologically compound estuary characterised by complex ecosystem dynamics and dependencies was used as a case study. The water quality dataset consists of 9 parameters collated annually at 31 locations within the study domain during the period 2007-2012. This dataset was used to produce WQI maps and ultimately to selected best-performance WQI model.

2.5.1 Generation of WQI

For each of the 7 WQI models, the generation of WQIs consist of four consecutive steps: (1) parameters selection, generation of (2) sub-indices, (3) weight values and (4) aggregation function. Steps (1) – (3) are identical for each model. Outputs of these steps are discussed below.With regards to the parameter selection, nine parameters were selected to determine WQI. The selection was based on recommendations given by each model developer, data availability, parameter cross-correlation and EPA recommendations. The list of parameters is shown in Table 1.

The generation of sub-indices in step (2) allows to convert dimensions and units of each parameters to a universal scale so the parameters can be intercompared. The process is described in section 2.3.4; sub-index values were determined for each parameter based on rules and criteria summarised in Table 3. In step (3) parameter weights are generated to rank an importance and contribution of induvial parameters to the overall water quality score. The rank of parameters on AHP scale of 1 to 9 is shown in Table 4. The numbers were assigned with respect to impact of a parameter on water quality and hence environmental conditions and ecosystem. From the assigned AHP ranks, the weights were calculated and are presented in Table 4. As the process of assignments of AHP sores is based on a set of subjective judgments in relation to a significance of the parameter, consistency of the set of judgments was evaluated using the Consistency Ratio, which was found to be close to 0 (< 0.1). This confirms that the judgments made are consistent throughout the dataset and there are no conflicts between assigned values. Consequently, the derived weights are consistently assigned and can be used in step (4).

Table 4: Estimated parameters weight values.

WQ Parameters	Weight values
DO	0.16
Temperature	0.16
Chl a	0.13
pH	0.13
Salinity	0.09
TP	0.09
Nitrate	0.09
TON	0.09
TA	0.05
Sum	1

Finally, in step (4) WQI are calculated for given sub-index and weight values using the aggregation function defined in section 2.3.2.6. Each model applies different aggregation function so the differences in WQI values obtained for various WQI models are directly related to the aggregation method used. Table 5 shows WQI values

(AMV) averaged spatially over 31 datasets (locations in Figure 1). All models (except Horton) operate on 0-100 scale; the higher the number is the better water quality. The Horton WQI model with value of 0 describes excellent water quality status while WQI >100 represents very poor conditions[19]. The WQIs are ultimately used to categorize water quality into classes. From the analysis of WQI it is apparent that for a given dataset the water quality is good to excellent depending on the applied model. Such discrepancies may lead to erroneous interpretations of the water quality status and result in inappropriate management decisions and actions.

Table 5: WQI values generated by WQI models (AMV) and interpolated using EBK model (APV) with average statistical error (ASE).

WQI Models	2007			2008			2009			2010			2011			2012		
	AMV	APV	ASE	AMV	APV	ASE	AMV	APV	ASE	AMV	APV	ASE	AMV	APV	ASE	AMV	APV	ASE
Horton	88.68	88.77	3.74	86.81	86.61	4.49	86.58	86.10	5.89	83.55	83.52	4.66	88.90	88.88	5.11	84.71	84.49	14.41
Bascaron	90.71	90.79	4.66	86.43	86.39	4.60	86.67	86.50	6.11	93.65	93.71	3.72	89.06	89.18	4.54	87.93	88.01	6.41
CCME	96.45	96.23	1.70	95.03	94.91	1.36	93.47	93.54	0.50	96.45	96.41	1.69	96.16	95.95	1.65	96.32	96.20	1.91
WJ	82.68	82.51	8.97	72.07	71.78	10.86	70.80	70.61	11.19	86.39	86.93	8.96	78.55	78.65	10.29	77.10	77.59	11.52
NSF	83.23	82.85	7.61	74.83	74.20	8.20	76.23	76.23	9.67	88.35	88.33	5.89	80.26	80.48	7.76	78.17	78.58	11.13
Hanh	47.87	47.70	6.70	32.73	34.28	14.91	47.33	47.93	5.23	51.45	51.78	4.57	47.87	47.76	6.49	49.17	49.17	2.37
SRDD	82.71	82.73	7.47	74.30	73.72	8.84	75.57	75.48	10.61	87.97	88.47	6.70	79.61	79.84	8.41	77.57	77.86	11.17

*AMV = Average measured values; APV = average predicted values; ASE = Average standard error

2.5.2 Model performance and uncertainty analysis

WQIs calculated for 31 monitoring stations were interpolated over the domain of Cork Harbour. From a range of interpolation techniques, the EBK was selected to perform the interpolation of WQI scores.

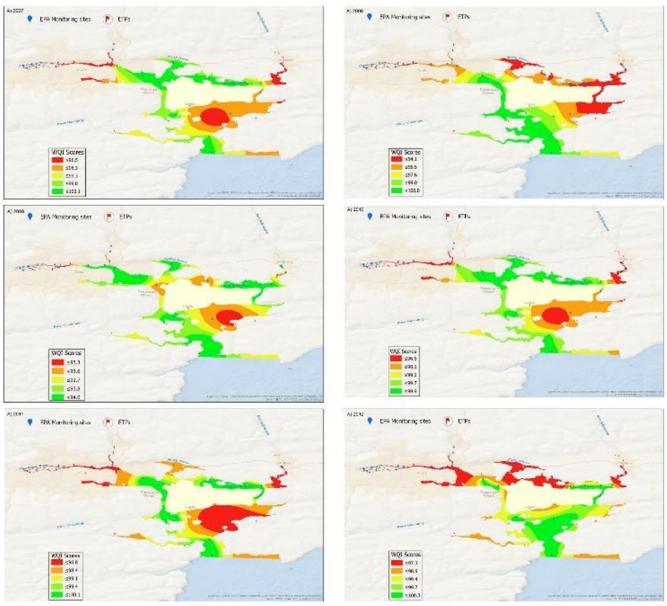


Figure 2. Maps of CCME WQIs spatially interpolated using EBK technique.

The cross-validation process was utilized to estimate the propagation of uncertainties in EBK predicted values. This analysis was conducted to establish for which of WQI models the EBK performs best. In general, the smallest RMSE and MAE values indicate the best performance of the EBK with the lowest propagation of uncertainties [3]. The CRPS scores were used to estimate the interpolation uncertainty [22].

Table 6: Statistical analysis of the EBK model performance.

Temporal variation	EBK model validation parameters	Applied WQI model						
		Horton	WJ	SRDD	NSF	Hanh	CCME	Bascaron
2007	ACRPS	2.065	4.48	3.728	3.649	3.209	**0.851**	2.123
	RMSE	3.991	8.84	7.072	6.827	10.22	**1.611**	4.04
	MSE	0.030	-0.021	-0.013	-0.028	0.243	**-0.056**	-0.012
	RMSSE	1.021	0.988	0.93	0.921	2.705	**0.903**	0.861
	ASE	3.908	9.154	7.673	8.089	7.466	**1.865**	4.837
2008	ACRPS	2.547	6.008	4.762	4.225	7.828	**0.677**	2.367
	RMSE	4.984	10.807	8.821	8.255	16.788	**1.421**	4.664
	MSE	0.001	-0.012	-0.029	-0.038	0.066	**-0.011**	-0.022
	RMSSE	1.117	0.994	0.99	0.954	1.181	**0.852**	0.866
	ASE	4.640	10.93	9.039	8.594	16.901	**1.604**	4.845
2009	ACRPS	2.822	5.68	5.264	4.847	3.157	**0.309**	3.053
	RMSE	4.942	10.382	9.419	8.851	10.187	**0.567**	5.438
	MSE	-0.064	-0.008	-0.002	0.002	0.228	**0.19**	-0.024
	RMSSE	0.952	0.89	0.89	0.893	2.381	**1.211**	0.918
	ASE	6.064	11.428	10.786	9.872	5.611	**0.502**	6.215
2010	ACRPS	2.467	4.598	3.61	2.878	2.653	**0.831**	1.902
	RMSE	4.439	9.06	7.012	5.884	10	**1.658**	3.716
	MSE	-0.005	0.047	0.053	-0.02	0.232	**0.015**	0.007
	RMSSE	0.974	1.078	1.09	0.937	2.665	**0.961**	0.984
	ASE	4.691	9.105	6.805	5.985	5.043	**1.714**	3.794
2011	ACRPS	2.702	5.429	4.569	4.173	3.127	**0.766**	2.422
	RMSE	4.750	10.187	8.367	7.862	10.325	**1.441**	4.471
	MSE	-0.005	0.031	0.044	0.053	0.271	**-0.046**	0.052
	RMSSE	0.961	1.106	1.098	1.153	2.912	**0.839**	1.122
	ASE	5.163	10.377	8.506	7.873	7.261	**1.738**	4.614
2012	ACRPS	7.350	6.567	6.172	6.225	1.186	**0.925**	3.664
	RMSE	19.534	12.5	12.087	12.157	2.357	**1.755**	7.381
	MSE	0.161	0.01	-0.004	0.002	0.007	**-0.03**	0.01
	RMSSE	2.121	1.013	0.962	0.971	1.102	**0.856**	1.046
	ASE	15.232	11.95	11.725	11.663	2.436	**2.072**	6.816

Table 6 summarizes statistics of EBK predictions for various WQI models. The lowest cross-validation parameter values were obtained by the CCME model for each year in the range 2007 – 2012. In contrast, the West-Java and Hanh models were generating the highest RMSE values, and as such the EBK for these model data exhibits worst performance. The EBK model uncertainty was estimated using the average continuous ranked probability score (CRPS) of predicted values. The lowest uncertainty was associated with the CCME WQI model while the highest with the NSF, SRDD and West Java models. Based on the uncertainty analysis, the EBK model was found to exhibit the best performance in conjunction with the CCME model outputs. Consequently, CCME is further used here to produce maps of water quality indices and ranks in Cork Harbour. Figure 2 presents distribution of WQI calculated using the CCME model and interpolated using EBK. In general, higher WQI scores (better water quality) are found at the Harbour mouth and along the western coastline while river inflows are characterized by low WQIs (worst water quality). This is a temporarily consistent spatial pattern. The water quality in Lower Cork Harbour varies substantially on the horizontal and temporal scale with generally high variability along eastern coastline

2.5.3 Ranking of the water quality

The CCME WQI model was employed to establish water quality status in Cork Harbour. Three ranks A1, A2 and A3 as described in the EC surface water quality guideline (1998) are adopted in this study. The WQI ranges corresponding to each class are shown in Table 7.

Table 7: WQI scores and corresponding water quality classes.

Best interpolated WQI	Categorization schemes	Water Classes*	Description
CCME model	95 - 100	A1	Excellent
	80 - 95 65 - 79	A2	Good
	45 - 64 0 - 44	A3	poor

**Based on EC guidelines for the surface water*

A ranked water quality map allows to determine spatial distribution of water quality, assess water quality status and enhance understanding of water quality spatial variability. Figure 3 shows that within the study period, the water quality varies from good to excellent and this confirms assessments conducted by the EPA, Ireland. There is no consistency in spatial or temporal variations, and this implies that Cork Harbour is a highly hydrologically dynamic system with many sources of instantaneous pollution.

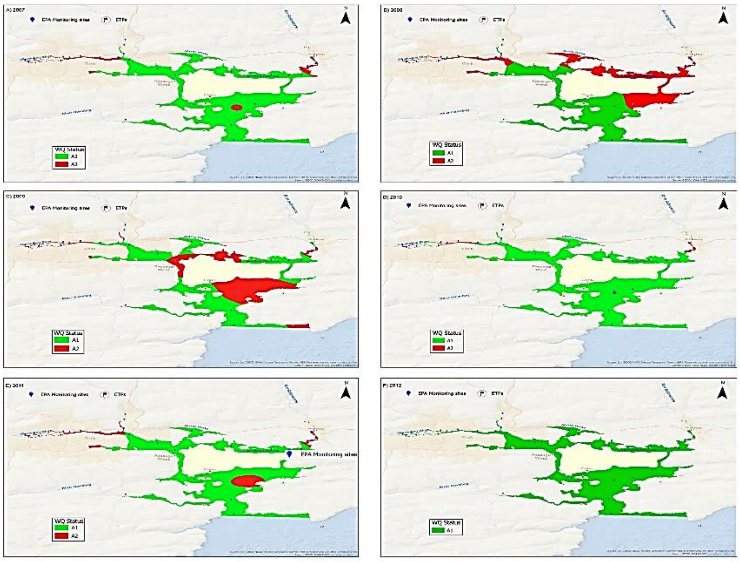


Figure 3. Maps of WQ ranks based on CCME WQIs.

2.6 Conclusion

The aim of this study was to apply various WQI models to assess surface water quality in Cork Harbour. To Authors knowledge the application of WQI to assess water quality is the first of this kind of studies in Ireland. Each model has been substantially modified in terms of parameter selection and aggregation method for the most accurate assessment of water quality.

The results show that water quality is good to excellent depending on the WQI model used. This implies that the right selection of WQI is paramount to a correct determination of water quality status. Also, a choice of the interpolation technique plays a fundamental role in understanding of spatial variations in water quality. The EBK interpolation model produces the least uncertainty levels when combined with the CCME model. The EBK interpolated WQIs were ultimately used to produce ranked water quality maps. Such maps are excellent tools to understand dynamics of water quality, optimize network of field observations, and to communicate status of the water quality and associated issues to non-expert stakeholders. Based on the analysis of WQI models, it was concluded that the Cork Harbour water quality was of ‘good’ to ‘excellent’ status during the period of analysis 2007-2012.

2.7 Acknowledgements

This research was funded by the Hardiman Scholarship Programme, NUI Galway. The authors would like to thank the Environmental Protection Agency for water quality data.

2.8 References

[1] Javed, S., Ali, A., Ullah, S., 2017. Spatial assessment of water quality parameters in Jhelum city (Pakistan). Environ. Monit. Assess. 189. https://doi.org/10.1007/s10661-017-5822-9
[2] Uddin, M.G., Nash, S., Olbert, A.I., 2020b. A review study of water quality index models and their use for assessing surface water quality. Manuscript submitted for publication.
[3] Uddin, M.G., Moniruzzaman, M., Quader, M.A., Hasan, M.A., 2018. Spatial variability in the distribution of trace metals in groundwater around the Rooppur nuclear power plant in Ishwardi, Bangladesh. Groundw. Sustain. Dev. 7. https://doi.org/10.1016/j.gsd.2018.06.002
[4] Abbasi, T., Abbasi, S.A., 2012. Water Quality Indices, Statistical Accounting of Water Resources. Elsevier publications.
[5] Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2017. Development of a water quality index for rivers in West Java Province, Indonesia. Ecol. Indic. 85, 966–982. https://doi.org/https://doi.org/10.1016/j.ecolind.2017.11.049
[6] Uddin, M.G., Moniruzzaman, M., Khan, M., 2017. Evaluation of Groundwater Quality Using CCME Water Quality Index in the Rooppur Nuclear Power Plant Area, Ishwardi, Pabna, Bangladesh. Am. J. Environ. Prot. https://doi.org/10.12691/env-5-2-2
[7] Zotou, I., Tsihrintzis, V.A., Gikas, G.D., 2018. Comparative Assessment of Various Water Quality Indices (WQIs) in Polyphytos Reservoir-Aliakmon River, Greece. Proceedings 2, 611. https://doi.org/10.3390/proceedings2110611
[8] Smith, D.G., 1990. A better water quality indexing system for rivers and streams. Water Res. 24, 1237–1244. https://doi.org/10.1016/0043-1354(90)90047-A

[9] Juwana, I., Muttil, N., Perera, B.J.C., 2016. Application of west Java water sustainability index to three water catchments in west Java, Indonesia. Ecol. Indic. 70, 401–408. https://doi.org/10.1016/j.ecolind.2016.06.017
[10] House, M.A., 1989. A Water Quality Index for River Management. Water Environ. J. 3, 336–344. https://doi.org/10.1111/j.1747-6593.1989.tb01538.x
[11] Pham, T.M.H., Sthiannopkao, S., Ba, D.T., Kim, K.W., 2011. Development of Water Quality Indexes to Identify Pollutants in Vietnam's Surface Water. J. Environ. Eng. 137, 273–283. https://doi.org/10.1061/(ASCE)EE.1943-7870.0000314.
[12] EPA, 2001. Parameters Of Water Quality: Interpretation and Standards, Environmental Protection Agency, Ireland. The Environmental Protection Agency, Ireland., Ireland. https://doi.org/10.1017/CBO9781107415324.004
[13] Jozaghi, A., Alizadeh, B., Hatami, M., Flood, I., Khorrami, M., Khodaei, N., Tousi, E.G., 2018. A comparative study of the AHP and TOPSIS techniques for dam site selection using GIS: A case study of Sistan and Baluchestan Province, Iran. Geosci. https://doi.org/10.3390/geosciences8120494
[14] Chandio, I.A., Matori, A.N.B., WanYusof, K.B., Talpur, M.A.H.,Balogun, A.L., Lawal, D.U., 2013. GIS-based analytic hierarchy processas a multicriteria decision analysis instrument: A review. Arab. J. Geosci. https://doi.org/10.1007/s12517-012-0568-8
[15] Dojlido, J.A.N., Raniszewski, J., Woyciechowska, J., 1994. Water Quality Index Applied to Rivers in the Vistula River Basin in Poland. Environ. Monit. Assess. 33, 33–42.
[16] Krivoruchko, K, 2012. Empirical Bayesian Kriging. ESRI Press.
[17] Carlin, B.P., Louis, T.A., 2009. Bayesian Methods for Analysis.
[18] Saaty, R.W., 1987. The analytic hierarchy process-what it is and how it is used. Math. Model. https://doi.org/10.1016/0270-0255(87)90473-8
[19] Horton, R.K., 1965. An Index Number System for Rating Water Quality. J. Water Pollut. Control Fed.
[20] European Union, 2009. S.I. No. 272/2009 - European Communities Environmental Objectives (Surface Waters) Regulations 2009. Electron. Irish Statut. B. 2009, 38–40.
[21] Gupta, A., Kamble, T., Machiwal, D., 2017. Comparison of ordinary and Bayesian kriging techniques in depicting rainfall variability in arid and semi-arid regions of north-west India. Environ. Earth Sci. https://doi.org/10.1007/s12665-017-6814-3
[22] Chilès, J.P., Delfiner, P., 2012. Geostatistics: Modeling Spatial Uncertainty: Second Edition, Geostatistics: Modeling Spatial Uncertainty: Second Edition. https://doi.org/10.1002/9781118136188

Study 3. Optimization of Parameters in a Water Quality Index Model using Principal Component Analysis

This study was published in the Proceedings of the 39th IAHR World Congress (Granada, 2022), on June 10, 2022. Details can be found at the following web resource:

https://doi.org/10.3850/IAHR-39WC2521711920221326

3.1 Abstract

The Water Quality Index (WQI) model is a simple method for evaluating water quality and determining pollution levels. This approach is becoming increasingly popular as a result of its simple architecture when compared to other hydrological models. The development and implementation processes of WQI are also simple. Parameter selection is a critical step towards the development of any hydrological model, including the WQI model. According to many researchers, model parameterization is one of the key sources of uncertainty in the WQI models. Across literature, a range of techniques are used to select essential water quality features - expert opinion and literature review are the most common tools. This study aims to establish a technique for selecting important water quality parameters. The principal component analysis (PCA) was applied to filter the relevant water quality parameters. A dataset from water quality monitoring in Cork Harbour was used to test a suitability of PCA. The PCA1 component explained 41.5 percent of the total variance with strong positive loading on dissolved inorganic nitrogen (DIN), total organic nitrogen (TON), Molybdate Reactive Phosphorus (MRP), and strong negative loading on pH, dissolved oxygen (DO), and water transparency. Water biological oxygen demand (BOD), chlorophyll, and total organic nitrogen (TOC) all contributed to 25.8% of the data variance. In total, the PCA technique recommended nine significant water quality parameters from the list of eleven in terms of their relative importance.

Keywords: Water Quality Index Model; Parameter Selection Process; Principal Component Analysis; Coastal Water Quality; Cork Harbour

3.2 Introduction

The water quality index model is an effective tool for assessing water quality while avoiding the complex mathematical functions of traditional models. It allows converting vast amounts of water quality data into a single unit with fewer values.

Recently, this model has been widely used in various fields due to its simplicity. In the meantime, several countries/agencies/environmental organizations developed various WQI models for various purposes, such as ground water (irrigation, health risk assessment) and surface water (lake, pond, and river water assessment). Commonly, a WQI index model is composed of four components, namely (i) parameters selection, (ii) sub-indexing process, (iii) weighting technique, and (iv) aggregation method (Uddin et al., 2021). Several studies reported considerable WQI model uncertainty and attributed this to the parameter selection as the main cause. This results in the WQI model not reflecting accurate information about water quality. Among the tools and techniques currently used for selecting water quality parameters in the WQI model are expert opinions, analytical hierarchical processes, and literature study techniques. A few studies have been conducted using the PCA technique for selecting important water quality parameters (Tripathi and Singal, 2019).

In this light, this research aims to establish a reliable technique for selecting important water quality parameters. Here the PCA technique for selecting the critical attributes of coastal water quality is used and the reliability of this technique in terms of extracting the relative importance of parameters is assessed.

3.3 Materials and methods

3.3.1 Data obtaining process

The Environmental Protection Agency (EPA), Ireland monitors all water bodies as part of their water quality management. In this research, the water quality data were collected from Cork Harbour, Ireland. In total, 29 monitoring sites in Cork Harbour were considered in this study, with ten water quality parameters. Table 1 provides the details of water quality parameters list and their measurement unit. The datasets of water quality are grouped into two categories: summer and winter. The present study used the 2019 monitored water quality data encompassing the following parameters: Water temperature (TEMP), pH, Dissolved oxygen (DOX), Total organic nitrogen (TON), Ammoniacal nitrogen (AMN), Molybdate Reactive Phosphorus (MRP), Biological Oxygen Demand (BOD5), Transparency (TRAN), Chlorophyll a (CHL) (as a measure of algae), and Dissolved inorganic nitrogen (DIN). Figure 1 shows the summary statistics between summer and winter for water quality data in Cork Harbour. All water quality data were obtained from the one-meter depth of the surface at each monitoring site. The EPA generally takes measurements at each location at approximately high and low tide on the same day in the winter and summer seasons, although the months of collection vary from year to year.

Table 1. Guide values of water quality parameters for surface water quality.

Parameter	unit	Std. threshold values
CHL	mg/m^3	8 - 25*(i)*
DOX	% sat	70 – 120*(ii)*
MRP	mg/l as P	0.015 – 0.030*(vi)*
DIN	mg/l	2.6*(v)*
AMN	mg/l	0.2 – 1.5*(iii)*
BOD5	mg/l	5 – 7*(iii)*
pH		5.5 – 8.5*(iii)*
Temp	^0C	25*(iii)*
TON	mg/l as N	1 - 2*(iii)*
Tran.	m/depth	> 1*(ii)*

[a]EPA, Ireland (2001), recommended values for the surface water/freshwater/river water/aquatic life.
(i) the Organisation for Economic Cooperation and Development (OECD) classification scheme for lake waters, 1982, adopted by (with modifications) EPA, Ireland.
(ii) bathing Water Quality Regulations 2008, (S.I. No. 79/2008).
(iii) the European Communities (Quality of surface water intended for the abstraction of drinking water) regulations, 1989 (S.I. No. 294/1989).
(iv) the European communities (Quality of Shellfish waters) regulations, 2006 (S.I. No. 268/2006).
(v) the Assessment of Trophic Status of Estuaries and Bays in Ireland (ATSEBI) System, 2001
(vi) EPA, Ireland (2001), recommended values for the surface water/freshwater/river water/aquatic life.

3.3.2 Data standardized and suitability check

For the purpose of this study, the statistical analysis was performed on the standardized water quality data sets. In order to meet the data standards, the z-scale transformation was used to avoid misclassification, as the water quality data was measured using the different orders of magnitude:

$$z = \frac{(x - \bar{x})}{\sigma} \qquad [1]$$

where, x is the target water quality variables, $\bar{x}$ is the mean of the intended variables and σ is the standard deviation of variables.

3.3.3 Correlation studies

3.3.4 Principal component analysis processes

The PCA is a vector transformation technique that allows the observe variables transform into a new uncorrelated variables vector position with loading linear combinations of the original data (Shrestha and Kazama, 2007). The new variables vector position composed with along the direction of the highest variance of original variables (Wang et al., 2013). The PCA statistical equation can be expressed as:

$$z_{in} = c_{f1}x_{1i} + c_{f2}x_{2i} + c_{f3}x_{3i} + \cdots + c_{fm}x_{mi} + e_{fi} \qquad [2]$$

where, z is the observed value of component score, c is the component loading, x is the observed value of variable, i is the number of variable, n is the sample number, f is the factor score, m is the total number of components, and e is the residual for considering errors or any variation of variables.

3.3.4.1 Extraction processes of PCA

The scree plot allows the selection of a number of principal components for PCA. Generally, the sum of squared distance (SSD) of variables vector length or eigenvalues (> 1) is used to pluck out the PCA (Mitra et al., 2018).

3.3.4.1.2 Reliability analysis of PCA technique

The outlier analysis technique was used for assessing reliability of the PCA extraction technique. This technique is widely used to detect the anomaly of data (Muharemi et al., 2019; Islam Khan et al., 2021)

3.4 Results and discussion

An overview of the statistical summary of water quality data in Cork Harbour is presented in Figure 1. In this study, a significant difference was found between summer and winter water quality, where all parameters were assessed as statistically significant at P = 0.05. The present study was found to have a significant level of less than 0.01.

The outliers were detected for DOX, DIN, MRP, AMN, TEMP, and TRAN during the summer season, and in CHL, DOX, BOD, and MRP through the winter period. The outlier results indicate that these water quality parameters had significant data variation. Those parameters have a significant impact on controlling water quality in Cork Harbour.

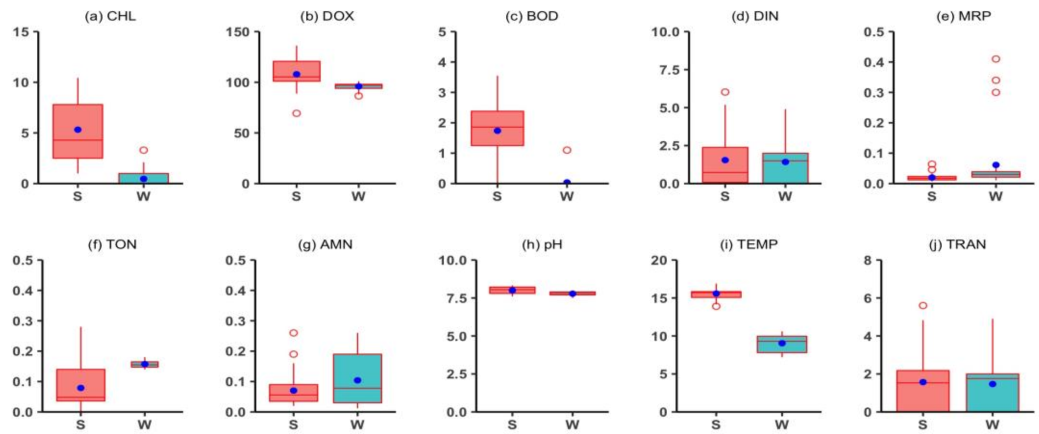


Figure 1. Statistical summary of water quality attributes in Cork Harbour respectively for summer (S) and winter (W) periods.

The PCA method was utilized to identify critical water quality parameters. The principal components of water quality variables were selected based on eigenvalues. Figure 2 shows the percentage of explained variances of total variables; two principal components were retained in this study during both seasons. The PCA results show that the components 1 and 2 explained 48% and 18.5% of the total variance during summer (Fig. 5a), respectively, while during winter, components 1 and 2 explained 43.5 % and 17.1 % of the total variance of water quality data in Cork Harbour (Fig. 5b).

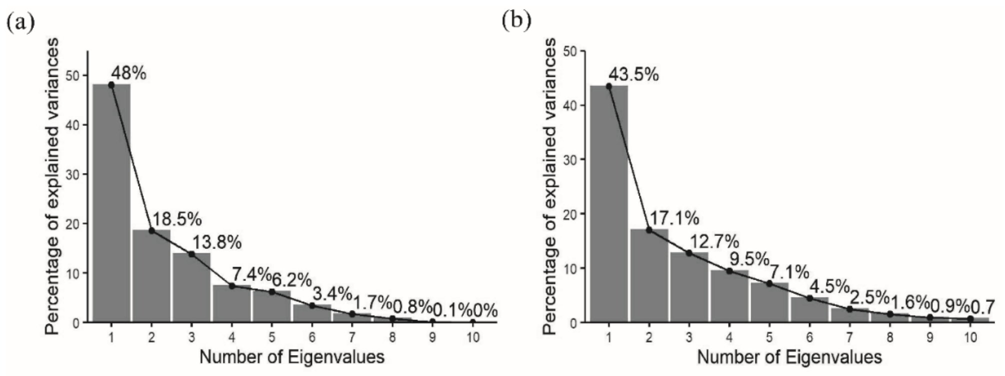


Figure 2. Scree plot for water quality parameters: (a) summer and (b) winter

In this study, the scree plot indicated that three principal components explain over 70% of the total variance of variables (Fig. 2). PCA degree of factor loading is determined using the significant level of correlation of covariance. There are three factor loading categories: strong (> 0.75), moderate (0.75 – 0.50) and weak (0.05 – 0.30) respectively (Liu et al., 2003). The present research considered the strong factor loading (>0.75) for extraction of the significant parameters. Figure 3 shows the loading factor results obtained from the variance analysis of PCA.

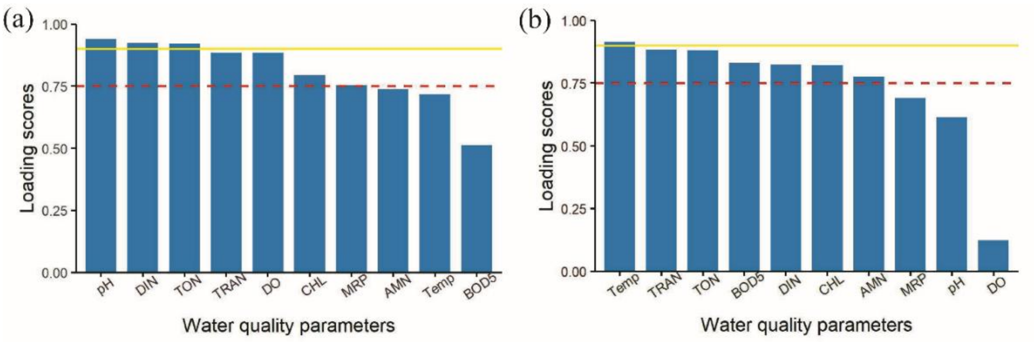


Figure 3. Critical water quality parameters in Cork Harbour: (a) summer and (b) winter. Red line indicates components loading threshold greater than 0.75 and yellow represents greater than 0.90.

Before conducting PCA, the Spearman correlation coefficients between the ten water quality parameters were calculated to identify correlations (p <0.01). A strong correlation coefficient was found between DIN and pH, TON and TRAN. Figure 4 presents the Spearman Correlation matrix with intercorrelations between water quality parameters.

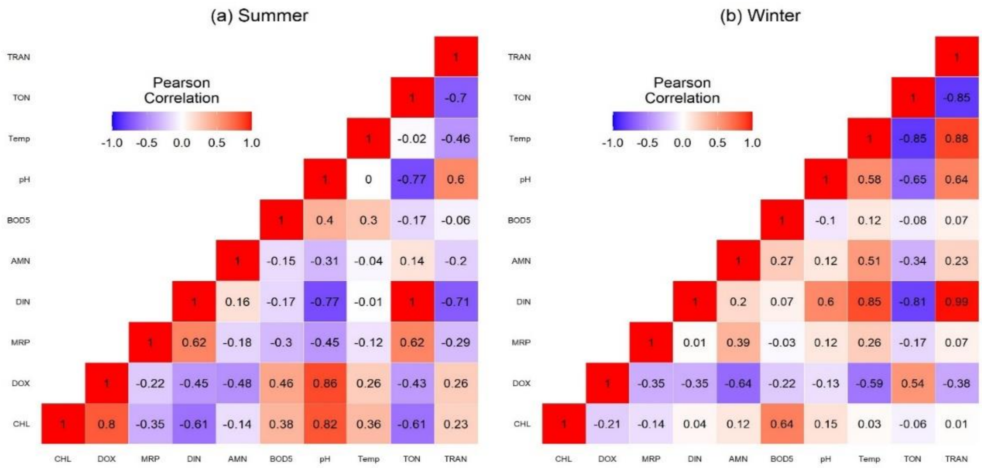


Figure 4. Correlation matrix of water quality parameters in Cork Harbour.

The PCA technique identified eight water quality parameters: pH, DIN, TON, TRAN, DO, CHL, MRP, and AMN, to be critically important during the summer season. These water quality indicators had been found to have a substantial impact on the quality of water in Cork Harbour in previous studies (Nash et al., 2011). The winter

PCA results suggested that seven parameters are important for monitoring water quality during this season: TEMP, TRAN, TON, BOD5, DIN, CHL, and AMN. All of these water quality attributes can have a significant impact on other variables (Ma et al., 2020).

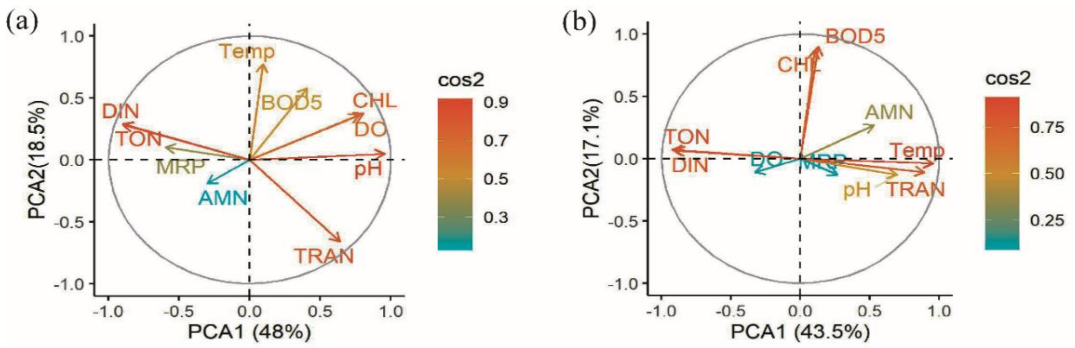


Figure 5. Loading of highly significant two principal components for water quality parameters in Cork Harbour: (a) summer and (b) winter

The findings of the PCA analysis imply that these water quality metrics are important in the context of temporal change of water quality in Cork Harbour. When comparing two datasets, it can be seen that the summer season has a higher data variance (66.5%). These findings suggest that the composition of water quality in the Harbour has a strong temporal component.

3.4.1 Understanding of reliability the PCA results

The box-plot outlier detection technique was used to assess the reliability of PCA results. As shown in (Figure 1), the outlier was detected in six water quality parameters, whereas the PCA results revealed that eight water quality parameters are important during the summer season. In winter, a significant variation was found between outlier detection and PCA results. The results of this study's PCA show that the technique may not be effective in determining critical water quality parameters for the coastal WQI model over the winter.

3.5 Conclusion

The purpose of this research is to evaluate the PCA technique as a tool for selecting critical water quality parameters in developing a WQI model for assessing coastal water quality. For the purpose of parameter selection, the present study applied PCA and boxplot techniques to assess the reliability of the PCA method by comparing results. This study found a significant difference between the PCA and boxplot analysis. In the boxplot analysis, MRP and AMN were found as an important during the summer, and DOX and MRP were also important for the winter analysis, respectively, but the PCA excluded these parameters from the analysis. However, the findings of this research revealed that the PCA technique may not effective tool to select crucial water quality parameters in terms of coastal water quality.

3.6 Acknowledgement

This research was funded by the Hardiman Research Scholarship of the National University of Ireland Galway, which funded the first author as part of his PhD program. The authors would like to thank the Environmental Protection Agency of Ireland for providing water quality data. MaREI, the SFI Research Centre for Energy, Climate, and Marine and Ryan Institute, NUIG, Galway, Ireland, also supported the research.

3.7 References

Islam Khan, M.S., Islam, N., Uddin, J., Islam, S., Nasir, M.K., 2021. Water quality prediction and classification based on principal component regression and gradient boosting classifier approach. J. King Saud Univ. - Comput. Inf. Sci. https://doi.org/10.1016/j.jksuci.2021.06.003

Liu, W.X., Coveney, R.M., Chen, J.L., 2003. Environmental quality assessment on a river system polluted by mining activities. Appl. Geochemistry 18, 749–764. https://doi.org/10.1016/S0883-2927(02)00155-5

Ma, X., Wang, L., Yang, H., Li, N., Gong, C., 2020. Spatiotemporal analysis of water quality using multivariate statistical techniques and the water quality identification index for the qinhuai river basin, east china. Water (Switzerland) 12. https://doi.org/10.3390/w12102764

Mitra, S., Ghosh, S., Satpathy, K.K., Bhattacharya, B.D., Sarkar, S.K., Mishra, P., Raja, P., 2018. Water quality assessment of the ecologically stressed Hooghly River Estuary, India: A multivariate approach. Mar. Pollut. Bull. 126, 592–599. https://doi.org/10.1016/j.marpolbul.2017.09.053

Muharemi, F., Logofătu, D., Leon, F., 2019. Machine learning approaches for anomaly detection of water quality on a real-world data set. J. Inf. Telecommun. https://doi.org/10.1080/24751839.2019.1565653

Nash, S., Hartnett, M., Dabrowski, T., 2011. Modelling phytoplankton dynamics in a complex estuarine system. Proc. Inst. Civ. Eng. - Water Manag. 164, 35–54. https://doi.org/10.1680/wama.800087

Primpas, I., Tsirtsis, G., Karydis, M., Kokkoris, G.D., 2010. Principal component analysis: Development of a multivariate index for assessing eutrophication according to the European water framework directive. Ecol. Indic. 10, 178–183. https://doi.org/10.1016/j.ecolind.2009.04.007

Shrestha, S., Kazama, F., 2007. Assessment of surface water quality using multivariate statistical techniques: A case study of the Fuji river basin, Japan. Environ. Model. Softw. https://doi.org/10.1016/j.envsoft.2006.02.001

Tripathi, M., Singal, S.K., 2019. Use of Principal Component Analysis for parameter selection for development of a novel Water Quality Index: A case study of river Ganga India. Ecol. Indic. 96, 430–436. https://doi.org/10.1016/j.ecolind.2018.09.025

Uddin, M.G., Nash, S., Olbert, A.I., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol. Indic. 122, 107218. https://doi.org/10.1016/j.ecolind.2020.107218

Wang, Y., Wang, P., Bai, Y., Tian, Z., Li, J., Shao, X., Mustavich, L.F., Li, B.L., 2013. Assessment of surface water quality via multivariate statistical techniques: A case study of the Songhua River Harbin region, China. J. Hydro-Environment Res. 7. https://doi.org/10.1016/j.jher.2012.10.003

Study 4. Development of a water quality index model - a comparative analysis of various weighting methods

This study has been accepted for publication in the Proceedings of the 3rd Springer Conference of the Arabian Journal of Geosciences (CAJG-3), Istanbul 2021.

4.1 Abstract

The Water Quality Index (WQI) model is a popular tool for the assessment of water quality (WQ) and its status classification. Over the last 50 years, many different WQI models have been developed; while the four-component structure remains common across the models, they vary in approaches in terms of parameter selection and their associated weightings, and the methods used for sub-indexing and aggregation. In this research, the parameter weight factors are investigated. The parameters are assigned weightings depending on their significance to the assessment. Recent research has revealed that that the WQI models generate a significant amount of uncertainty as a result of this process. Most of the WQI models widely used the expert opinion or analytical hierarchy process (AHP) to estimate the parameters' weight values. Many researchers have argued that these methods do not accurately represent the importance of parameters. The aim of this study is to compare various statistical weighting approaches and propose the most accurate method for calculating weight values in terms of uncertainty. To estimate the weight value of parameters, four statistical attribute weighting methods were used: (i) rank sum (RS), (ii) rank reciprocal (RR), (iii) rank order centroid (ROC), and (iv) equivalent (EQ). In this study, the Guide to the Expression of Measurement Uncertainty (GUM) approach was used to quantify uncertainty of the weighting process by implementing Monte Carlo simulation (MCS) technique. The finding of this study show that the ROC method produces the highest uncertainty, while the RS and EQ methods generate relatively lower uncertainties. In terms of uncertainty, the results suggest that the rank sum method is an effective method to estimate the weight value in developing a WQI model.

Keywords: Water Quality Index Model; Monte Carlo simulation; Weight Values; Weighting Methods; Uncertainty; Random Forest, Rating Methods

4.2 Introduction

Water quality index (WQI) model is a popular tool due to its simple architecture and easy to application. Commonly, an ideal WQI model comprises including four components: (i) parameter selection, (ii) sub-index process, (iii) parameter weighting and (iv) aggregation function. This model is becoming increasingly popular and utilized to assess and classify water quality. Nevertheless, recent research has revealed that WQI has uncertainty problems in different stages [1-2]. The weighting technique is one of them. The present WQI used a variety of methods (such as expert opinions, analytical hierarchy process, literatures) for generating parameters weight values. These methods have received much criticism due to its reliability in terms of uncertainty [3]. The present study have been carried out using amalgamation approaches with machine-learning (ML) and multi-attributes (MA) statistical techniques. This approach was implemented by following two sequential steps. The first step of this process was to obtain the water quality rank for assigning degree of significant, then parameters weight values were estimated using four common rank-based weighting methods. However, the purpose of this study is to explore an effective weighting method in order to reduce model uncertainty in developing a WQI model.

4.3 Materials and Methods

4.3.1 Data Description

For this study, data on water quality obtained from https://www.catchments.ie/data/. The Irish Environmental Protection Agency (EPA) has been collecting water quality data from 32 different monitoring sites in the Cork harbour in 2020 that was used in the current research as a case study. This study used the average concentration of water quality data from eleven parameters: ammonia (AMN), biological oxygen demand (BOD), dissolved oxygen (DO), chlorophyll a (CHL), molybdate reactive phosphorus (MRP), water pH, total organic carbon (TOC), total organic nitrogen (TON), water transparency (TRAN), dissolved inorganic nitrogen (DIN), and water temperature (TEMP).

4.3.2 Parameters ranking procedures

In this research, we conducted a study using ten widely used machine-learning (ML) algorithms for ranking water quality parameters based on their real-time relative importance. For ranking, this study utilized surface water quality guidelines that adopted by the Environmental Protection Agency (EPA) of Ireland. The random forest (RF) algorithm was found to be the most efficient for assigning parameter rankings

[4]. In this research, the RF is used in order to provide the rank of water quality parameters. The RF prediction function defined as follows:

$$f(x) = \sum_{m=1}^{M} c_m \prod (x, R_m) \qquad (1)$$

where *M* denotes the number of regions in the features space, R_m is the region that corresponds to m, c_m is a constant that relates to m.

$$\prod (x, R_m) = \{ \begin{matrix} 1, & if\ x, R_m \\ 0, & otherwise \end{matrix} \qquad (2)$$

The Gini scores are obtained by voting scores of each decision tree. Finally, the important features are chosen from the new subset based on the Gini score of the features [4].

2.3.3 Estimating parameters weight values

The present study was used the four direct rating subjective methods to estimate weight value of water quality parameters. These methods may avoid the problems highlighted by recent studies. These functions are defined as follow:

(i) Rank Sum (RS) method: $w_i = \frac{n+1-i}{\sum_{j=1}^{n} j} = \frac{2(n+1-i)}{n(n+1)}, i = 1,2,3 \ldots \ldots., n$ (3)

(ii) Rank Reciprocal (RR) method: $w_i = \frac{1/i}{\sum_{j=1}^{n} 1/j}, i = 1,2,3 \ldots \ldots \ldots, n$ (4)

(iii) Rank Order Centroid (ROC) method: $w_i = \frac{1}{n} . \sum_{j=1}^{n} \frac{1}{j}, i = 1, 2, 3 \ldots \ldots \ldots, n$ (5)

(iv) equal Weight (EQ) method: $w_i = \frac{1}{n}, i = 1,2,3 \ldots, n$ (6)

where, *n* is the total number of attributes; *i* is the *i*th attribute rank; *j* is the summation of rank and *w* is the weight value.

The present study was used Monte Carlo simulation (MCS) approaches by following the Guide to the Expression of Measurement Uncertainty (GUM) method to calculate uncertainties in different weighting methods. In this study, the MCS run 103 trials for MC simulation.

4.4 Results

4.4.1 Ranks of water quality parameters

Figure 1 presents the rank of different water quality parameters were obtained from the RF method. The results showed that the TOC, TON, TRAN and DIN are most important parameters in terms of water quality standards. AMN and temperature were found to have no significance in the analysis of water quality for this study.

4.4.2 Comparative analysis of weighting methods

In this study, parameter weight values were estimated using four weighting methods. In terms of weight variability of parameter, there was a significant difference between the four weighting methods. Table 1 shows the weight values of different water quality variables for different techniques respectively.

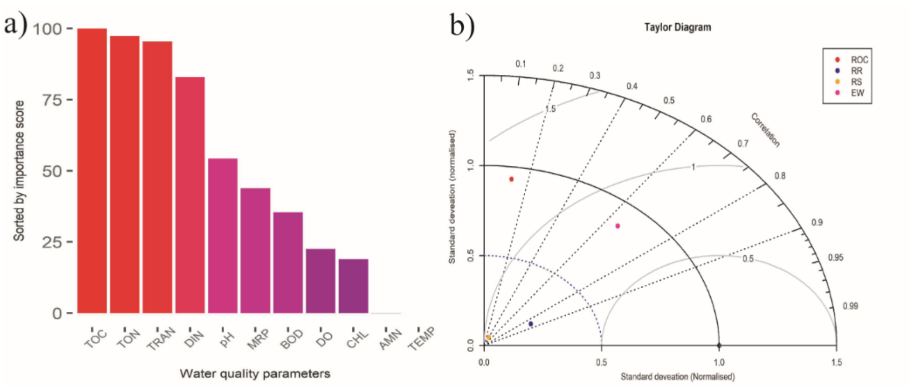


Figure 1. (a) Importance of water quality parameters; and (b) Cross-validation of the four weighting methods using Taylor diagram.

Table 1. Estimating weight values of water quality parameters.

WQ parameters	Rank	ROC	RR	RS	EW
TOC	1	0.4083	0.4082	0.2857	0.1667
TON	2	0.2417	0.2041	0.2381	0.1667
TRAN	3	0.1583	0.1361	0.1905	0.1667
DIN	4	0.1028	0.1020	0.1429	0.1667
pH	5	0.0611	0.0816	0.0952	0.1667
MRP	6	0.0278	0.0680	0.0476	0.1667

4.4.3 Uncertainty analysis

The current study investigated into a significant difference in weight variation of water quality parameters between weighting methods. Table 2 shows the summary statistics of probability distributions of ROC, RR, and RS weighting methods were triangular and EW method was normal distribution.

Table 2. Different-weighting methods and related PDFs

Weighting methods	PDFs	PDF parameters
ROC	Triangular	a = 0.0278; b = 0.4083; c = 0.16667
RR	Triangular	a = 0.0680; b = 0.4082; c = 0.16667
RS	Triangular	a = 0.0476; b = 0.2857; c = 0.16667
EW	Normal	Mean = 0.1667; SD = 0.00

As seen in Figure 2, it shows the summary of MCS results. Table 3 provides comparative statistical scenarios between various weighting procedures. According to MCS results, the ROC method produced the highest weighting uncertainty, while the RS method produced the lowest. Table 4 presents the uncertainty results obtained from the MCS analysis for different weighting methods.

Table 3. Descriptive statistics of different weighting techniques.

Ranking methods	Descriptive statistics				
	Minimum	Maximum	Mean	SE	Std.
ROC	0.0278	0.4083	0.1667	0.0573	0.1404
RR	0.0680	0.4082	0.1667	0.0522	0.1279
RS	0.0476	0.2857	0.1667	0.0364	0.0891
EQ	0.1667	0.1667	0.1667	0.0000	0.000

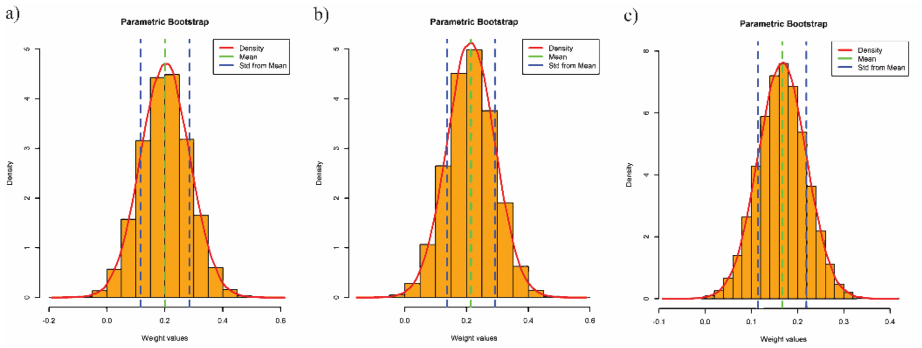


Fig. 2. Density plots for input PDFs of water quality parameters obtained from by MCS method: (a) ROC; (b) RR; (c) RS

4.4.5 Cross-validation of uncertainty results

The effectiveness of the methods was compared and visualized using a Tylor diagram. The correlation coefficient (R), root mean square difference (RMSD), and standard deviation (SD) between any prediction and observation weight values are shown in this diagram. The RS method, as shown in Figure 1b, falls into lines with the lowest RMSD and SD between predicted and observed weighted values. The findings suggest that the RS method could help improve the weighting system's accuracy.

Table 4. Uncertainty with 95% coverage probability of different weighting methods.

Ranking methods	Uncertainty parameters			
	SU[1]	EDF[2]	CF[3]	EU[4]
ROC	0.0320	5	2.57	0.0823
RR	0.0292	5	2.57	0.0751
RS	0.0198	5	2.57	0.0509
EQ	0.0	5	2.57	0.0

4.5 Discussion

As mentioned in the recent research, the weighting method contributes to the uncertainty in the WQI model. Six water quality parameters out of eleven were found to be significant in the current study in order to assess water quality in Cork Harbour, Ireland. The finding confirms that different weighting methods resulted in significant differences in parameter weight values. Figure 1b shows the summary statistics for different weighting methods. In contrast to four weighting methods, different methods show significant variation, which is consistent with previous literature. From the figure 1b, it can be seen that the RS method produced the lowest uncertainty relatively the highest weight variation was produced by ROC methods. However, recent research has revealed that the rank order centroid (ROC) weights lead to the highest performance in identifying the best alternative under the ranked attribute weights due to its sharpness and non- linear function. The findings of this study suggest that the rank sum method is an effective technique for estimating weight value in developing a WQI model.

4.6 Conclusions

The present study examined the performance of four statistical weighting methods in order to estimate weight values of water quality parameters. In terms of contribution to uncertainty in WQI model, the results indicate that the rank sum method is robust method to estimate the weight value than other methods. This new study could aid in reducing uncertainty and improving the WQI model's performance. The present study has confirmed the finding of recent studies, which revealed that the weighting method contributes to the uncertainty in WQI model. Therefore, according to analysis the weighting values had a slight significant impact on producing uncertainty in WQI model. Statistically, it could be held statistically accountable to estimate weight values in the WQI model due to this study was calculated less than two percent uncertainty in weighting process.

4.7 Acknowledgement

This research was funded by the Hardiman Research Scholarship of the National University of Ireland, Galway, which funded the first author as part of his PhD program. The authors would like to thank the Environmental Protection Agency of Ireland for providing water quality data.

4.8 References

1. Sutadian, A.D., Muttil, N., Yilmaz, A.G., Perera, B.J.C., 2017. Using the Analytic Hierarchy Process to identify parameter weights for developing a water quality index. Ecol. Indic. 75, 220–233. https://doi.org/10.1016/j.ecolind.2016.12.043
2. Uddin, M.G., Nash, S., Olbert, A.I., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol. Indic. 122, 107218. https://doi.org/10.1016/j.ecolind.2020.107218
3. Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment. Water Res. 219, 118532. https://doi.org/10.1016/j.watres.2022.118532
4. Jović, A., Brkić, K., Bogunović, N., 2015. A review of feature selection methods with applications. 2015 38th Int. Conv. Inf. Commun. Technol. Electron. Microelectron. MIPRO 2015 - Proc. 1200–1205. https://doi.org/10.1109/MIPRO.2015.7160458

Study 5. A comparison of geocomputational models for validating geospatial distribution of water quality index

This study (Book Chapter) has been accepted for publication in the "**Computational Statistical Methodologies and Modeling for Artificial Intelligence**" Book series, Edited by Priyanka Harjule, Azizur Rahman, Basant Agarwal and Vinita Tiwari, CRC Press, Taylor & Francis Publisher, USA

5.1 Abstract

Water resources management is a vital component of maintaining good water quality. The surveillance program is one of the essential tools for regularly monitoring water quality. But, it's a very expensive and long term process. To date, several tools and techniques have been developed for assessing water quality. The water quality index (WQI) is one of them. Recently, this technique has been widely used for assessing water quality. Its application has increased rapidly due to its allows converting a vast amount of water quality information into a unitless numerical expression using simple mathematical functions. For the purposes of predicting WQIs at each grid point, various geospatial techniques were used. The aim of this research was to identify the best geospatial predictive model for the spatial distribution of WQIs for coastal water quality. In this research, eight widely used interpolation techniques were utilized for the interpolation of WQIs: local polynomial interpolation (LPI), global polynomial interpolation (GPI), inverse distance weighted interpolation (IDW), radial basis function (RBF), simple kriging (SK), universal kringing (UK), disjunctive kriging (DK), and empirical Bayesian kriging (EBK). This study has been carried out in Cork Harbour, Ireland, as a case study for assessing coastal water quality using the weighted quadratic mean (WQM) WQI model. According to the cross-validation results, the UK (RMSE = 6.0, MSE = 0.0, MAE = 4.3, and R^2 = 0.8) and EBK (RMSE = 6.2, MSE = 0.0, MAE = 4.6, and R^2 = 0.78) methods performed excellently in predicting WQIs at each grid point in Cork Harbour, respectively. The findings of this study reveal that the EBK geospatial computational model could be effective in predicting WQIs in Harbour.

Keywords: Coastal Water Quality; Cork Harbour; Water Quality Index Model; Geostatistical Simulation Models; Spatial Distribution of WQI.

5.2 Introduction

Water resources management is an essential task to maintain to ensure good water quality in aquatic ecosystems. It will be extremely difficult for future generations in the world to maintain “good water quality status” in all states, since the quality of the water deteriorates over time gradually due to the association of various factors, manmade intervention being one of them. Industrialisation and urbanisation have accelerated day by day in order to ensure a better quality of life. As consequences, freshwater consumption has significantly increased over the decades (Javed et al., 2017; Uddin et al., 2020a). Therefore, surface and ground water quality degradation has been occurring very rapidly due to the both anthropogenic activities and natural processes (Uddin et al., 2021; Uddin et al., 2020b).

In order to ensure the good water quality status, sustainable management plans, policies, and adequate resources are required. Water resources management is a complex and critical process that involves a variety of components such as institutional framework, skilled labour, legislations and financial framework, resources availability, etc. It is a challenging process not only for developing countries but also recently addressed by developed countries and agencies. Several countries have formulated various action plans to maintain good water quality status in all water bodies but have run into frequent issues when implementing and adopting management programs.

In Europe, the European Union (EU) is mainly responsible for formulating plans and policy for ensuring good water quality in the member states. The Water Framework Directive (WFD) is one of the important tools for managing quality of water and ecosystems (Carsten Von Der Ohe et al., 2007; Zotou et al., 2020). This tool provides in detail guidelines for the management of aquatic environments, but it has not defined any specific tools or techniques that should be used to assess water quality globally in EU member states. While it recommended adopting monitoring programs for surveillance of water quality in all member states, this is very costly and time consuming. Thus, many countries have been suffering these challenges and trying to overcome them.

To date, a variety of tools and techniques are used for assessing water quality and the water quality index (WQI) model is one of them. The WQI model is a simple mathematical tool whose uses have been increasing very rapidly around the world due to its ease of application compared to other traditional models. It allows converting a range of water quality information into a single unit-less numerical value. Commonly, this technique consists of four crucial components: (i) water quality parameter selection using several techniques to identify the important parameters; (ii) sub-index process to convert different dimensional variables into universal form; (iii) weighting of water quality parameters is the process to assign the parameters weight based on their relative importance; and (iv) aggregation function is the final and most important step of the WQI model to transfer sub-index and weight values into a single numerical value (Gupta and Gupta, 2021; Parween et al., 2022; Sutadian et al., 2016; Uddin et al., 2021). Details of the WQI models and their uses can be found in Uddin et. al. (2021). Recently, several studies have revealed that the WQI model produces considerable uncertainty by its own process (Abbasi and Abbasi, 2012; Uddin et al., 2022d; 2022e). As a result, accurate water quality information does not reflect its outcomes. Many researchers have developed various techniques to reduce the uncertainty in the WQI model (Juwana et al., 2016). Recently, we carried out a comprehensive study on the WQI model. In our study, we compared eight aggregation functions (five are widely used and three are newly proposed by the authors) to identify the best aggregation method in terms of uncertainty (Uddin et al., 2022). That study revealed that the new weighted quadratic mean (WQM) aggregation functions gave excellent performance in assessing coastal water quality. For that reason, in this study, we used the WQM-WQI model to calculate WQIs for coastal water quality in Cork Harbour, Ireland.

For the limitation of surveillance programme, WQI simulation or prediction is essential to estimate WQI's value at unknown location or grid points. Many tools and techniques are widely used to predict unknown point values and spatial interpolation technique is one of the most common approaches (Farzaneh et al., 2022). Up to now, many interpolation techniques have been utilized to predict the spatial distribution of water quality (Antal et al., 2021; Borges et al., 2016; Uddin et al., 2018). But they are mainly categorised into two groups: (i) deterministic and (ii) geostatistical methods.

Deterministic geocomputational interpolation methods well known as the exact interpolator technique. Usually, this technique is used for creating surfaces (polynomial trend surface) from known points using the extent of the similarity or the degree of smoothing (radial basis function) (Adhikary and Dash, 2017). Polynomial trend surface analysis is one of the popular techniques used for global interpolation where measured data is fitted with a linear or quadratic function in order to create the interpolated surface within the geospatial extent (Verma et al., 2019). It can be classified into two groups; one is global approaches and the other one is local. Whereas the global approaches are used for the prediction of the entire geospatial extent using the entire dataset, the local methods predict unknown grid point values from the measured grid points within neighborhoods. Generally, this technique is widely used to predict unknown grid points across a smaller area within a large geospatial extent (Pellicone et al., 2018). A number of deterministic geocomputational methods are commonly used for prediction of unknown grid points, including inverse distance weighted (IDW), spline, Thiessen polygon, and linear regression (Verma et al., 2019).

Usually, the geostatistical interpolation techniques applies for predicting unknown grid points data using the statistical properties of the known points within given dataset (Adhikary and Dash, 2017). This technique is a well-known kriging method for analysing spatial distribution of measured data. In terms of statistical approaches, it is a very effective interpolation technique because it allows spatial correlation among grid points of an entire area (Adhikary and Dash, 2017; Al-Mamoori et al., 2021). Several kringing/geostatistical methods are widely used to interpolate or predict unknown grid values; there are simple kriging (SK), ordinary kriging (OK), universal kriging (UK), co-kriging, regression kriging, indicator kriging, etc. (Bronowicka-Mielniczuk et al., 2019; Han et al., 2020; Jalili Pirani and Modarres, 2020; Wu et al., 2019).

Recently, several studies have been carried out for interpolating various environmental factors such as climatic variables (Amini et al., 2019; Attorre et al., 2007; Verma et al., 2019; Yan et al., 2005); wind speed prediction (Luo et al., 2008); air temperature; snowmelt prediction (Hock, 2003); surface water quality variable predictions (Khouni et al., 2021; Murphy et al., 2010; Uddin et al., 2020a; Wu et al., 2019); soil pH and salinity in coastal water (Emadi and Baghernejad, 2014); heavy metal distribution analysis in rivers (Madhloom et al., 2018); and rainfall/precipitation interpolation (Antal et al., 2021; Bárdossy and Pegram, 2013; Borges et al., 2016; Jalili Pirani and

Modarres, 2020; Liu et al., 2020; Pellicone et al., 2018; Wang et al., 2014; Zhang and Srinivasan, 2009). A number of studies have utilized various interpolation techniques for spatial distribution of water quality index for assessing surface water quality (Kawo and Karuppannan, 2018; Kumar et al., 2022; Muzenda et al., 2019; Nikitin et al., 2021). Moreover, for the purposes of performance analysis and to identify the best interpolation/prediction techniques, recently, a few studies have been carried out comparing various geostatistical interpolation methods (Adhikary and Dash, 2017; Antal et al., 2021; Attorre et al., 2007; Emadi and Baghernejad, 2014; Farzaneh et al., 2022; Liu et al., 2020; Luo et al., 2008; Meng et al., 2013; Murphy et al., 2010; Uddin et al., 2020a; Verma et al., 2019; Wang et al., 2014; Wu et al., 2019). The present study applied eight interpolation techniques including four deterministic: local polynomial interpolation (LPI), global polynomial interpolation (GPI), inverse distance weighted interpolation (IDW), and radial basis function (RBF) and four geostatistical models: simple kriging (SK), universal kringing (UK), disjunctive kriging (DK), and empirical bayesian kriging (EBK) to determine the best interpolation/prediction model for predicting WQM-WQIs value for coastal water. Finally, the model performance was evaluated using the cross-validation (CV) approach, a technique widely used to evaluate prediction model performance (Belete and Huchaiah, 2021; Agarwal et al. 2022a; Agarwal et al. 2022b).

Therefore, the aim of this study was to identify the appropriate geocomputational-interpolation method for the spatial distribution of WQM-WQIs properly at each unknown grid point in Cork Harbour, Ireland. This study can directly support the water quality-monitoring program by providing an insightful application of the WQI model. For the purposes of achieving the goals of this research, a few specific objectives have been carried out as follows:

- To calculate WQIs using WQM-WQI model for coastal water quality in Cork Harbour.
- To utilize eight geocomputational-interpolating techniques to predict the spatial distribution of WQIs.
- To identify the best geocomputational model by comparing eight interpolation techniques in order to predict WQIs accurately at each monitoring site.

The chapter is structured as follows: Section 2 describes the study domain, Section 3 provides the descriptions of various geostatistical and other statistical methods for assessing the models (Harjule et al. 2021), Section 4 presents results and discusses the output of the prediction models, and Section 5 summarizes the main conclusions of this research.

5.3 Application domain: A case study in Cork Harbour

The present study was conducted in Cork Harbour, a Special Protection Area (SPA) that is relatively the deepest and longest (17.72 km) surface waterbody in Ireland (Hartnett and Nash, 2015; Nash et al., 2011). The harbour is a large surface area (85.85 km2) and brackish estuary on the south coast of Ireland (Nash et al., 2011). It is a macro-tidal harbour with a typical spring tide range of 4.2 m at the entrance to the harbour (Hartnett and Nash, 2015). The Cork city is the industrial hub of the Irish southwest region and the surrounding hinterlands are subject to relatively intense agricultural activities, which impact water quality in the region (EPA, 2017). Recently, several annual environmental reports from the EPA revealed that Cork and Donegal received the highest raw discharge wastewater directly without any treatment from the various sources (EPA, 2017). Moreover, the Cork Harbour geological patterns are vital for harbour area ecosystem and freshwater quality. It has been identified as a SPA under the 1979 Wild birds Directive (79/409/EEC).

5.4 Methods and materials

5.4.1 Data obtaining process

For the purposes of this study, the water-quality data was obtained from 29 monitoring sites out of 32 across the Cork Harbour monitoring data in the year 2020. Details of the monitoring sites are illustrated in Figure 1. Typically, the Irish Environmental Protection Agency (EPA) monitors the water quality of Cork Habour frequently. In this study, water-quality data was considered at one-meter below water surface at approximately high and low tides over the year. In order to calculate WQI values, in total 11 water-quality parameters were obtained from the EPA water quality-monitoring database of Cork Harbour. These were temperature (TEMP), pH, dissolved oxygen (DOX), salinity (SAL), ammonia (AMN), total organic nitrogen (TON), ammoniacal nitrogen (AMN), molybdate reactive phosphorus (MRP), biological oxygen demand (BOD), transparency (TRAN), and Chlorophyll a (CHL). Details of the data can be found at the following web resource: www.catchments.ie/data. These parameters were selected for this study based on the availability of variables in the monitoring database and taking account of the spatial distribution of monitoring sites.

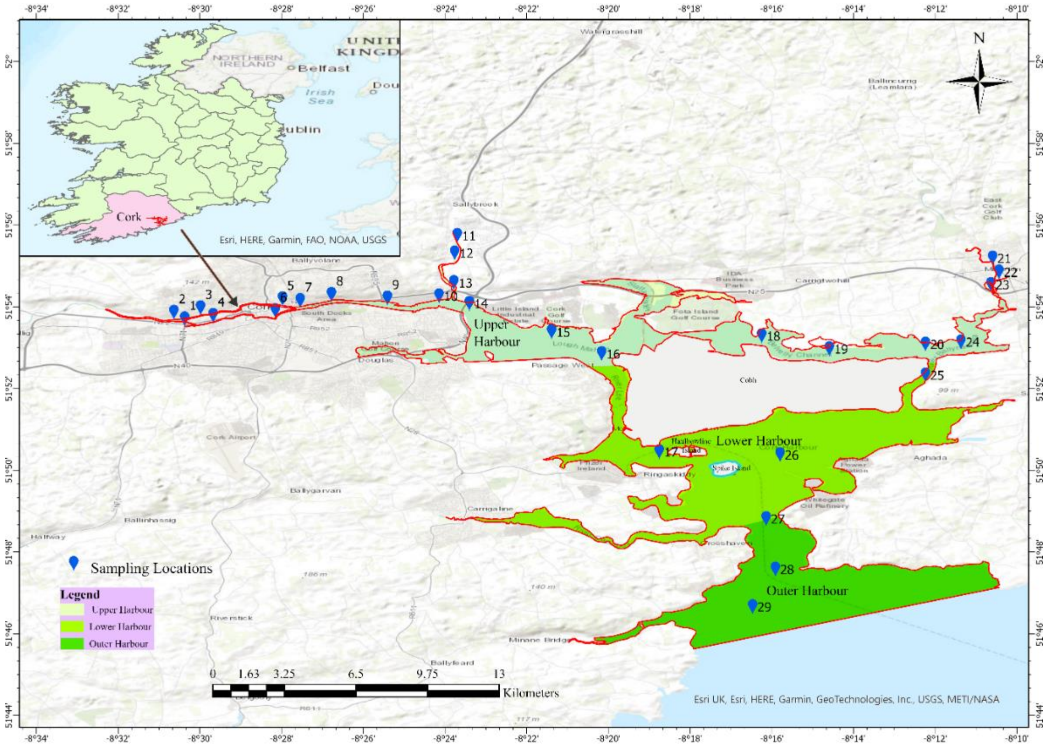


Fig. 1. Study domain: Cork Harbour, Ireland.

5.4.2 WQI calculation

To date, a range of WQI models have been used to calculate the WQI values. Its application has increased sequentially due to its simple mathematical functions and ease of application. Commonly, an ideal WQI model comprises four components: (i) water indicators selection, (ii) sub-index function, (iii) indicator weight value generation, and (iv) aggregation function. The existing literature on WQI models is extensive and focuses particularly on details of WQI models and their uses (Gupta and Gupta, 2021; Sutadian et al., 2016; Uddin et al., 2021, 2022a). In this research, WQI values were calculated using the weighted quadratic mean (WQM) WQI model, a technique performed based on the conceptual framework proposed by Uddin et al. (2022b). The WQM-WQI function can be expressed as follows:

$$WQM - WQI = \sqrt{\sum_{i=1}^{n} w_i s_i^2} \qquad (1)$$

where w_i is the weight value and s_i is refers to the sub-index value of water quality ith indicators.

5.4.3 Prediction techniques

Thus far, several geocomputational tools and techniques have been used to analyse the spatial distribution of water quality. Geocomputational-interpolation techniques allow to calculate unknown grid point values using the weighted means of sampled data by applying a set of mathematical, statistical, and spatial approaches (Rahman, 2020; Das et al., 2018; McManus et al., 2020, 2021; Rahman et al., 2013; Rahman & Harding, 2016; Uddin et al., 2018; Uddin et al., 2020a; Verma et al., 2019; Xie et al., 2011; Zandi et al., 2011). In this study, eight geocomputational prediction models were utilized to compare their performances to find the best model to properly predict WQI values.

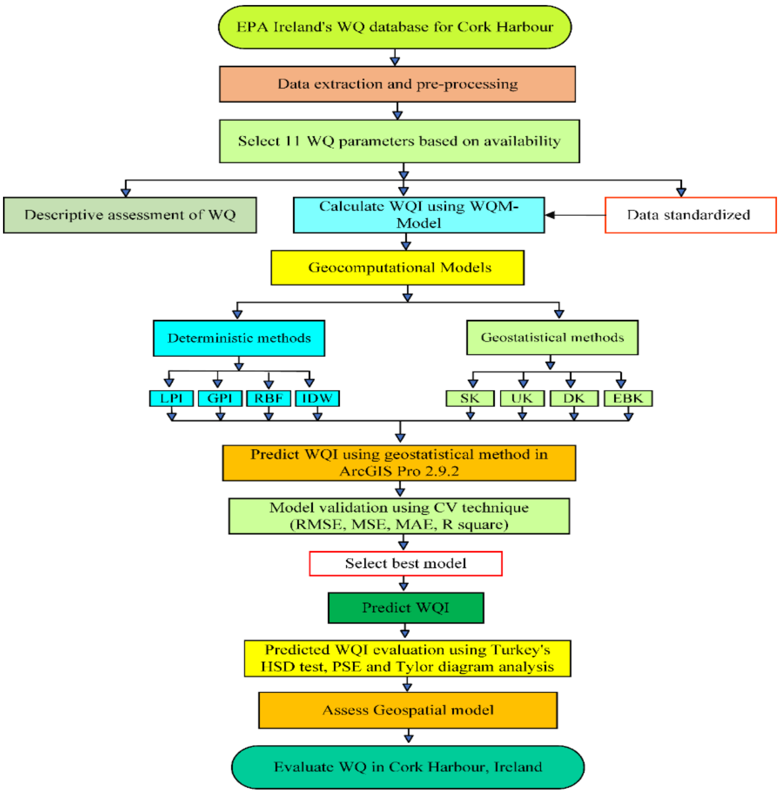


Fig. 2. A comprehensive framework for the assessment of geospatial distribution tools for predicting WQIs.

5.4.3.1 Spatial computational methods

Available geocomputational-interpolation techniques can be classified into two groups: deterministic and geostatistical (Rahman and Harding, 2016). In this research, in total eight interpolation techniques were selected from two groups, with four techniques included in each group. These techniques were selected for this study based on their application and literature resources. A short description of various interpolation techniques and details of the methodological framework are presented in Figure 2.

5.4.3.1.1 Deterministic interpolation methods

(a) Deterministic technique

In general, the geometric properties of the samples are the main attributes of the deterministic techniques, whereas the spatial autocorrelations of the target variables are the main attributes of the geocomputational techniques (Verma et al., 2019). The four techniques used in this research are as follows.

(i) Global polynomial interpolation (GPI)

GPI is an effective interpolation technique to predict the lowest data variability space. It fits a smooth surface that is defined by a polynomial mathematical function to the unknown sample point (Wang et al., 2014). This technique enables to capture coarse-scale pattern in the data where the global polynomial surface changes gradually (Antal et al., 2021; ESRI, n.d.; Verma et al., 2019). The polynomial of degree n is fitted for the surface changes and is defined as follows:

$$z = ax + by + c \qquad (2)$$

where z is the value of target variable, a, b, and c are input parameters, and x and y are the coordinates of sample.

(ii) Local polynomial interpolation (LPI)

LPI is completely different than the GPI approach. This technique is effective to predict short-range surface area whereas GPI is performed for long-range data variation (Luo et al., 2008; Wang et al., 2014). LPI fits the local polynomial using known points only within a specific neighbourhood instead of all the data. The neighbourhood is able to overlap after the polynomial has been fitted using any kind of kernel, and the surface value in the neighborhood's centre predicts an unknown value (Antal et al., 2021). The LPI can be defined as:

$$l = \left(1 - \frac{d_i}{N}\right) p \qquad (3)$$

where d_i is the range between actual and predicted WQI values, N refers to the neighbourhood area, and p is the order of the polynomial function that is defined by the operators.

(iii) Radial basis function (RBF)

Unlike GPI and LPI, RBF requires the surface to pass through all actual data points (Wang et al., 2014). It is a sequence of actual interpolation techniques that utilizes the basic mathematical equation depending on the detachment between the known point and unknown grid point (Uddin et al., 2018). This technique enables to predict the unknown value of any roughness surface effectively whereas other interpolation methods are suitable only for the plain surface (Amini et al., 2019). The RBF can be defined as (Uddin et al., 2018):

$$K(y) = \sum_{i=1}^{p} C_i f_i(y) + \sum_{i=1}^{q} E_j \emptyset\left(d_j\right) \qquad (4)$$

where (dj) expresses the radial basis functions and E_j the distance from the observation point to projection point y trend function is fi(y), C is member of a basis for the space of polynomials of degree <p. Ej are calculated and the coefficients Ci through means of the determination of the subsequent coordination of q + p linear equations; and q is the whole number of selected points used in the interpolation.

(iv) Inverse distance weighted interpolation (IDW)

IDW is a widely used interpolation technique that calculates an unknown grid value using a linear combination of known grid points. It allows predicting the value of any unknown grid point using actual values surrounding the prediction location. Likely, the closest predicted point is highly influenced by the nearest known sample point, and its farthest points gradually decrease (ESRI, n.d.). Commonly, this technique predicts the value at each point using the weighted average of the nearest known points. Whereas the weight values are estimated using the inverse distance between known and predicted sample points (Uddin et al., 2018; Xiao et al., 2016). Measurements of distances can be defined as:

$$D = \frac{\sum_{1}^{n} \frac{z_i}{d_i^p}}{\sum_{1}^{n} \frac{1}{d_i^p}} \qquad (5)$$

where D refers to the predicted point, n is the number of neighbours nominated for the prediction, p is the power of distance, z_i is the known point of ith observation, and d_i denotes to the distance between unknown and known points.

3.3.1.2 Geostatistical methods

(i) Simple or ordinary kriging (SK)

Compared to the deterministic methods, SK is the most powerful interpolation method to precisely predict unknown grid values more. It is considered a spatial and statistical correlation between known and unknown grid values (Wang et al., 2014). This technique assumes that the mean of the known points is constant, whereas the unknown focuses on spatial attributes, and it uses only local known points within a neighbourhood to predict the unknown point value. Recently, several studies have revealed that the SK methods provide the smallest standard error in order to predict unknown values of any grid point within a surface (Verma et al., 2019; Wang et al., 2014). SK can be expressed as:

$$K_s = \sum_{i=1}^{n} w_i M(X_i) \qquad (6)$$

where K is the predicted unknown value, w_i is the unknown values of the known point, and $M(X_i)$ is the known vale of ith grid points.

(ii) Universal Kriging (UK)

The UK technique is an extension of the SK and is applied to predict unknown point values more accurately. This technique was developed by the mathematician Georges Matheron in 1963 (Borges et al., 2016). The UK assumes the spatial interpolation model as:

$$Z(s) = \mu(s) + \varepsilon(s) \qquad (7)$$

where $\mu(s)$ is a few deterministic functions that are obtained using SK concepts, and $\varepsilon(s)$ is the errors of the samples obtained from the randomly modelled data (ESRI, n.d.).

(iii) Disjunctive kriging (DK)

The DK predicts unknown values using the regionalised variable theory. It calculates the conditional probabilities; that is, the known values of samples of interest equal or exceed the defined thresholds. This technique involves defining a new disjoint parameter from the original continuous variable where the parameters values equal to or exceed the threshold, then it accepts 1, and 0 otherwise (Oliver, 1991). DK assumes a model that can be defined as:

$$f\big(Z(s)\big) = \mu_1 + \varepsilon(s) \qquad (8)$$

where $\mu_1$is the unknown constant and $f(Z(s))$is an arbitrary function of Z(s) and $\varepsilon(s)$is the errors of the samples that estimates from the predictive errors randomly.

(iv) Empirical Bayesian kriging (EBK)

EBK is a robust geostatistical interpolation technique that interpolates unknown point values automatically within most difficult aspects and optimizes the model parameters with an instinctive process of subsetting and simulation (Krivoruchko, 2012; Konstantin Krivoruchko, 2012; Mainuri and Owino, 2017; Pellicone et al., 2018; Uddin et al., 2020a). A few researchers have revealed that the EBK technique is more reliable for predicting unknown grid values with minimum errors (Antal et al., 2021; Gupta et al., 2017; K Krivoruchko, 2012; Mainuri and Owino, 2017; Payblas,2018;; Uddin et al., 2020a). Unlike other kriging approaches, the EBK generates the unknown points prediction values considering model uncertainty while other kriging techniques predict unknown value using the semivariogram of known data points (ESRI, 2016, 2007; Gupta et al., 2017; Kumari et al., 2018). Consequently, the EBK estimates prediction outputs more accurately than other kriging methods (Gupta et al., 2017; Mainuri and Owino, 2017; Payblas,2018. Several studies have successfully applied the EBK technique for predicting unknown locations data and analysis of prediction data uncertainty (Acharya and Panigrahi, 2016; Çaldırak and Kurtuluş, 2018; Gunarathna et al., 2016; Hussain et al., 2016; Kumari et al., 2018; Pandey et al., 2015; Payblas,2018; Pellicone et al., 2018). The empirical semivariogram was calculated using the following equation;

$$\gamma\,(h \pm \delta) = \frac{1}{2|N(h \pm \delta|} \sum_{(i,j)\in N(h\pm\delta)} \left|z_i - z_j\right|^2 \qquad (9)$$

where h is the distance between unkown points, δ is the tolerance range between points, and N(h ± δ) is a set of points $N(h\ \pm\ \delta) \equiv \{(S_{i,}S_j): |S_iS_j| = h \pm \delta; i,j =$

$1,2, \ldots, N\}$. The $|z_i - z_j|^2$ are the squared variances between observations. The squared variances are added and normalized by the natural number N (h ± δ). The empirical transformation function was employed to predict the probability distribution of the aggregation value of the WQI model.

In this research, all interpolation techniques were performed using the Geostatistical tool from ArcGIS Pro 2.9.2 and other relevant statistical analysis and graphical presentations have been carried out using the R programming language on R Studio.

5.4 Methods and materials

5.4.1 Data obtaining process

For the purposes of this study, the water-quality data was obtained from 29 monitoring sites out of 32 across the Cork Harbour monitoring data in the year 2020. Details of the monitoring sites are illustrated in Figure 1. Typically, the Irish Environmental Protection Agency (EPA) monitors the water quality of Cork Habour frequently. In this study, water-quality data was considered at one-meter below water surface at approximately high and low tides over the year. In order to calculate WQI values, in total 11 water-quality parameters were obtained from the EPA water quality-monitoring database of Cork Harbour. These were temperature (TEMP), pH, dissolved oxygen (DOX), salinity (SAL), ammonia (AMN), total organic nitrogen (TON), ammoniacal nitrogen (AMN), molybdate reactive phosphorus (MRP), biological oxygen demand (BOD), transparency (TRAN), and Chlorophyll a (CHL). Details of the data can be found at the following web resource: www.catchments.ie/data. These parameters were selected for this study based on the availability of variables in the monitoring database and taking account of the spatial distribution of monitoring sites.

To evaluate the performance of the geocomputational model, the present study used four evaluation criteria of the CV technique: (i) root mean square error (RMSE), (ii) mean absolute error (MAE), (iii) mean square error (MSE), and (iv) coefficient of determination (R2). Recently, several studies have utilized this technique to compare performance among geocomputational interpolation methods (Adhikary and Dash, 2017; Amini et al., 2019; Antal et al., 2021; Bronowicka-Mielniczuk et al., 2019; Farzaneh et al., 2022; McManus et al., 2020, 2021; Rahman et al., 2013; Rahman & Harding, 2016; Xie et al., 2011). In this research, a 10-fold cross-validation (CV) technique was applied to calculate the evaluation criteria. Details technique can be found in Xiong et al., (2020). Except for R2, the performance criteria expect a predictive model's performance to be as small as possible (Al-Mamoori et al., 2021). In general, the R2 value refers to how well the models fit with the model inputs and predicted data (Uddin et al., 2022c; Wu et al., 2019). It is expected to be close to 1 (He et al., 2015). Model evaluation criteria are measured as follows:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \quad (10)$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \quad (11)$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \quad (12)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \hat{y})^2} \quad (13)$$

where $y_i$and $\hat{y}$are the ith observed and mean of the predicted values, respectively. n is the number of observations.

5.5.2 Prediction uncertainty analysis

For the purposes of uncertainty analysis in water quality models, several techniques are used, such as Monte Carlo simulation, ML algorithms, etc. In approaching a geospatial model, several studies have used the prediction standard errors (PSEs) technique by performing the geocomputational-interpolation method (Antal et al., 2021). In this study, the UK model was used to calculate the PSE in various interpolation models, and excellent prediction performance was found for the UK interpolation model. For the analysis of prediction uncertainties, predicted WQI scores of each interpolation technique were used to calculate the PSE by implementing the optimized hyper-parameter settings of the UK model. The details of the hyper-parameters of the UK can be found in Table 3. Figure 11 presents the uncertainty results of the WQI scores obtained from the various interpolation models.

5.5.3 Model suitability analysis

The suitable model was identified by comparing all interpolation models using the Tylor diagram. This technique is commonly used to compare various methods, techniques, or models in terms of data deviation. It is effective to identify an appropriate model because it allows three statistical measures, including the correlation between observations and predictions, the root-mean-square deviation (RMSD), and their standard deviations (SD), which help in understanding model reliability (Calim et al., 2018). Recently, a few studies have utilized this technique to select the best performer (Seifi et al., 2020; Xu et al., 2016). Figure 12 compares the summary statistics for various geospatial prediction techniques.

5.6 Results and discussion

5.6.1 Descriptive assessment of water quality

The general characteristics of the studied physicochemical parameters and the statistical relationship among them are summarized and visualized in Table 1 and in Figure 3. The surface water temperature varied between 13.90°C and 16.90°C with a mean value of 15.58 ± 0.74°C (Table 1). The maximum and minimum water pH was observed to be 8.33 and 7.6 with a mean value of 8.00 ± 0.23 while the range of salinity varied from 0.83 to 30.10 PSU with a mean value of 16.87 ± 12.00 PSU (Table 1). Water transparency was found within the guideline value of greater than 1 m/depth (Table 1) and showed significant positive association with water pH ($r = 0.60$, $p < 0.01$) (Fig. 3). The highest concentration of DOX (136.17 % sat) exceeded the upper standard threshold value while minimum (69.33 % sat) and mean (107.90 % sat) concentration of DOX were found within the prescribed limit (Table 1) and the DOX were significantly correlated with water pH ($r = 0.86$, $p < 0.01$) (Fig. 3), which was previously well documented by Hoque et al. (2015).

Table 1. Descriptive statistics of water quality parameter in Cork Harbour.

Parameter	Unit	Min.	Max.	Mean	SD	Variance	Skewness	Kurtosis	Standard threshold*	
									Lower	Upper
Temp.	˚C	13.9	16.90	15.58	0.74	0.54	-0.36	0.01	-	25
pH	-	7.60	8.33	8.00	0.23	0.05	-0.22	-1.55	5	9
TRAN	m/depth	0.00	5.60	1.57	1.5	2.17	1.00	1.05	> 1	-
DOX	% sat	69.3	136	108	15.2	230.52	-0.18	0.18	72	128
BOD	mg/l	0.00	3.55	1.74	0.87	0.76	-0.27	0.17	0	7

DIN	mg/l	0.04	6.02	1.54	1.78	3.18	1.18	0.39	0.0	1.20
TON	mg/l as N	0.00	6.00	1.47	1.78	3.19	1.21	0.49	0.0	2
MRP	mg/l as P	0.01	0.06	0.02	0.01	0.00	2.13	5.91	0.0	0.05
AMN	mg/l	0.02	0.26	0.07	0.05	0.003	1.89	3.92	0	1.5
CHL	mg/m3	1.00	10.4	5.32	3.2	10.36	0.29	-1.53	0.0	14.2

* EPA (2001)

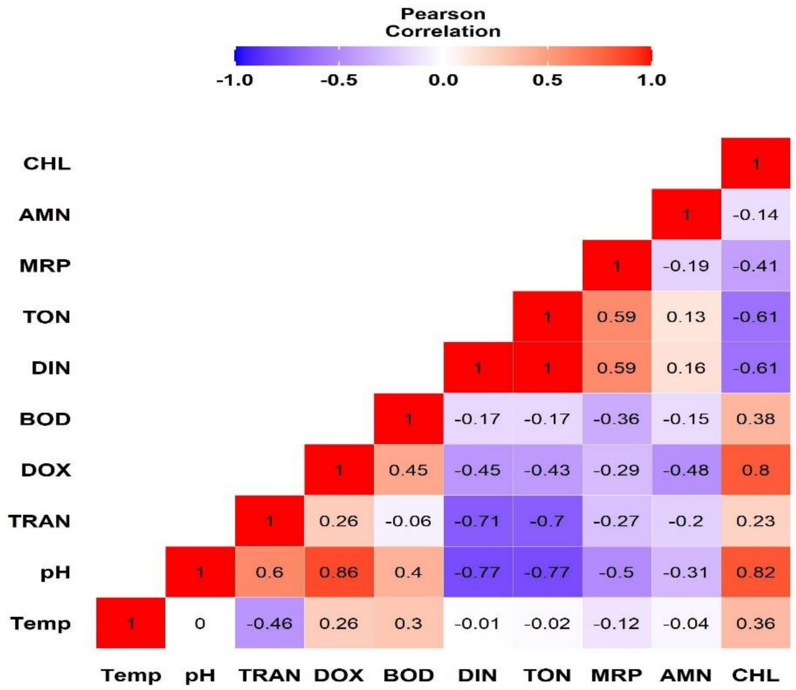


Fig. 3. Correlation between water quality parameters in Cork Harbour.

Concentration of BOD in the harbour was found with a mean value of 1.74 ± 0.87 mg/l, which was below that of upper threshold level. Except DIN, mean concentration of TON (1.47 ± 1.78 mg/l), MRP (0.02 ± 0.01 mg/l), and AMN (0.07±0.05 mg/l) were found within the upper standard limit (Table 1). However, maximum concentration of TON (6.00 mg/l) and MRP (0.06 mg/l) exceeded the upper threshold level (Table 1). The DIN correlated positively with TON ($r = 1.00$, $p < 0.01$) whereas both parameters displayed significant negative correlation with water pH ($r = -0.77$, $p < 0.01$) and with TRAN ($r = -0.70$, $p < 0.01$) and significant moderate positive correlation with MRP ($r = 0.59$, $p < 0.01$) (Fig. 3). Concentration of CHL was found ranging from 1.00 mg/m3 to 10.43 mg/m3 with a mean value of 5.32 ± 3.22 mg/m3, which implied the concentration of CHL was within the guideline value (Table 1). The concentration of chlorophyll-a showed significant positive association with water pH ($r = 0.82$, $p <$

0.01) and with DOX (r = 0.80, p < 0.01) where significant negative correlation was found with DIN and TON (r = -0.61, p < 0.01) (Fig. 3).

5.6.2 Assessing water quality using WQI models

The WQI is a widely used tool to assess water quality by the simple mathematical transformation of water quality data into numerical values. In this research, the WQI values were obtained from the WQM-WQI model. The WQI values ranged from 33 to 73, with an average of 56.19. Figure 4 shows the WQI and water quality status in Cork Harbour during the study period, respectively. As can be seen from

Table 2. Proposed new classification scheme for assessing coastal water quality using WQI model (Uddin et al., 2022).

Classification scheme	Range of score
(i) Good	80-100
(ii) Fair	50-79
(iii) Marginal	30-49
(iv) Poor	0-29

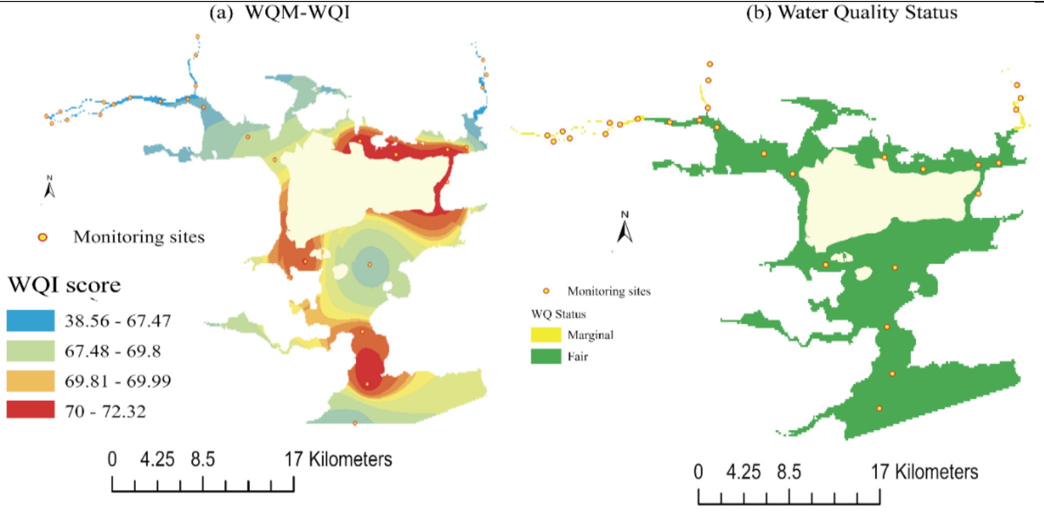


Fig. 4. Water quality in Cork Harbour: (a) WQM-WQI values and (b) water quality status over the study period.

Figure 4a, higher WQI values were found at the lower and outer monitoring sites in Cork harbour, while the lowest WQI values were obtained for the upper monitoring sites in the Harbour (Fig. 4a). Once the WQI values were obtained, the water quality was classified using the WQM water quality classification scheme (Table 2). As seen in Figure 4b, the WQM evaluated two water quality classes. These varied from "marginal" to "fair". The marginal class water quality was evaluated in the upper Lee estuary and the upper part of the river Owenacurra (Midleton). The past decade has seen an increase in the use of the effluent treatment plant (ETPs) in this area. Consequently, the ETPs can contribute to raw wastewater discharges into the estuary directly without treatment (Hartnett and Nash, 2015). As a result, it is expected that the water quality in the upper part of the Harbour's had depleted due to the overloaded wastewater and this might have also contributed to this trend. The remaining part of the Harbour was dominated by the "fair" water quality over the study period (Fig. 4b). These results reflect those of Uddin et al., (2022a) and Wall et al., (2020); both studies also found similar water states in Cork Harbour.

5.6.3 Comparison of geostatistical perdition models

In this research, eight interpolation models, including four commonly used deterministic geocomputational-interpolation methods (LPI, GPI, RBF, and IDW) and four advanced geostatistical (EBK, SK, UK, and DK) models, were utilised to identify the best geocomputational technique for predicting WQI values. Figure 6 presents the predicted WQIs spatial distribution in Cork Habour for various geostatistical prediction models. For the purposes of model evaluation, the present study used the CV approaches to optimise the hyper-parameters of the predictive model. Table 3 provides the list of optimized hyper-parameters for eight geocomputational models. In order to evaluate the prediction performance, the present study utilized four evaluation metrics, including RMSE, MSE, MAE, and R2, which indicate the model prediction (Antal et al., 2021; Uddin et al., 2018).

Table 3. Optimized hyper-parameters of various geocomputational prediction models.

Hyper-parameters	Geostatistical prediction models							
	EBK	SK	UK	DK	LPI	GPI	IDW	RBF
(i) Model settings								
Output	Prediction	prediction	prediction	prediction	predicti on	predict ion	predict ion	predict ion
subset size	100	100	100	-	100	-	-	-
Power	-	-	-	-	1	2	2	-
overlap factor	1	1	1	-	1	-	-	-
Number of simulation	1000	1000	1000	-	1000	-	-	-
Number of simulation	1000	1000	-	-	-	-	-	-
(ii) Transformation	Empirical	normal score	-	normal score		-	-	-

approximation	-	density Skew	-	density Skew		-	-	-
Kernels	Exponential	-	-	8	Exponential	-	-	CRP*
base distribution	-	Empirical	-	Student's t-distribution		-	-	-
(iii) Neighborhood searching type	standard circular	standard	standard		standard	-	standard	standard
Neighbors to include	15	5	5	5	1000	-	15	15
Include at least	10	2	2	2	10	-	10	10
Sector type	full	4 and 45 degree	4 and 45 degree	5 and 45 degree	full	-	full	full
Major semiaxis	-	14374.34	9541.8	-	10046.94	-	11588	11588
Minor semiaxis	-	14374.34	9541.8	-	10046.94	-	11588	11588
radius	16510.28	-	-	-	-	-	-	-
Angle	-	0	0	-	0		0	0
(iv) Variogram	-	covariance	semivariogram	covariance	-	-	-	-
number of lags	-	12	12	12	-	-	-	-
lag size	-	1647.17	1091.93	1,766.94	-	-	-	-
Nugget	-	0	27.14	0	-	-	-	-
(v) Model type	-	stable	stable	stable	-	-	-	-
parameter	-	1.075	2	0.7941	-	-	-	0.0031
partial sill	-	1.18	112.97	0.9725	-	-	-	-
Anisotropy	-	No	No	No	-	-	-	-
range	-	14374.34	9541.8	14399.2	-	-	-	-

*Completely Regularized Spline

Figure 5 presents the CV results of various interpolation models. The lower prediction errors were found for the all geocomputational models. Compared to four geostatistical models, robust performance was shown by the UK (RMSE = 6.0, MSE = 0.0, and MAE = 4.3) and the EBK models (RMSE = 6.2, MSE = 0.0, and MAE = 4.6), respectively, whereas the remaining two, DK and SK, also well performed to predict WQI values. On the other hand, all deterministic models (GPI, IDW, LPI, and RBF) including the widely used IDW technique also had higher prediction errors in this study. A similar finding was also investigated by Adhikary and Dash, (2017). Her finding revealed that the UK method outperformed when predicting water quality. It can be seen from Figure 5 that higher RMSE, MSE, and MAE were obtained for those models. Surprisingly, the IDW and RBF methods had the highest prediction errors among the most popular techniques (Fig. 5). These findings are in line with previous research, which found similar results for the LPI, GPI, IDW, and RBF methods (Antal et al., 2021).

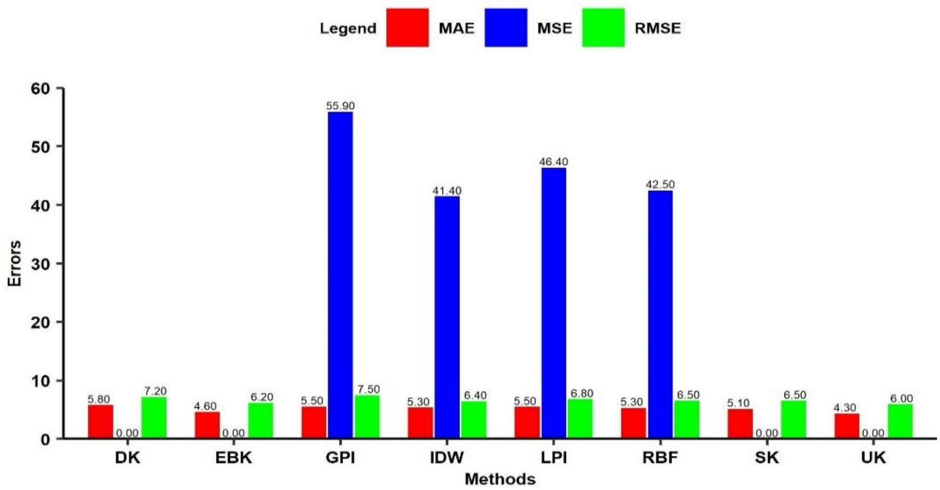


Fig. 5. Cross-validation results of various geostatistical prediction model.

As shown in Figure 6, all geocomputational-interpolation models produced similar spatial distribution patterns of predicted WQIs except the LPI and GPI methods. Even though all prediction models predicted higher WQI values in the upper and outer part of the Harbour, those models (LPI and GPI) differ from others (Fig. 6f; Fig. 6g). The GPI model predicted the higher WQIs in the lower-eastern part of the Harbour (Fig. 6g), whereas the LPI showed a completely different pattern of spatial distribution of WQIs in the Harbour (Fig. 6f). Moreover, the present study utilized the coefficient of determination for assessing the relationship between model predictors and response. Figure 7 presents the scatter plots of actual and predicted WQI values. Based on the results of R2, a strong relationship between the actual and predicated WQI values was observed for all models except the RBF technique (R2 = 0.51). This finding is contrary to previous studies, which have suggested that the RBF model performed the best in predicting river water quality (Wu et al., 2019).

To validate the model performance, a comparison scenario was generated between actual and predicted WQI values for each deterministic and geostatistical model. Figure 8 provides a comparison overview between predicted and actual WQI values at each monitoring site in Cork harbour. As can be seen from Figure 8, all models performed well in this study, but they did not accurately predict WQI at each point. Comparison results of each site indicate that all the models followed the trend to the actual WQI values, whereas a slight difference was observed in the outer Harbour monitoring sites.

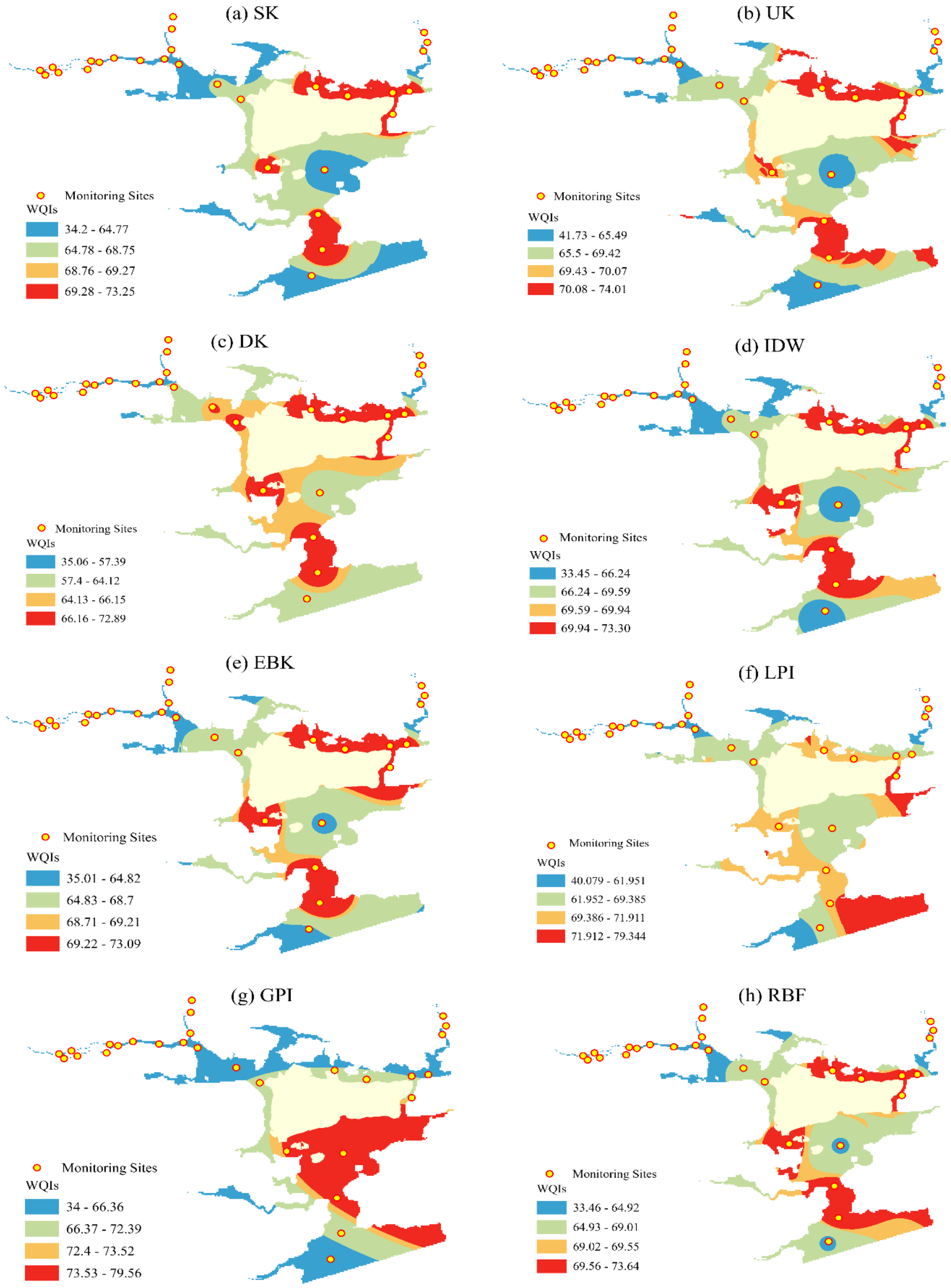


Fig. 6. Spatial distribution of WQI in Cork Harbour; maps obtained from various geocomputational prediction models.

Figure 9 presents a comparative result of various statistical measures for the predicted and actual WQIs in boxplots. In Figure 9a, boxplots show the deterministic interpolation methods are different from the geostatistical techniques in several statistical measures. It can be seen from that the predicted mean and median values differ for each group, whereas similar statistical measures were found for the UK methods when comparing actual statistics. Figure 9b shows the cumulative distribution function (CDF) of the eight methods. The CDF results indicate that 98% of monitoring sites were predicted correctly except the UK methods.

However, it is very hard to determine the best method using CV and R2 analysis. Hence, Turkey's HSD analysis was performed for the purposes of comparing among interpolation methods. Recently, several studies have utilized this technique to identify the unique method from groups by comparing overall and pairwise aspects (Nanda et al., 2021; Rouder et al., 2016). Figure 10 presents the multiple comparison results of pair-wise various deterministic and geostatistical models with a 95% CI from Tukey's HSD. The results of the Tukey's HSD indicate that there were no statistically significant differences among methods at $p < 0.05$.

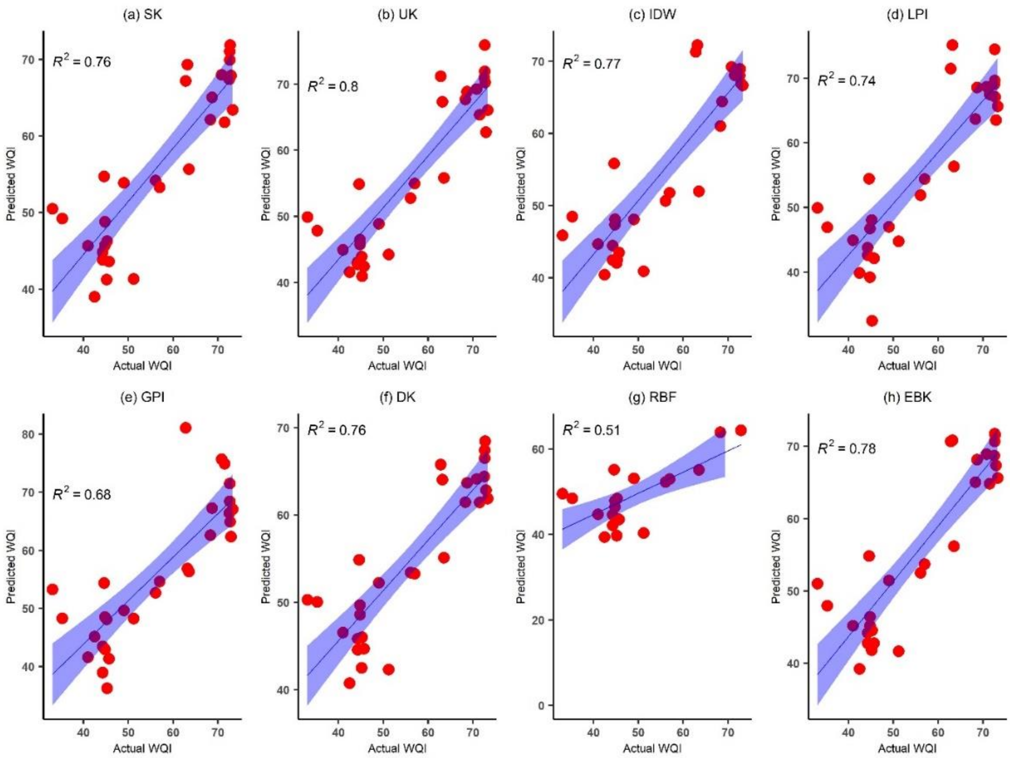


Fig. 7. Scatter plots of actual vs predicted WQI scores based on the model testing dataset of different geocomputational prediction models.

5.6.4 Evaluation of uncertainty of geocomputational-interpolation models

For real-world applications, model uncertainty is a major concern. All models, including prediction models, contain inherent uncertainties (Antal et al., 2021; Farrance and Frenkel, 2012; Seifi et al., 2020) and therefore it is critical to figure out how much data variance the model contains. It is essential to understand the level of uncertainty in the modelled spatial distribution of predicted WQIs in order to assess the reliability of prediction data for assessing water quality; otherwise, the predicted data can not reflect the actual water quality indicators. As a result, misinterpretation/wrong information can be transferred to water managers. In order to assess the prediction uncertainty of various interpolation techniques, the present study utilized the PSE value of the predicted WQIs of various interpolation techniques.

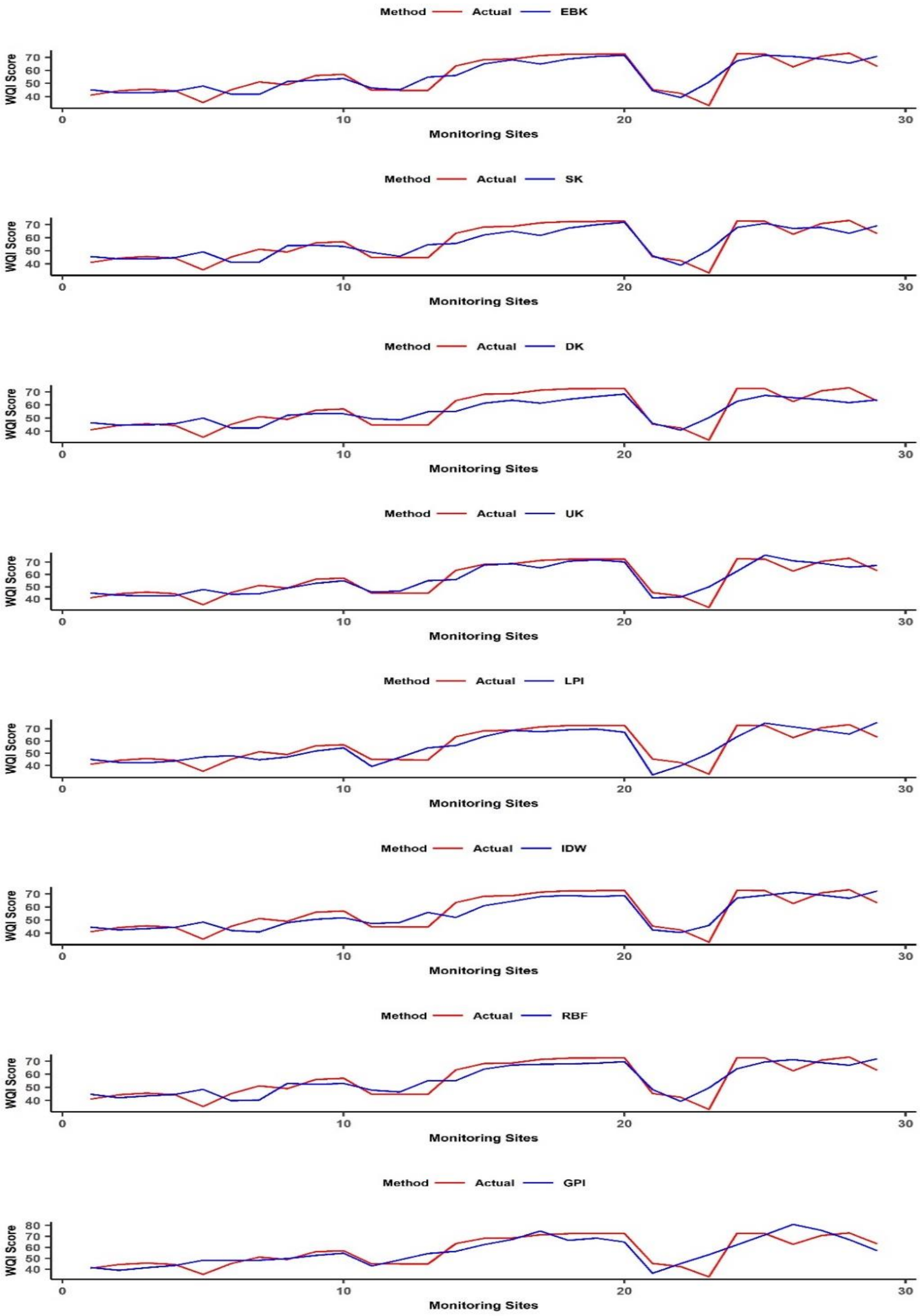


Fig. 8. Comparison of the model validation performance between predicted and actual WQI values at each monitoring sites.

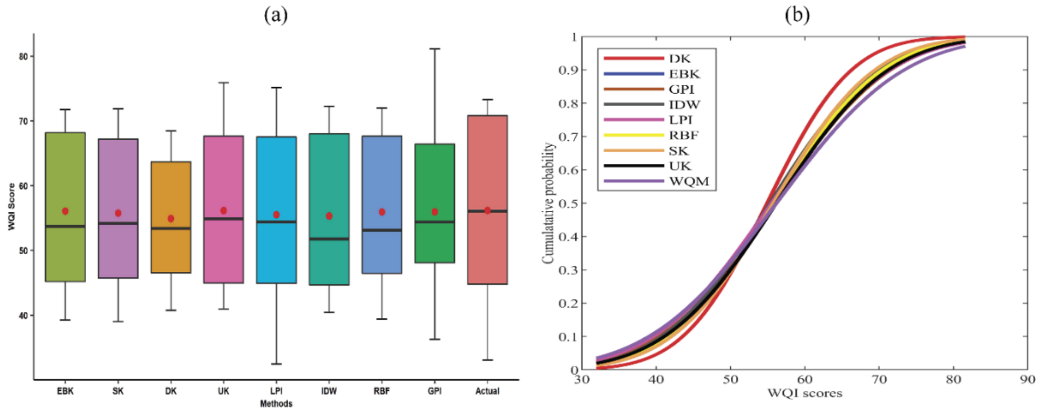


Fig. 9. Comparison of predicted WQI from various geocomputational models: (a) Boxplots show a comparison between actual and predicted WQI scores and (b) CDF comparison of predicted WQI scores of various techniques.

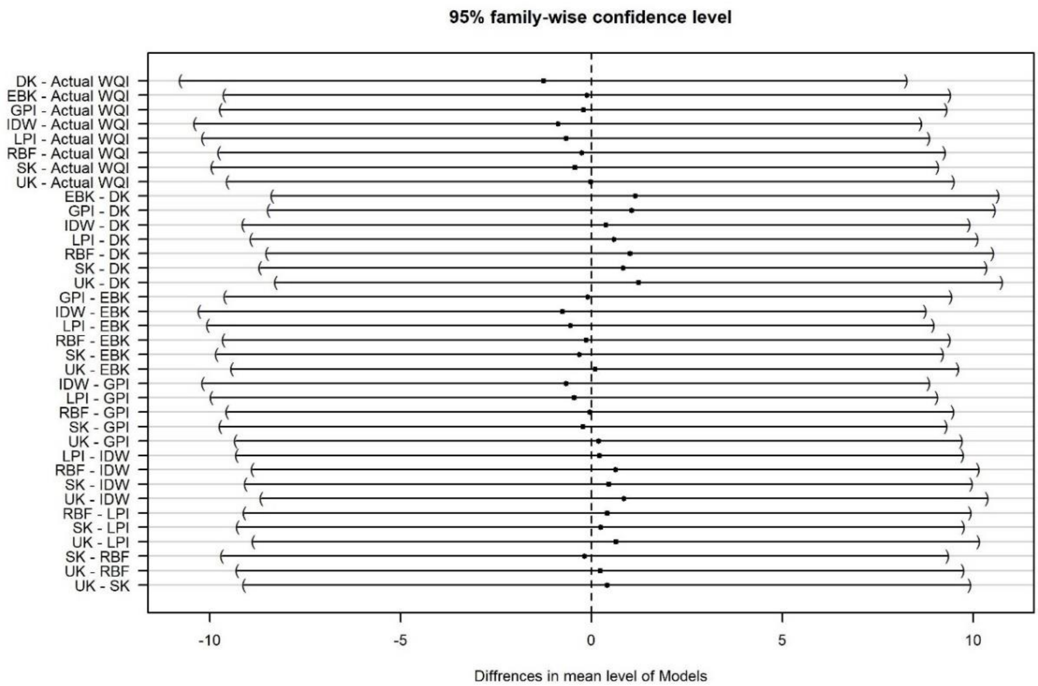


Fig. 10. Multiple comparison results of pair-wise geocomputational models with 95% CI from Tukey's HSD, the vertical dashed line indicates the point where the difference between the means is equal to zero or similarity of model statistics, the refers to the means are equal of both models.

As shown in Figure 11, all of interpolation models overestimated the WQIs in the outer part of the Harbour. In comparison of various geostatistical interpolation methods, the present study found small PSE (PSE: 0.67 to 8.64) for the EBK method (Fig. 11e), whereas the largest PSE (PSE: 2.62 to 12.9) was produced by the DK method (Fig. 11c). On the other hand, compared to the deterministic methods, the GPI model produced the highest interpolation PSE values; it ranged from 1.45 to 12.56 (Fig. 11g). Surprisingly, the LPI generated the lowest PSE values (0.16 to 7.03) while this technique showed poor prediction performance (RMSE= 6.8, MSR= 46.40, MAE = 5.5, and R2 = 0.74). Wang et al., (2014) reported that the LPI outperformed in estimating the spatial distribution of precipitation.

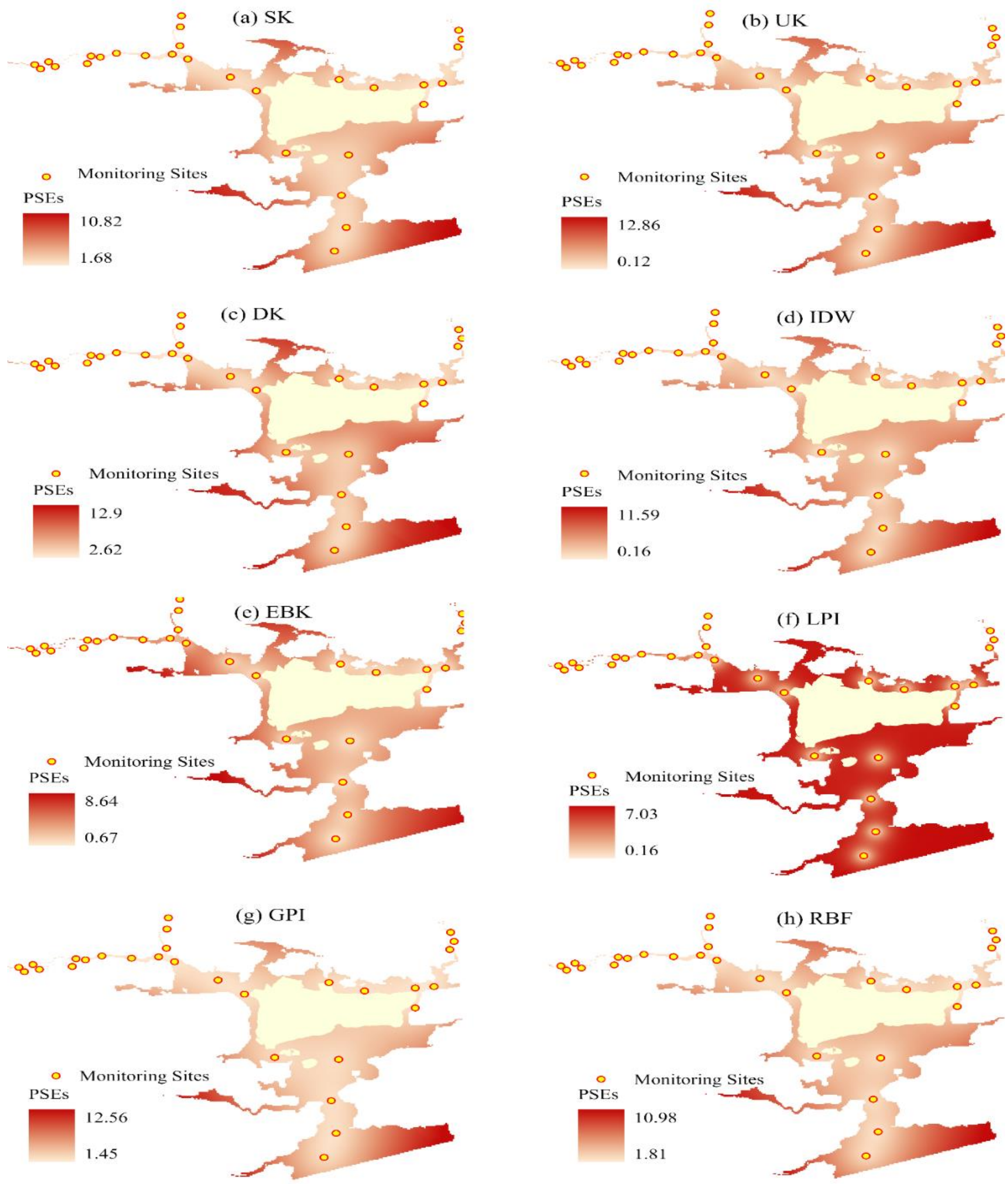


Fig. 11. WQIs prediction uncertainties of various geocomputational-interpolation models.

The comparison results of deterministic and geostatistical methods indicate that the geostatistical model could be effective to predict WQM-WQIs for coastal water quality. Similar results are in accord with recent studies indicating that the geostatistical interpolation model outperformed deterministic methods (Antal et al., 2021; Pellicone et al., 2018). Higher PSE values were generated in the outer Harbour of monitoring locations over the study period by all interpolation methods. The higher

PSE in the outer Harbour found may be due to the inadequate sampling locations (Antal et al., 2021; Borges et al., 2016). The results of uncertainties of various models reveals that the EBK model could be effective and reliable to predict spatial distribution of WQIs in Cork Harbour. The studies by Antal et al., (2021) and Al-Mamoori et al., (2021) both revealed that the EBK method is the best interpolation technique for spatial distribution analysis.

5.7 Comparison of model suitability for the prediction of WQIs

To identify the suitable model for predicting WQIs, Tylor diagram analysis was utilized in this research. Recently, this approach has been widely used to compare various methods/datasets/models in terms of data variances (Annapoorna et al., 2016 Xu et al., 2016). This technique is more effective in identifying the best model by comparing three-dimensional statistics, including centred root-mean-square deviation (RMSD), their standard deviations (SD), and correlation between predicted and actual values (Seifi et al., 2020). Figure 12 provides insight into how the model performed in terms of three statistical measures, where statistics were obtained from various interpolation techniques by using actual and predicted WQI values in Cork Harbour, respectively.

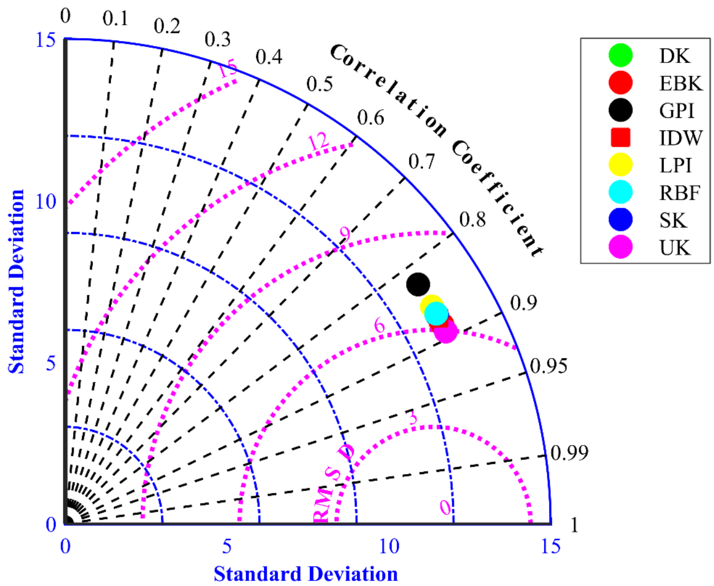


Fig. 12. Various geospatial predictive models comparison using Tylor diagram.

As seen in Figure 12, the GPI showed poor performance compared to other geocomputational-interpolation methods, whereas the remaining methods showed good agreement with statistical measures. The results from Tylor statistics indicate there were no statistically significant differences between models with $p < 0.05$.

However, the present study compared various geocomputational-interpolation methods using the cross-validation results and coefficient of determination analysis. To determine the best model in order to predict WQIs appropriately, CV results were utilized in this research. According to the CV results of interpolation models, the UK (RMSE = 6.0, MSE = 0.0, MAE = 4.30 and R2 = 0.8) and EBK (RMSE = 6.2, MSE = 0.0, MAE = 4.60, and R2 = 0.78) had the lowest prediction errors, respectively, compared to the other techniques. Results of the CV reveal that the UK method could be effective to interpolate the WQIs in Cork Harbour. This study also compared between actual and predicted WQIs of various geocomputational using Tukey's HSD test and Tylor diagram. The results of those tests revealed that there were no statistically significant differences between predicted and actual WQI values for all geocomputational predictive models, except for the deterministic GPI. But when comparing the CV and uncertainty results of the geocomputational-interpolation methods, the findings of this study suggest that the EBK method could be a useful technique for reducing the uncertainty in WQI spatial distribution analysis.

5.8 Conclusion

The aim of this research was to identify the best geocomputational-interpolation technique for predicting spatial distribution of WQIs by comparing various interpolation methods. To achieve this goal, eight widely used interpolation techniques (LPI, GPI, IDW, RBF, SK, UK, DK, and EBK) were performed in this study. Predictive models were validated using the cross-validation process. The key findings of this research are as follows:

- Geostatistical interpolation methods showed better performance than deterministic techniques.
- The CV results reveal that the UK and the EBK methods could be effective in predicting the spatial distribution of the WQIs, whereas these methods showed robust performance (RMSE = 6.0, MSE = 0.0, MAE = 4.3, and R2 = 0.8) and (RMSE = 6.2, MSE = 0.0, MAE = 4.6, and R2 = 0.78), respectively.

- Tukey's HSD family-wise multi-comparison results reveal there was no significant difference between predicted and actual WQIs among geocomputational models.
- Compared to the uncertainty of the spatial distribution of WQIs, the lowest PSE was found for the EBK, where PSE ranged from 1.01 to 13.31.

However, geospatial EBK predictive models could be effective to interpolate WQIs more precisely to reduce uncertainty in predicting WQIs. The findings of this research could be useful in predicting the geospatial distribution of WQIs more accurately in order to assess coastal water quality. Further studies should be carried out in order to validate the other geostatistical methods in terms of predicting WQIs. Although the conclusion of this study was drawn based on the findings of analysis it is critical to compare between the results of this study and findings of the literatures because most of the recent studies have only focused on surface (river, lakes) and groundwater quality whereas previous studies are limited to coastal water quality.

5.9 Declaration of Competing Interest

The authors state that there are no competing financial interests or personal relationships that influenced the work reported in this chapter.

5.10 Acknowledgments

This research was funded by the Hardiman Research Scholarship of the National University of Ireland, Galway, which funded the first author as part of his PhD program. The authors would like to thank the Environmental Protection Agency of Ireland for providing water quality data. The research was also supported by MaREI, the SFI Research Centre for Energy, Climate, and Marine and Ryan Institute, NUIG, Galway, Ireland. The authors also sincerely acknowledge Charles Sturt University for providing all necessary supports to this PhD project through the international co-supervision.

5.11 References

Abbasi, T., Abbasi, S., 2012. Water Quality Indices, Water Quality Indices. https://doi.org/10.1016/C2010-0-69472-7

Acharya, S.S., Panigrahi, M.K., 2016. Evaluation of factors controlling the distribution of organic matter and phosphorus in the Eastern Arabian Shelf: A geostatistical reappraisal. Cont. Shelf Res. https://doi.org/10.1016/j.csr.2016.08.001

Adhikary, P.P., Dash, C.J., 2017. Comparison of deterministic and stochastic methods to predict spatial variation of groundwater depth. Appl. Water Sci. 7, 339–348. https://doi.org/10.1007/s13201-014-0249-8

Al-Mamoori, S.K., Al-Maliki, L.A., Al-Sulttani, A.H., El-Tawil, K., Al-Ansari, N., 2021. Statistical analysis of the best GIS interpolation method for bearing capacity estimation in An-Najaf City, Iraq. Environ. Earth Sci. 80, 1–14. https://doi.org/10.1007/s12665-021-09971-2

Agarwal, B., Agarwal, A., Harjule, P., & Rahman, A. (2022a). Understanding the intent behind sharing misinformation on social media. Journal of Experimental and Theoretical Artificial Intelligence, 1-15. https://doi.org/10.1080/0952813X.2021.1960637

Agarwal, B., Rahman, A., Patnaik, S., & Poonia, R. C. (Eds.) (2022b). Proceedings of International Conference on Intelligent Cyber-Physical Systems. (Algorithms for Intelligent Systems). Springer. https://www.springer.com/gp/book/9789811671357.

Amini, M.A., Torkan, G., Eslamian, S., Zareian, M.J., Adamowski, J.F., 2019. Analysis of deterministic and geostatistical interpolation techniques for mapping meteorological variables at large watershed scales. Acta Geophys. 67, 191–203. https://doi.org/10.1007/s11600-018-0226-y

Antal, A., Guerreiro, P.M.P., Cheval, S., 2021. Comparison of spatial interpolation methods for estimating the precipitation distribution in Portugal. Theor. Appl. Climatol. 145, 1193–1206. https://doi.org/10.1007/s00704-021-03675-0

Attorre, F., Alfo, M., De Sanctis, M., Francesconi, F., Bruno, F., 2007. Comparison of interpolation methods for mapping climatic and bioclimatic variables at regional scale. Int. J. Climatol. 27, 1825–1843. https://doi.org/10.1002/JOC.1495

Bárdossy, A., Pegram, G., 2013. Interpolation of precipitation under topographic influence at different time scales. Water Resour. Res. 49, 4545–4565. https://doi.org/10.1002/WRCR.20307

Belete, D.M., Huchaiah, M.D., 2021. Grid search in hyperparameter optimization of machine learning models for prediction of HIV/AIDS test results. Int. J. Comput. Appl. https://doi.org/10.1080/1206212X.2021.1974663

Borges, P. de A., Franke, J., da Anunciação, Y.M.T., Weiss, H., Bernhofer, C., 2016. Comparison of spatial interpolation methods for the estimation of precipitation distribution in Distrito Federal, Brazil. Theor. Appl. Climatol. 123, 335–348. https://doi.org/10.1007/S00704-014-1359-9/FIGURES/9

Bronowicka-Mielniczuk, U., Mielniczuk, J., Obroślak, R., Przystupa, W., 2019. A Comparison of Some Interpolation Techniques for Determining Spatial Distribution of Nitrogen Compounds in Groundwater. Int. J. Environ. Res. 13, 679–687. https://doi.org/10.1007/s41742-019-00208-6

Çaldırak, H., Kurtuluş, B., 2018. Evidence of Possible Recharge Zones for Lake Salda (Turkey). J. Indian Soc. Remote Sens. https://doi.org/10.1007/s12524-018-0779-x

Calim, M.C., Nobre, P., Oke, P., Schiller, A., Siqueira, L.S.P., Castelão, G.P., 2018. A new tool for model assessment in the frequency domain – Spectral Taylor Diagram: application to a global ocean general circulation model with tides. Geosci. Model Dev. https://doi.org/10.5194/gmd-2018-5

Carsten Von Der Ohe, P., Prüß, A., Schäfer, R.B., Liess, M., De Deckere, E., Brack, W., 2007. Water quality indices across Europe - A comparison of the good ecological status of five river basins. J. Environ. Monit. 9, 970–978. https://doi.org/10.1039/b704699p

Emadi, M., Baghernejad, M., 2014. Comparison of spatial interpolation techniques for mapping soil pH and salinity in agricultural coastal areas, northern Iran. Arch. Agron. Soil Sci. 60, 1315–1327. https://doi.org/10.1080/03650340.2014.880837

Das, S., Rahman, A., Ahamed, A., & Rahman, S. T. (2018). Multi-level models can benefit from minimizing higher-order variations: an illustration using child malnutrition data. Https://Doi.Org/10.1080/00949655.2018.1553242, 89(6), 1090–1110. https://doi.org/10.1080/00949655.2018.1553242

EPA, 2017. Urban Waste Water Treatment, Official Journal of the European Union.

ESRI, 2016. How inverse distance weighted interpolation works—Help | ArcGIS for Desktop [WWW Document]. ARCMAP.

ESRI, 2007. How Inverse Distance Weighted (IDW) interpolation works. ArcGIS 9.2 Deskt. Help.

ESRI, n.d. How global polynomial interpolation works—ArcGIS Pro | Documentation [WWW Document]. URL https://pro.arcgis.com/en/pro-app/2.7/help/analysis/geostatistical-analyst/how-global-polynomial-interpolation-works.htm (accessed 4.9.22a).

ESRI, n.d. Understanding universal kriging—ArcGIS Pro | Documentation [WWW Document]. URL https://pro.arcgis.com/en/pro-app/2.7/help/analysis/geostatistical-analyst/understanding-universal-kriging.htm (accessed 4.9.22b).

Farrance, I., Frenkel, R., 2012. Uncertainty of measurement: A review of the rules for calculating Uncertainty components through functional relationships. Clin. Biochem. Rev. 33, 49–75.

Farzaneh, G., Khorasani, N., Ghodousi, J., Panahi, M., 2022. Application of geostatistical models to identify spatial distribution of groundwater quality parameters. Environ. Sci. Pollut. Res. https://doi.org/10.1007/s11356-022-18639-8

Gunarathna, M.H.J.P., Nirmanee, K.G.S., Kumari, M.K.N., 2016. Are geostatistical interpolation methods better than deterministic interpolation methods in mapping salinity of groundwater? Int. J. Res. Innov. Earth Sci.

Gupta, A., Kamble, T., Machiwal, D., 2017. Comparison of ordinary and Bayesian kriging techniques in depicting rainfall variability in arid and semi-arid regions of north-west India. Environ. Earth Sci. https://doi.org/10.1007/s12665-017-6814-3

Gupta, S., Gupta, S.K., 2021. A critical review on water quality index tool: Genesis, evolution and future directions. Ecol. Inform. 63, 101299. https://doi.org/10.1016/j.ecoinf.2021.101299

Han, H., Lee, K.H., Jeon, Y., Yoon, J.W., 2020. Comparison of various interpolation techniques to infer localization of audio files using ENF signals. Proc. - 2020 Int. Conf. Softw. Secur. Assur. ICSSA 2020 46–51. https://doi.org/10.1109/ICSSA51305.2020.00015

Hartnett, M., Nash, S., 2015. An integrated measurement and modeling methodology for estuarine water quality management. Water Sci. Eng. 8, 9–19. https://doi.org/10.1016/j.wse.2014.10.001.

Harjule, P., Rahman, A., & Agarwal, B. (2021). A cross-sectional study of anxiety, stress, perception and mental health towards online learning of school children in India during COVID-19. Journal of Interdisciplinary Mathematics, 24(2), 411–424. https://doi.org/10.1080/09720502.2021.1889780

He, X., Gou, W., Liu, Y., Gao, Z., 2015. A Practical Method of Nonprobabilistic Reliability and Parameter Sensitivity Analysis Based on Space-Filling Design 2015.

Hock, R., 2003. Temperature index melt modelling in mountain areas. J. Hydrol. 282, 104–115. https://doi.org/10.1016/S0022-1694(03)00257-9

Hoque, M.M., Mustafa Kamal, A.H., Idris, M.H., Ahmed, O.H., Saifullah, A.S.M., Billah, M.M., 2015. Status of some fishery resources in a tropical mangrove estuary of Sarawak, Malaysia. Mar. Biol. Res. https://doi.org/10.1080/17451000.2015.1016970

Hussain, M.M., Bari, S.H., Tarif, M.E., Rahman, M.T.U., Hoque, M.A., 2016. Temporal and spatial variation of groundwater level in Mymensingh district, Bangladesh. Int. J. Hydrol. Sci. Technol. https://doi.org/10.1504/IJHST.2016.075587

Jalili Pirani, F., Modarres, R., 2020. Geostatistical and deterministic methods for rainfall interpolation in the Zayandeh Rud basin, Iran. Hydrol. Sci. J. 65, 2678–2692. https://doi.org/10.1080/02626667.2020.1833014

Javed, S., Ali, A., Ullah, S., 2017. Spatial assessment of water quality parameters in Jhelum city (Pakistan). Environ. Monit. Assess. 189. https://doi.org/10.1007/s10661-017-5822-9

Juwana, I., Muttil, N., Perera, B.J.C., 2016. Uncertainty and sensitivity analysis of West Java Water Sustainability Index - A case study on Citarum catchment in Indonesia. Ecol. Indic. 61, 170–178. https://doi.org/10.1016/j.ecolind.2015.08.034

Kärnä, T., Baptista, A.M., 2016. Evaluation of a long-term hindcast simulation for the Columbia River estuary. Ocean Model. 99, 1–14. https://doi.org/10.1016/j.ocemod.2015.12.007

Kawo, N.S., Karuppannan, S., 2018. Groundwater quality assessment using water quality index and GIS technique in Modjo River Basin, central Ethiopia. J. African Earth Sci. 147, 300–311. https://doi.org/10.1016/J.JAFREARSCI.2018.06.034

Khouni, I., Louhichi, G., Ghrabi, A., 2021. Use of GIS based Inverse Distance Weighted interpolation to assess surface water quality: Case of Wadi El Bey, Tunisia. Environ. Technol. Innov. 24, 101892. https://doi.org/10.1016/j.eti.2021.101892

Krivoruchko, K, 2012. Empirical Bayesian Kriging. ESRI Press.

Krivoruchko, Konstantin, 2012. Empirical Bayesian Kriging Implemented in ArcGIS Geostatistical Analyst. ArcUser.

Kumar, A., Bojjagani, S., Maurya, A., Kisku, G.C., 2022. Spatial distribution of physicochemical-bacteriological parametric quality and water quality index of Gomti River, India. Environ. Monit. Assess. 194. https://doi.org/10.1007/S10661-022-09814-Y

Kumari, M.K.N., Sakai, K., Kimura, S., Nakamura, S., Yuge, K., Gunarathna, M.H.J.P., Ranagalage, M., Duminda, D.M.S., 2018. Interpolation methods for groundwater quality assessment in tank cascade landscape: A study of ulagalla cascade, Sri Lanka. Appl. Ecol. Environ. Res. https://doi.org/10.15666/aeer/1605_53595380

Liu, D., Zhao, Q., Fu, D., Guo, S., Liu, P., Zeng, Y., 2020. Comparison of spatial interpolation methods for the estimation of precipitation patterns at different time scales to improve the accuracy of discharge simulations. Hydrol. Res. 51, 583–601. https://doi.org/10.2166/NH.2020.146

Luo, W., Taylor, M.C., Parker, S.R., 2008. A comparison of spatial interpolation methods to estimate continuous wind speed surfaces using irregularly distributed data from England and Wales. Int. J. Climatol. 28, 947–959. https://doi.org/10.1002/JOC.1583

Madhloom, H.M., Al-Ansari, N., Laue, J., Chabuk, A., 2018. Modeling spatial distribution of some contamination within the lower reaches of Diyala river using IDW interpolation. Sustain. 10. https://doi.org/10.3390/su10010022

Mainuri, Z.G., Owino, J.O., 2017. Spatial Variability of Soil Aggregate Stability in a Disturbed River Watershed. Eur. J. Econ. Bus. Stud. https://doi.org/10.26417/ejes.v9i1.p278-290

McManus, S., Rahman, A., Coombes, J., & Horta, A. (2021). Uncertainty assessment of spatial domain models in early stage mining projects – A review. Ore Geology Reviews, 133, 104098. https://doi.org/10.1016/J.OREGEOREV.2021.104098

McManus, S., Rahman, D. A., Coombes, D. J., & Horta, D. A. (2021). Comparison of interpretation uncertainty in spatial domains using portable x-ray fluorescence and ICP data. Applied Computing and Geosciences, 12, 100067. https://doi.org/10.1016/J.ACAGS.2021.100067

McManus, S., Rahman, A., Horta, A., & Coombes, J. (2020). Applied Bayesian Modeling for Assessment of Interpretation Uncertainty in Spatial Domains. Statistics for Data Science and Policy Analysis, 3–13. https://doi.org/10.1007/978-981-15-1735-8_1

Meng, Q., Liu, Z., Borders, B.E., 2013. Assessment of regression kriging for spatial interpolation – comparisons of seven GIS interpolation methods. Cartogr. Geogr. Inf. Sci. 40, 28–39. https://doi.org/10.1080/15230406.2013.762138

Murphy, R.R., Curriero, F.C., Ball, W.P., 2010. Comparison of Spatial Interpolation Methods for Water Quality Evaluation in the Chesapeake Bay. J. Environ. Eng. 136, 160–171. https://doi.org/10.1061/(asce)ee.1943-7870.0000121

Muzenda, F., Masocha, M., Misi, S.N., 2019. Groundwater quality assessment using a water quality index and GIS: A case of Ushewokunze Settlement, Harare, Zimbabwe. Phys. Chem. Earth, Parts A/B/C 112, 134–140. https://doi.org/10.1016/J.PCE.2019.02.011

Nanda, A., Mohapatra, D.B.B., Mahapatra, Abikesh Prasada Kumar, Mahapatra, Abiresh Prasad Kumar, Mahapatra, Abinash Prasad Kumar, 2021. Multiple comparison test by Tukey's honestly significant difference (HSD): Do the confident level control type I error. Int. J. Stat. Appl. Math. 6, 59–65. https://doi.org/10.22271/maths.2021.v6.i1a.636

Nash, S., Hartnett, M., Dabrowski, T., 2011. Modelling phytoplankton dynamics in a complex estuarine system. Proc. Inst. Civ. Eng. - Water Manag. 164, 35–54. https://doi.org/10.1680/wama.800087

Nikitin, A., Tregubova, P., Shadrin, D., Matveev, S., Oseledets, I., Pukalchik, M., 2021. Regulation-based probabilistic substance quality index and automated geo-spatial modeling for water quality assessment. Sci. Reports 2021 111 11, 1–14. https://doi.org/10.1038/s41598-021-02564-w

Oliver, M.A., 1991. Disjunctive Kriging - an Aid to Making Decisions on Environmental Matters. Area 23, 19–24.

Pandey, P.C., Kumar, P., Tomar, V., Rani, M., Katiyar, S., Nathawat, M.S., 2015. Modelling spatial variation of fluoride pollutant using geospatial approach in the surrounding environment of an aluminium industries. Environ. Earth Sci. https://doi.org/10.1007/s12665-015-4563-8

Payblas, C., 2018,. Evolution of Ground Water Quality and Source Tracking of Nitrate Contamination in the Seymour Aquifer of Texas. Boller Rev. https://doi.org/10.18776/tcu/br/3/86

Parween, S., Siddique, N.A., Mahammad Diganta, M.T., Olbert, A.I., Uddin, Md.G., 2022. Assessment of urban river water quality using modified NSF water quality index model at Siliguri city, West Bengal, India. Environmental and Sustainability Indicators 16, 100202. https://doi.org/10.1016/j.indic.2022.100202

Pellicone, G., Caloiero, T., Modica, G., Guagliardi, I., 2018. Application of several spatial interpolation techniques to monthly rainfall data in the Calabria region (southern Italy). Int. J. Climatol. https://doi.org/10.1002/joc.5525

Rahman, A., Harding, A., Tanton, R., & Liu, S. (2013). Simulating the characteristics of populations at the small area level: New validation techniques for a spatial microsimulation model in Australia. Computational Statistics & Data Analysis, 57(1), 149–165. https://doi.org/10.1016/J.CSDA.2012.06.018

Rahman, A., & Harding, A. (2016). Small area estimation and microsimulation modeling. Small Area Estimation and Microsimulation Modeling, 1–521. https://doi.org/10.1201/9781315372143

Rahman, A., (2020). Statistics for Data Science and Policy Analysis. In Statistics for Data Science and Policy Analysis. Springer Singapore. https://doi.org/10.1007/978-981-15-1735-8

Rouder, J.N., Engelhardt, C.R., McCabe, S., Morey, R.D., 2016. Model comparison in ANOVA. Psychon. Bull. Rev. 23, 1779–1786. https://doi.org/10.3758/s13423-016-1026-5

Seifi, A., Dehghani, M., Singh, V.P., 2020a. Uncertainty analysis of water quality index (WQI) for groundwater quality evaluation: Application of Monte-Carlo method for weight allocation. Ecol. Indic. 117, 106653. https://doi.org/10.1016/j.ecolind.2020.106653

Seifi, A., Dehghani, M., Singh, V.P., 2020b. Uncertainty analysis of water quality index (WQI) for groundwater quality evaluation: Application of Monte-Carlo method for weight allocation. Ecol. Indic. 117, 106653. https://doi.org/10.1016/j.ecolind.2020.106653

Sutadian, A.D. hany, Muttil, N., Yilmaz, A.G. okhan, Perera, B.J.C., 2016. Development of river water quality indices-a review. Environ. Monit. Assess. 188, 58. https://doi.org/10.1007/s10661-015-5050-0

Uddin, M.G., Moniruzzaman, M., Quader, M.A., Hasan, M.A., 2018. Spatial variability in the distribution of trace metals in groundwater around the Rooppur nuclear power plant in Ishwardi, Bangladesh. Groundw. Sustain. Dev. 7. https://doi.org/10.1016/j.gsd.2018.06.002

Uddin, M.G., Olbert, A.I., Nash, S., 2020a. Assessment of water quality using Water Quality Index (WQI) models and advanced geostatistical technique, in: Civil Engineering Research Association of Ireland (CERAI). pp. 594–599.

Uddin, M.G., Stephen Nash, Olbert, A.I., 2020b. Application of Water Quality Index Models to an Irish Estuary, in: Kieran Runae, V.J. (Ed.), Civil and Environmental Research. Civil and Environmental Research, Cork, Ireland, pp. 576–581.

Uddin, M.G., Nash, S., Olbert, A.I., 2021. A review of water quality index models and their use for assessing surface water quality. Ecol. Indic. https://doi.org/10.1016/j.ecolind.2020.107218

Uddin, M. G., Nash, S., Olbert, A. I., & Rahman, A. (2022a). Development of a water quality index model - a comparative analysis of various weighting methods. In Prof. Dr. A. Çiner (Ed.), Mediterranean Geosciences Union Annual Meeting (MedGU-21) (pp. 1–6).

Uddin, M. G., Nash, S., Rahman, A., & Olbert, A. I. (2022b). A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment. Water Research, 118532. https://doi.org/10.1016/J.WATRES.2022.118532

Uddin, Md.G., Nash, S., Talas, M., Diganta, M., Rahman, A., Olbert, A.I., 2022c. Robust machine learning algorithms for predicting coastal water quality index, Journal of Environmental Management. https://doi.org/10.1016/j.jenvman.2022.115923

Uddin, Md.G., Nash, S., Rahman, A., Olbert, A.I., 2022d. A novel approach for estimating and predicting uncertainty in water quality index model using machine learning approaches. Manuscript submitted for publication.

Uddin, MD. Galal and Nash, Stephen and Rahman, Azizur and Olbert, Agnieszka I., 2022e. Performance Analysis of the Water Quality Index Model for Predicting Water State Using Machine Learning Techniques. Available at http://dx.doi.org/10.2139/ssrn.4270761

Verma, P.A., Shankar, H., Saran, S., 2019. Comparison of Geostatistical and Deterministic Interpolation to Derive Climatic Surfaces for Mountain Ecosystem. Remote Sens. Northwest Himal. Ecosyst. 537–547. https://doi.org/10.1007/978-981-13-2128-3_24

Wall, B., Cahalane, A., Derham, J., 2020. Ireland’s Environment - An Integrated Assessment.

Wang, S., Huang, G.H., Lin, Q.G., Li, Z., Zhang, H., Fan, Y.R., 2014. Comparison of interpolation methods for estimating spatial distribution of precipitation in Ontario, Canada. Int. J. Climatol. 34, 3745–3751. https://doi.org/10.1002/JOC.3941

Wu, C.Y., Mossa, J., Mao, L., Almulla, M., 2019. Comparison of different spatial interpolation methods for historical hydrographic data of the lowermost Mississippi River. Ann. GIS 25, 133–151. https://doi.org/10.1080/19475683.2019.1588781

Xiao, Y., Gu, X., Yin, S., Shao, J., Cui, Y., Zhang, Q., Niu, Y., 2016. Geostatistical interpolation model selection based on ArcGIS and spatio-temporal variability analysis of groundwater level in piedmont plains, northwest China. Springerplus 5. https://doi.org/10.1186/s40064-016-2073-0

Xie, Y., Chen, T.-B. Bin, Lei, M., Yang, J., Guo, Q.-J.J., Song, B., Zhou, X.-Y.Y., 2011. Spatial distribution of soil heavy metal pollution estimated by different interpolation methods: Accuracy and uncertainty analysis. Chemosphere 82, 468–476. https://doi.org/10.1016/j.chemosphere.2010.09.053

Xiong, Z., Cui, Y., Liu, Z., Zhao, Y., Hu, M., Hu, J., 2020. Evaluating explorative prediction power of machine learning algorithms for materials discovery using k-fold forward cross-validation. Comput. Mater. Sci. 171, 109203. https://doi.org/10.1016/j.commatsci.2019.109203

Xu, Z., Hou, Z., Han, Y., Guo, W., 2016. A diagram for evaluating multiple aspects of model performance in simulating vector fields. Geosci. Model Dev. 9, 4365–4380. https://doi.org/10.5194/gmd-9-4365-2016

Yan, H., Nix, H.A., Hutchinson, M.F., Booth, T.H., 2005. Spatial interpolation of monthly mean climate data for China. Int. J. Climatol. 25, 1369–1379. https://doi.org/10.1002/JOC.1187

Study 6. Development of an efficient water quality model using cutting-edge artificial intelligence techniques

The abstract was presented (online) in the "**Australia and New Zealand Regional Science Association International 45th Annual Conference, 1-2 December, 2022**". Charles Sturt University, Wagga Wagga, 286 Pine Gully Rd, Charles Sturt University NSW 2678 , Australia, pp. 19.

Abstract

For achieving the target level of satisfaction of water quality, several tools and techniques are utilized. The water quality index model is one of the widely used techniques. Recently, this approach has received much criticism in terms of model reliability and inconsistence assessment results. Since the development of the WQI model in 1965, the model's application has increased tremendously due to its simple mathematical architecture and ease of application. Many studies have revealed that the existing technique produces a significant amount of uncertainty in the final assessment. In order to obtain reliability and consistency of assessment results, it should be optimized and improved, considering the existing limitations of the model. Therefore, here, we present the Irish Water Quality Index (IEWQI) model for assessing transitional and coastal water quality in an effort to improve the method and develop a tool that can be used by environmental regulators to abate water pollution in Ireland. The developed model has been associated with the adoption of water quality standards formulated for coastal and transitional waterbodies according to the water framework directive legislation by the environmental regulator of Irish water.

The model consists of five identical components, including (i) indicator selection technique to select the crucial water quality indicator; (ii) subindex (SI) function for rescaling various water quality indicators' information into a uniform scale; (iii) indicators' weight method for estimating the weight values based on the relative significance of real-time information on water quality; (iii) aggregation function for computing the water quality index (WQI) score; and (v) score interpretation scheme for assessing the state of water quality. Each component of the model has been tested and validated using cutting-edge artificial intelligence and machine learning techniques in order to avoid the intervention of experts or humans in terms of reducing model uncertainty. The findings of this study reveal that the IEWQI model could be an efficient and reliable technique for the assessment of transitional and coastal water

quality more accurately in any geospatial domain.

Keywords: coastal water quality; water quality index model; uncertainty; Irish water quality model; artificial intelligence

Study 7. Sensitivity of indicator weights in the water quality index model for assessing coastal water quality

The abstract is accepted for presentation and publication on digital proceedings of the **"16th SDEWES Conference on Sustainable Development of Energy, Water and Environment Systems"** to be held from October 10 - 15, 2021 in Dubrovnik, Croatia.

Abstract

The water quality index (WQI) model is a widely used tool for assessing water quality. It allows converting vast amounts of water quality information into a single dimensionless numerical expression. An ideal WQI model is composed of five consecutive components, including (i) the indicator selection process, (ii) sub-index functions, (iii) indicator weighting processes, (iv) the aggregation function, and (v) the score interpretation scheme. Since developing this technique, its application has increased tremendously day by day due to its simple architecture and ease of application. Recently, several studies have revealed that existing WQI model(s) produce a significant amount of uncertainty in their own processes, whereas the indicators' weight value generation technique is one of the sources. Many water research studies have reported that a considerable amount of uncertainty contributes to the final assessment of water quality due to the inappropriate weight estimation procedures. For the purposes of assessing the effect of indicator weight values of various indicators, the present study has been carried out as a comparison study between the weighted and unweighted WQI models. In this research, two completely new developed water quality indices, including weighted based weighted quadratic mean (WQM)-WQI and unweighted root mean square (RMS)-WQI, were used for assessing coastal water quality in Dublin Bay, Ireland. This research has been carried out during the summer and winter seasons for the purposes of determining the spatio-temporal effects of weight values of various indicators on the WQI model. The result of this study shows that there was no significant difference between weighted and unweighted WQI model scores during both seasons. Both WQI models recommended a "good" and "fair" state of water quality in Dublin Bay during both the summer and winter periods. The findings of this research reveal that the indicator weight values had no significant impact on the model outcomes. Although the present study did not consider the impact of the geospatial resolution on models, this study only applied to a domain. Studies should be carried out on different waterbodies to determine the

sensitivity of models in terms of different geospatial resolutions. However, the findings of this study could be useful for further improvement of the water quality index model in terms of reducing model uncertainty from the final assessment.

Keywords: Coastal Water Quality, Water Quality Index Model, Indicator Weight Estimation, Model Uncertainty

List of Appendix

Appendix 2. WQIs, application domains, types of water bodies, and references materials

WQIs	Application Domain	Types of water bodies	References materials
	Algeria	Tafna, coastal region and Macta basins	Hamlat, Tidjani, Yebdri, Errih, & Guidoum, 2014
	Egypt	Lake Mariout	Sameh et al., 2017
	Turkey	Coruh River Basin	Bilgin, 2018
	Turkey	Kucuk Menderes River Basin	(Boyacioglu, 2010)
	Nigeria	river Asa	Ahaneku & Animashaun, 2013
	Ghana	Aboabo River	Gyamfi et al., 2013
	Grece	Mediterranean Lakes	Alexakis et al., 2016
	Maharashtra, India	Purna River Basin	D. H. Tambekar, S. M. Waghode, 2008
	Iraq	Tigris River	Mahmood, 2018
	Maharashtra, India	Kadava River Basin	Wagh, Panaskar, Muley, & Mukate, 2017
	Karbala City, Iraq	Al-Hussainiya River	Bayati et al., 2017
	India	Yamuna River	Sharma & Kansal, 2011
	Bangladesh	Surma River	Ray, Sourav Bari & Shuvro, 2015
	Iran	River	Mirrasooli, Ghorbani, & Molaei, 2017
	Iran	Karun River	Mojahedi & Attari, 2009
	Iran	Kashkan River	Mostafaei, 2014
	India	Khadakwasla reservoir	Hansda, Swain, Vaidya, & Jagtap, 2018
	India	Damodar River	Haldar, Halder, Das (Saha), & Halder, 2016
CCME	India	River	Dohare et al., 2014
	India	Kadava River Basin	Wagh et al., 2017
	Iraq	Al-Hussainiya River	Bayati et al., 2017
	Iraq	Tigris River	Zahraw Al-Janabi, Jawad Al-Obaidy, & Al-Kubaisi, 2015
	Nepal	Kathmandu Valley	Regmi et al., 2017
	Philiphine	River	Faith, Martinico-Perez, Hara, & Cabrestante, 1996
	Pakistan	River Soan,	Nazeer et al., 2014
	Brazil	Marine water	Ferreira et al., 2011
	Canada	Atlantic coast	El-Jabi et al., 2014
	Canada	River, Ontario	Lumb et al., 2011
	Atlantic region of Canada	Dunk River,	Khan et al., 2003
	Canada	Mackenzie River Basin	Lumb et al., 2006
	Quebec, Canada	Mine water	de Rosemond et al., 2009
	China	New Tongyang Canal,Taizhou	Yan et al., 2016
	Costa Rica	Purires River,	Chacón et al., 2018
	Central North America	Lakes and Rivers	Davies, 2006
	Philippine	Basig River	Regmi and Mishra, 2016
	Srilanka	Kelani River	Mahahamage et. al.,2015

NSFQ	Pará, Brazil	Arapiranga and Murucupi rivers	Medeiros et al., 2017
	Brazil	Amazon River	Lobato et al., 2015
	Nigeria	Warri River	Egborge & Benka-Coker, 1986
	South Korea	Sapgyo River	Song & Kim, 2009
	Iran	Ghezel Ozan River basin	Misaghi, Delgosha, Razzaghmanesh, & Myers, 2017
	Iran	Karun River	Mojahedi & Attari, 2009
	Chania	Taihu Basin	Wu, Wang, Chen, Cai, & Deng, 2018
	Turkey	Aksu River	Şener, Şener, & Davraz, 2017
	Iran	Aydughmush River	Hoseinzadeh, Khorsandi, Wei, & Alipour, 2015
	Bangladesh	Titas River	Islam, Rasul, Alam, & Haque, 2010
	Indonesia	Ciambulawung River	Effendi, Romanto, & Wardiatno, 2015
	Tanzania	Ruvu River	Alphayo & Sharma, 2018
	Nepal	Mardi River	Shah, 2014
	Indonesia	Ciambulawung River	Effendi et al., 2015
	Italy	Imera Meridionale River	Bonanno and Giudice, 2010
	Iraq	Tigris Rive	Ewaid, 2016
	Croatia	Sava and Drava river	Tomas et al., 2017
	Colombia	Magdalena River Basin	Ortega et al., 2016
SRDD (Scottish)	Portugal	river Febros	Carvalho, Cortes, & Bordalo, 2011
	Greece	Douro River	Bordalo, Teixeira, & Wiebe, 2006
	Iran	Karun River	Dadolahi-Sohrab, Arjomand, & Fadaei-Nasab, 2012
	Uttarakhand, India	River	Banerjee & Srivastava, 2009
	Chania	Changjiang River	Yan et al., 2015
	Thailand	Bangpakong river	Agastya, 2009
Horton Index	Southern Iraq	Al-Gharraf river	Shukla, Ojha, & Garg, 2017
	India	Godavari River	Akkaraboyina & Raju, 2012
	India	Andaman Sea	Jha et al., 2015
	Nepal	River system	Kannel et al., 2007
	India	Rangit river	Gupta et al., 2016
	Ghana	River system	(Yidana and Yidana, 2009)
	France	Surface watersheds	(Sánchez et al., 2007)
West Java Index	Indonesia	West Java Sea	Sutadian, Muttil, Yilmaz, & Perera, 2018
MWQI (Malaysian WQI)	Malaysia	Perlis River	Amneera, Najib, Mohd Yusof, & Ragunathan, 2013
		Chini Lake	Shuhaimi-Othman, Lim, & Mushrifah, 2007
		Marine Water	(Aminah et al., 2017)
		Klang river	(Othman and Alaa Eldin, 2012)
		River	(Sim et al., 2015)
		Kinta River	(Gazzaz et al., 2012)
		River system	(Naubi et al., 2016)
		Selangor River	(Fulazzaky et al., 2010)
Oregon WQI	Oregon, USA	Tualatin River	Cude, 2001
	Oregon, USA	Willamette river basin	Dunnette, 1979
Environmental Quality Index (EQI) or Great Lakes Nearshore Index (GLNI)	North America	The Great Lakes	Dojlido et al., in 1994
	India	Assi River	Javed et al., 2018
Dalmatian WQI Model	Southern Croatia	Sea	(Nives, 1999)
British Colombia Water Quality Index (BCWQI)	The Colombia state, USA	Brunette and Salmon River	Paul, 1998

Dojlido WQI	The Vistula River Basin,	Poland	Dojlido et al., 1994
Dinius Index	USA	Surface water	Dinius, 1987
Ross WQI	USA	-	-
Said WQI	USA	Stream water	(Said et al., 2004)
Hanh Index	Vietnam	surface water	(Hanh et al., 2010)
Liou Index	Taiwan	Keya River	(Liou et al., 2004)
Almeida's Index	Argentina	River Water (Recreational water)	(Almeida et al., 2012)
Bascaron Index	Argentina China	Suquia river Dongjiang River	(Pesce and Wunderlin, 2000) (Sun et al., 2016)
	Central Chili	Chill´ an River	(Debels et al., 2005)
	Turkey	Mediterranean basin	(Koçer and Sevgili, 2014)
Smith Index	New Zealand	River water	Smith, 1990
	India	Sabarmati River	(Shah and Joshi, 2017)
House Index	USA	Surface water	House, 1989
Fuzzy Interface System (FIS)	Iran	Jajrood River	(Nikoo et al., 2011)
	Iran	Cane agricultural water system	(Sami et al., 2014)
	India	River water	(Mahapatra et al., 2011)
	Spain	Mediterranean Sea after	(Ocampo-Duque et al., 2006)
	Sichuan province, China	Jialing River	(Li et al., 2016)
	China	River water	(Yan et al., 2010)
	China	Huai River Basin	(Xia and Chen, 2014)
	Morocco	River water	(Mourhir et al., 2014)
	Brazil	Ribeira do Iguape River watershed	(Lermontov et al., 2009)
	Malaysia	River water	(Bai Varadharajan et al., 2009)
	Malaysia	River water	(Che Osmi et al., 2016)
	Colombia	Cauca River	(Ocampo-Duque et al., 2013)

Appendix 3. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment

Table 3.S1 Averaged summer concentrations and computed pollution status used for input to XGBoost model. The guideline values adopted for the research are included at the bottom and values in bold indicate compliance failures.

Monitoring sites	CHL (mg/m^3)	DOX (% sat)	MRP (µg/l as P)	DIN (mg/l)	AMN (mg/l)	BOD5 (mg/l)	pH -	Temp (^{0}C)	TON (mg/l as N)	Tran. (m/depth)	PS*
LE030	1	**69.333**	0.012	**3.423**	0.26	1.37	7.6	15	**3.17**	0	1
LE040	1.9	103.333	0.011	**2.258**	0.06	3.55	7.93	15.43	**2.2**	0	1
LE110	2.033	98	0.015	**1.992**	0.025	1.3	7.73	16.8	1.97	0	1
LE120	1.45	93.333	0.018	**2.64**	0.039	1.33	7.67	16.13	**2.6**	**0**	1
LE130	2.5	89.333	0.028	**2.394**	0.06	1.25	7.77	15.83	**2.3**	1.5	1
LE140	2.067	93.333	0.025	**2.357**	0.057	1.2	7.7	15.53	**2.3**	**0**	1
LE150	4.283	90.167	0.025	1.001	0.11	1.86	7.81	15.83	0.89	2.18	0
LE160	3.25	88.833	0.027	1.105	0.16	0	7.83	15.75	0.95	2.26	0
LE170	7.518	102	0.019	0.731	0.12	2	7.97	15.84	0.65	1.77	0
LE180	7.8	109.167	0.014	0.709	0.1	0	8.05	15.68	0.61	1.9	0
LE200	2.6	101.333	**0.064**	**6.021**	0.021	1.9	7.7	14.83	**6**	**0**	1
LE210	2	103	0.046	**4.587**	0.02	0	7.77	14.77	**4.57**	**0**	1
LE220	5.967	101	0.023	**1.351**	0.068	2.17	7.93	16.6	1.28	**0.75**	1
LE310	7.6	112.5	0.015	0.584	0.09	2.48	8.25	15.7	0.14	1.53	0
LE330	9.442	123.667	0.011	0.246	0.11	2.38	8.24	15.82	0.14	1.65	0
LE340	10.233	121.333	0.011	0.234	0.09	2.48	8.25	15.7	0.14	1.53	0
LE380	10.433	119.5	0.008	0.12	0.056	2.55	8.21	15.57	0.064	1.83	0
LE420	8.85	**136.167**	0.022	0.092	0.035	2.7	8.33	16.6	0.057	1.53	1
LE430	9.6	**130.833**	0.012	0.077	0.028	2.25	8.28	16.17	0.048	1.8	1
LE450	7.65	120.667	0.034	0.076	0.036	1.1	8.23	15.4	0.04	2.3	0
LE500	3.15	106.667	0.024	**4.861**	0.027	2	7.8	16.27	**4.83**	**0**	1
LE505	1.8	104.333	0.021	**5.186**	0.19	1.3	7.8	15.07	**5.17**	**0**	1
LE510	9.82	**133.2**	0.02	**2.382**	0.064	3.2	8.16	16.9	**2.318**	1.05	1
LE540	9.8	124	0.008	0.066	0.03	1.1	8.25	15.65	0.036	2.03	0
LE550	6.467	121.833	0.013	0.075	0.038	2.48	8.22	15.73	0.037	2.23	0
LE620	5.06	110.333	0.007	0.052	0.04	1.68	8.18	14.5	0.017	3.87	0

LE630	4.175	105.333	0.014	0.064	0.036	2	8.15	14.17	0.28	3.4	0
LE810	3.167	113.667	0.018	0.056	0.031	1.65	8.16	14.8	0.026	5.6	0
LE820	2.7	103	0.017	0.038	0.038	1.1	8.13	13.9	0	4.83	0
Criteria	**0 - 14.2**	**72 - 128**	**0 - 0.057**	**0 - 1.208**	**0 - 1.5**	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	

PS = Pollution Status; 0 = unpolluted; 1= polluted; bolded underline is breached the criteria

Table 3.S2 Averaged winter concentrations and computed pollution status used for input to XGBoost model. the guideline values adopted for the research are included at the bottom and values in bold indicate compliance failures.

Monitoring sites	CHL (mg/ m^3)	DOX (% sat)	MRP (µg/l as P)	DIN (mg/l)	AMN (mg/l)	BOD5 (mg/l)	pH -	Temp (^{0}C)	TON (mg/l as N)	Tran. (m/depth)	PS*
LE030	0	97	0.03	0.29	0.26	0	7.5	8.7	**6.6**	**0**	1
LE040	0	98	0.014	**4.028**	0.028	0	7.5	7.8	**4**	**0**	1
LE110	0	98	0.022	**3.832**	0.032	0	7.5	8.3	**3.8**	**0**	1
LE120	0	98	0.024	**4.33**	0.03	0	7.6	8.3	**4.3**	**0**	1
LE130	0	98	0.034	**4.543**	0.043	0	7.6	7.6	**4.5**	**0**	1
LE140	0	99	0.027	**4.347**	0.047	0	7.6	7.7	**4.3**	**0**	1
LE150	1	86.5	0.032	**2.26**	0.16	0	7.65	9.83	**2.1**	1.95	1
LE160	0	88	**0.34**	**2**	0.16	0	7.7	9.7	1.96	2.2	1
LE170	3.3	92	0.045	**1.99**	0.22	1.1	7.7	9.75	1.78	2	1
LE180	1.6	92.25	0.037	1.34	0.19	0	7.85	9.9	1.15	2	0
LE200	1.7	100	0.052	**6.73**	0.03	0	7.8	7.4	**6.7**	**0**	1
LE210	0	101	0.034	**6.324**	0.024	0	7.8	8.4	**6.3**	**0**	1
LE220	0	98	0.036	**3.61**	0.11	0	7.7	7.7	**3.5**	**0**	1
LE310	0	92	0.039	1.15	0.21	0	7.85	9.8	0.94	2	0
LE330	0	95.25	**0.41**	**1.77**	0.22	0	7.9	10	1.55	1.76	1
LE340	0	94.5	**0.3**	0.89	0.175	0	7.9	10.1	0.715	1.7	0
LE380	0	95.25	0.04	**1.76**	0.22	0	7.9	9.97	1.54	1.9	1
LE420	0	92	0.039	1.145	0.21	0	7.85	9.8	0.94	2	0
LE430	1.1	96	0.031	1.121	0.091	0	7.9	8.45	1.03	1.5	0
LE450	0	94	0.026	0.863	0.078	0	7.95	9.2	0.785	1.8	0
LE500	0	100	0.021	**5.213**	0.013	0	7.7	7.3	**5.2**	**0**	1
LE505	0	99	0.011	**5.618**	0.018	0	7.8	7.4	**5.6**	**0**	1
LE510	1.4	99	0.017	**5.512**	0.012	0	7.8	7.2	**5.5**	**0**	1
LE540	2.1	97	0.029	0.694	0.084	0	7.95	9.3	0.61	2.1	0
LE550	1.2	94	0.025	0.665	0.075	0	8	10.5	0.59	2	0
LE620	0	96.5	0.016	0.36	0.2	0	7.95	10.6	0.16	4.3	0
LE630	0	97	0.014	0.174	0.034	0	7.9	10.6	0.14	4.9	0

LE810	0	98	0.016	0.204	0.024	0	7.9	10.4	0.18	4.5	0
LE820	0	97	0.016	0.167	0.017	0	7.9	10.5	0.15	4	0
Criteria	**0 - 14.7**	**71 - 129**	**0 - 0.059**	**0 - 1.336**	**0 - 1.5**	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	

* PS = Pollution Status; 0 = unpolluted; 1 = polluted; bolded underline is breached the criteria

Table 3.S3 Water quality guideline values for the entire range of salinities using the ATSEBI system.

Salinity Median psu	DIN Median mg/l N	MRP Median µg/l P	Chlorophyll Median µg/l	Chlorophyll 95 %ile µg/l	Dissolved Oxygen % Saturation 5 %ile	Dissolved Oxygen % Saturation 95 %ile
0	2.600	60	15.0	30.0	70	130
1	2.529	60	15.0	30.0	70	130
2	2.459	60	15.0	30.0	70	130
3	2.388	60	15.0	30.0	70	130
4	2.318	60	15.0	30.0	70	130
5	2.247	60	15.0	30.0	70	130
6	2.176	60	15.0	30.0	70	130
7	2.106	60	15.0	30.0	70	130
8	2.035	60	15.0	30.0	70	130
9	1.965	60	15.0	30.0	70	130
10	1.894	60	15.0	30.0	70	130
11	1.824	60	15.0	30.0	70	130
12	1.753	60	15.0	30.0	70	130
13	1.682	60	15.0	30.0	70	130
14	1.612	60	15.0	30.0	70	130
15	1.541	60	15.0	30.0	70	130
16	1.471	60	15.0	30.0	70	130
17	1.400	60	15.0	30.0	70	130
18	1.336	59	14.7	29.4	71	129
19	1.272	58	14.4	28.9	71	129
20	1.208	57	14.2	28.3	72	128
21	1.144	56	13.9	27.8	72	128
22	1.081	54	13.6	27.2	73	127
23	1.017	53	13.3	26.7	73	127
24	0.953	52	13.1	26.1	74	126
25	0.889	51	12.8	25.6	74	126
26	0.825	50	12.5	25.0	75	125
27	0.761	49	12.2	24.4	76	124
28	0.697	48	11.9	23.9	76	124
29	0.633	47	11.7	23.3	77	123
30	0.569	46	11.4	22.8	77	123
31	0.506	44	11.1	22.2	78	122
32	0.442	43	10.8	21.7	78	122
33	0.378	42	10.6	21.1	79	121
34	0.314	41	10.3	20.6	79	121
35	0.250	40	10.0	20.0	80	120

Table 3.S4 Eclipsing impacts on aggregation process by comparing actual water quality parameters and qualitative status of water quality using different WQI models in Cork Harbour during summer season.

Monitoring sites	Attributes criteria							Weighted WQI models				Unweighted WQI models			
	TRAN (m/depth)	DIN (mg/l)	TEMP (^{0}C)	CHL (mg/m^3)	AMN (mg/l)	MRP (µg/l as P)	BOD5 (mg/l)	NSF	WQM	SRDD	WJ	RMS	AM	Hanh	CCME
LE030	0	3.423	15	1	0.26	0.012	1.37	Marginal	Fair	Poor	Poor	Fair	Fair	Fair	Good
LE040	0	2.258	15.43	1.9	0.06	0.011	3.55	Marginal	Fair	Poor	Poor	Fair	Fair	Fair	Good
LE110	0	1.992	16.8	2.033	0.025	0.015	1.3	Marginal	Fair	Poor	Poor	Fair	Fair	Fair	Good
LE120	0	2.64	16.13	1.45	0.039	0.018	1.33	Marginal	Fair	Poor	Poor	Fair	Fair	Fair	Good
LE130	1.5	2.394	15.83	2.5	0.06	0.028	1.25	Fair	Fair	Fair	Poor	Good	Fair	Fair	Good
LE140	0	2.357	15.53	2.067	0.057	0.025	1.2	Marginal	Fair	Poor	Poor	Fair	Fair	Fair	Good
LE150	2.18	1.001	15.83	4.283	0.11	0.025	1.86	Fair	Fair	Fair	Fair	Fair	Fair	Fair	Good
LE160	2.26	1.105	15.75	3.25	0.16	0.027	0	Fair	Fair	Fair	Fair	Good	Fair	Fair	Good
LE170	1.77	0.731	15.84	7.518	0.12	0.019	2	Fair	Fair	Fair	Fair	Fair	Fair	Fair	Good
LE180	1.9	0.709	15.68	7.8	0.1	0.014	0	Fair	Fair	Fair	Fair	Good	Fair	Fair	Good
LE200	0	6.021	14.83	2.6	0.021	0.064	1.9	Marginal	Fair	Poor	Poor	Fair	Fair	Fair	Good
LE210	0	4.587	14.77	2	0.02	0.046	0	Marginal	Fair	Poor	Poor	Fair	Fair	Fair	Good
LE220	0.75	1.351	16.6	5.967	0.068	0.023	2.17	Fair	Fair	Marginal	Poor	Fair	Fair	Fair	Good
LE310	1.53	0.584	15.7	7.6	0.09	0.015	2.48	Good	Fair	Fair	Fair	Fair	Fair	Fair	Good
LE330	1.65	0.246	15.82	9.442	0.11	0.011	2.38	Good	Fair	Fair	Good	Good	Fair	Fair	Good
LE340	1.53	0.234	15.7	10.233	0.09	0.011	2.48	Good	Fair	Fair	Good	Good	Fair	Fair	Good
LE380	1.83	0.12	15.57	10.433	0.056	0.008	2.55	Good	Fair	Fair	Good	Good	Good	Fair	Good
LE420	1.53	0.092	16.6	8.85	0.035	0.022	2.7	Good	Fair	Fair	Good	Good	Fair	Fair	Good
LE430	1.8	0.077	16.17	9.6	0.028	0.012	2.25	Good	Good	Good	Good	Good	Good	Fair	Good
LE450	2.3	0.076	15.4	7.65	0.036	0.034	1.1	Good	Good	Good	Good	Good	Good	Fair	Good
LE500	0	4.861	16.27	3.15	0.027	0.024	2	Marginal	Fair	Poor	Poor	Fair	Fair	Fair	Good

LE505	0	5.186	15.07	1.8	0.19	0.021	1.3	Marginal	Fair	Poor	Poor	Fair	Fair	Fair	Good
LE510	1.05	2.382	16.9	9.82	0.064	0.02	3.2	Fair	Fair	Marginal	Poor	Fair	Fair	Fair	Good
LE540	2.03	0.066	15.65	9.8	0.03	0.008	1.1	Good	Good	Good	Good	Good	Good	Fair	Good
LE550	2.23	0.075	15.73	6.467	0.038	0.013	2.48	Good	Good	Good	Good	Good	Good	Fair	Good
LE620	3.87	0.052	14.5	5.06	0.04	0.007	1.68	Good	Good	Good	Good	Good	Good	Good	Good
LE630	3.4	0.064	14.17	4.175	0.036	0.014	2	Good	Good	Good	Good	Good	Good	Good	Good
LE810	5.6	0.056	14.8	3.167	0.031	0.018	1.65	Good	Good	Good	Good	Good	Good	Good	Good
LE820	4.83	0.038	13.9	2.7	0.038	0.017	1.1	Good	Good	Good	Good	Good	Good	Good	Good
	Breached criteria			Underestimate eclipsing				Overestimate eclipsing							

Table 3.S5 Eclipsing impacts on aggregation process by comparing actual water quality parameters and qualitative status of water quality using different WQI models in Cork Harbour during winter season.

Monitoring sites	Attributes of criteria					Weighted WQIs				Unweighted WQIs			
	TON (mg/l as N)	DIN (mg/l)	pH -	TRAN (m/depth)	DOX (% sat)	NSF	WQM	SRDD	WJ	RMS	AM	Hanh	CCME
LE030	6.6	0.29	7.5	0	97	Marginal	Fair	Poor	Poor	Fair	Fair	Fair	Fair
LE040	4	4.028	7.5	0	98	Poor	Marginal	Poor	Poor	Fair	Marginal	Poor	Fair
LE110	3.8	3.832	7.5	0	98	Poor	Marginal	Poor	Poor	Fair	Marginal	Poor	Fair
LE120	4.3	4.33	7.6	0	98	Poor	Marginal	Poor	Poor	Fair	Marginal	Poor	Fair
LE130	4.5	4.543	7.6	0	98	Poor	Marginal	Poor	Poor	Fair	Marginal	Poor	Fair
LE140	4.3	4.347	7.6	0	99	Poor	Marginal	Poor	Poor	Fair	Marginal	Poor	Fair
LE150	2.1	2.26	7.65	1.95	86.5	Poor	Fair	Poor	Poor	Fair	Fair	Poor	Fair
LE160	1.96	2	7.7	2.2	88	Poor	Fair	Poor	Poor	Fair	Fair	Poor	Fair
LE170	1.78	1.99	7.7	2	92	Marginal	Fair	Poor	Poor	Fair	Fair	Marginal	Fair
LE180	1.15	1.34	7.85	2	92.25	Marginal	Fair	Poor	Poor	Fair	Fair	Fair	Fair
LE200	6.7	6.73	7.8	0	100	Poor	Marginal	Poor	Poor	Fair	Marginal	Poor	Fair
LE210	6.3	6.324	7.8	0	101	Poor	Marginal	Poor	Poor	Fair	Marginal	Poor	Fair

LE220	3.5	3.61	7.7	0	98	Poor	Marginal	Poor	Poor	Fair	Marginal	Poor	Fair
LE310	0.94	1.15	7.85	2	92	Fair	Fair	Marginal	Marginal	Fair	Fair	Fair	Fair
LE330	1.55	1.77	7.9	1.76	95.25	Marginal	Fair	Poor	Poor	Fair	Fair	Marginal	Fair
LE340	0.715	0.89	7.9	1.7	94.5	Fair	Fair	Marginal	Fair	Fair	Fair	Fair	Fair
LE380	1.54	1.76	7.9	1.9	95.25	Marginal	Fair	Poor	Poor	Fair	Fair	Marginal	Fair
LE420	0.94	1.145	7.85	2	92	Fair	Fair	Marginal	Marginal	Fair	Fair	Fair	Fair
LE430	1.03	1.121	7.9	1.5	96	Fair	Fair	Poor	Marginal	Fair	Fair	Fair	Fair
LE450	0.785	0.863	7.95	1.8	94	Fair	Fair	Marginal	Fair	Fair	Fair	Fair	Fair
LE500	5.2	5.213	7.7	0	100	Poor	Marginal	Poor	Poor	Fair	Marginal	Poor	Fair
LE505	5.6	5.618	7.8	0	99	Poor	Marginal	Poor	Poor	Fair	Marginal	Poor	Fair
LE510	5.5	5.512	7.8	0	99	Poor	Marginal	Poor	Poor	Fair	Marginal	Poor	Fair
LE540	0.61	0.694	7.95	2.1	97	Fair	Fair	Fair	Fair	Good	Good	Good	Good
LE550	0.59	0.665	8	2	94	Fair	Fair	Fair	Fair	Good	Fair	Fair	Good
LE620	0.16	0.36	7.95	4.3	96.5	Good	Good	Fair	Good	Good	Good	Good	Good
LE630	0.14	0.174	7.9	4.9	97	Good	Good	Good	Good	Good	Good	Good	Good
LE810	0.18	0.204	7.9	4.5	98	Good	Good	Good	Good	Good	Good	Good	Good
LE820	0.15	0.167	7.9	4	97	Good	Good	Good	Good	Good	Good	Good	Good

	Breached criteria		Underestimate eclipsing		Overestimate eclipsing

Table 3.S6 Calculated sub-index values using Eq. (3.4) – Eq. (3.6), WQI scores of various WQI methods and ambiguity problems of aggregation functions during summer season.

Monitoring sites	Sub-index of water quality parameters							Weighted WQIs				Unweighted WQIs			
	TRAN	DIN	TEMP	CHL	AMN	MRP	BOD5	NSF	WQM	[a]SRDD	[a]WJ	RMS	AM	Hanh	[b]CCME
LE030	0.0	0.0	100.0	93.0	82.7	79.0	80.0	37	58	14	0	74	62	65	95
LE040	0.0	0.0	100.0	86.6	96.0	80.7	48.6	37	58	13	0	71	59	62	94
LE110	0.0	0.0	100.0	85.7	98.0	73.7	81.4	37	59	14	0	75	63	64	94
LE120	0.0	0.0	100.0	89.8	97.3	68.4	81.4	37	59	14	0	74	62	65	93
LE130	100.0	0.0	100.0	82.4	96.0	50.9	81.4	72	83	52	0	80	73	77	94
LE140	0.0	0.0	100.0	85.4	96.0	56.1	82.9	36	57	13	0	72	60	63	93
LE150	100.0	17.1	100.0	69.8	92.7	56.1	72.9	75	82	56	62	78	73	74	99
LE160	100.0	8.5	100.0	77.1	89.3	52.6	100.0	74	83	54	53	82	75	78	99
LE170	100.0	39.5	100.0	47.1	92.0	66.7	71.4	78	82	61	72	77	74	68	99
LE180	100.0	41.3	100.0	45.1	93.3	75.4	100.0	79	83	63	74	83	79	70	99
LE200	0.0	0.0	100.0	81.7	98.7	0.0	72.9	33	56	11	0	67	50	56	93
LE210	0.0	0.0	100.0	85.9	98.7	19.3	100.0	35	57	12	0	73	58	61	94
LE220	75.0	0.0	100.0	58.0	95.3	59.7	68.6	61	70	37	0	72	65	65	93
LE310	100.0	51.7	100.0	46.5	94.0	73.7	64.3	81	84	65	77	79	76	69	99
LE330	100.0	79.6	100.0	33.5	92.7	80.7	65.7	86	88	74	82	82	79	64	99
LE340	100.0	80.6	100.0	27.9	94.0	80.7	64.3	86	89	73	81	82	78	60	99
LE380	100.0	90.1	100.0	26.5	96.0	86.0	62.9	88	91	78	83	84	80	60	99
LE420	100.0	92.4	100.0	37.7	97.3	61.4	61.4	89	91	79	85	82	79	66	99
LE430	100.0	93.6	100.0	32.4	98.0	79.0	67.1	89	92	80	85	85	81	65	99
LE450	100.0	93.7	100.0	46.1	97.3	40.4	84.3	90	92	80	87	84	80	71	99

LE500	0.0	0.0	100.0	77.8	98.0	57.9	71.4	35	56	12	0	70	58	60	94
LE505	0.0	0.0	100.0	87.3	87.3	63.2	81.4	36	57	13	0	72	60	63	94
LE510	100.0	0.0	100.0	30.9	96.0	64.9	54.3	67	79	45	0	73	64	55	94
LE540	100.0	94.5	100.0	31.0	98.0	86.0	84.3	90	93	81	86	88	85	65	99
LE550	100.0	93.8	100.0	54.5	97.3	77.2	64.3	92	93	84	90	86	84	76	99
LE620	100.0	95.7	100.0	64.4	97.3	87.7	75.7	94	95	88	93	90	89	83	99
LE630	100.0	94.7	100.0	70.6	97.3	75.4	71.4	94	94	88	93	88	87	84	99
LE810	100.0	95.4	100.0	77.7	98.0	68.4	75.7	94	95	89	94	89	88	86	99
LE820	100.0	96.9	100.0	81.0	97.3	70.2	84.3	95	96	91	95	91	90	89	99

a = underestimating ambiguity and b = overestimation ambiguity

Table 3.S7 Calculated sub-index values using Eq. (3.4) – Eq. (3.6), WQI scores of various WQI methods and ambiguity problems of aggregation functions during winter season.

Monitoring sites	Sub-index of water quality parameters					Weighted WQIs				Unweighted WQIs			
	TON	DIN	pH	TRAN	DOX	NSF	WQM	[a]SRDD	[a]WJ	RMS	AM	[b]Hanh	[b]CCME
LE030	0	78.29	100	0	89.66	39	59	16	0	70	54	56	92
LE040	0	0	100	0	93.1	19	44	4	0	61	39	0	92
LE110	0	0	100	0	93.1	19	44	4	0	61	39	0	92
LE120	0	0	100	0	93.1	19	44	4	0	61	39	0	92
LE130	0	0	100	0	93.1	19	44	4	0	61	39	0	92
LE140	0	0	100	0	96.55	20	44	4	0	62	39	0	92
LE150	0	0	100	100	53.45	27	51	7	0	68	51	0	93
LE160	2	0	100	100	58.62	28	51	8	0	68	52	18	93
LE170	11	0	100	100	72.41	33	52	11	0	71	57	34	93
LE180	42.5	0	100	100	73.28	47	59	22	0	74	63	54	97
LE200	0	0	100	0	100	20	44	4	0	63	40	0	93
LE210	0	0	100	0	96.55	20	44	4	0	62	39	0	93
LE220	0	0	100	0	93.1	19	44	4	0	61	39	0	92
LE310	53	13.92	100	100	72.41	55	63	31	45	75	68	62	97
LE330	22.5	0	100	100	83.62	38	55	15	0	74	61	45	93
LE340	64	33.38	100	100	81.03	66	70	43	61	80	76	73	97
LE380	23	0	100	100	83.62	39	55	15	0	74	61	46	93
LE420	53	13.92	100	100	72.41	55	63	31	45	75	68	62	97
LE430	48.5	16.17	100	100	86.21	54	63	30	45	78	70	65	97
LE450	60.5	35.63	100	100	79.31	65	69	42	61	79	75	72	97
LE500	0	0	100	0	100	20	44	4	0	63	40	0	92
LE505	0	0	100	0	96.55	20	44	4	0	62	39	0	93
LE510	0	0	100	0	96.55	20	44	4	0	62	39	0	93
LE540	69.5	48.35	100	100	89.66	72	75	53	70	84	82	80	97
LE550	70.5	49.85	100	100	79.31	73	75	53	71	82	80	78	97
LE620	92	73.05	100	100	87.93	89	90	79	89	91	91	89	97
LE630	93	87.28	100	100	89.66	93	93	87	93	94	94	93	97
LE810	91	85.03	100	100	93.1	92	92	84	92	94	94	93	97
LE820	92.5	87.28	100	100	89.66	93	93	86	93	94	94	93	97

a = underestimating ambiguity and b = overestimation ambiguity

Appendix 4. A comprehensive framework for estimating and predicting uncertainty in water quality index model using machine learning approaches

Table 4.S1 Monitored water quality parameters, concentration and calculated WQI values for different WQI models over the summer season in the Cork Harbour, Cork, Ireland (2019). This dataset also used as input for developing the GPR prediction model.

Monitoring sites	Water quality Parameters							Weighted WQI models				Unweighted WQI models			
	TRAN	DIN	TEMP	CHL	AMN	MRP	BOD5	NSF	WQM	SRDD	WJ	RMS	AM	Hanh	CCME
LE030	0	3.423	15	1	0.26	0.012	1.37	37	58	14	0	74	62	65	95
LE040	0	2.258	15.43	1.9	0.06	0.011	3.55	37	58	13	0	71	59	62	94
LE110	0	1.992	16.8	2.033	0.025	0.015	1.3	37	59	14	0	75	63	64	94
LE120	0	2.64	16.13	1.45	0.039	0.018	1.33	37	59	14	0	74	62	65	93
LE130	1.5	2.394	15.83	2.5	0.06	0.028	1.25	72	83	52	0	80	73	77	94
LE140	0	2.357	15.53	2.067	0.057	0.025	1.2	36	57	13	0	72	60	63	93
LE150	2.18	1.001	15.83	4.283	0.11	0.025	1.86	75	82	56	62	78	73	74	99
LE160	2.26	1.105	15.75	3.25	0.16	0.027	0	74	83	54	53	82	75	78	99
LE170	1.77	0.731	15.84	7.518	0.12	0.019	2	78	82	61	72	77	74	68	99
LE180	1.9	0.709	15.68	7.8	0.1	0.014	0	79	83	63	74	83	79	70	99
LE200	0	6.021	14.83	2.6	0.021	0.064	1.9	33	56	11	0	67	50	56	93
LE210	0	4.587	14.77	2	0.02	0.046	0	35	57	12	0	73	58	61	94
LE220	0.75	1.351	16.6	5.967	0.068	0.023	2.17	61	70	37	0	72	65	65	93
LE310	1.53	0.584	15.7	7.6	0.09	0.015	2.48	81	84	65	77	79	76	69	99
LE330	1.65	0.246	15.82	9.442	0.11	0.011	2.38	86	88	74	82	82	79	64	99
LE340	1.53	0.234	15.7	10.233	0.09	0.011	2.48	86	89	73	81	82	78	60	99
LE380	1.83	0.12	15.57	10.433	0.056	0.008	2.55	88	91	78	83	84	80	60	99
LE420	1.53	0.092	16.6	8.85	0.035	0.022	2.7	89	91	79	85	82	79	66	99
LE430	1.8	0.077	16.17	9.6	0.028	0.012	2.25	89	92	80	85	85	81	65	99
LE450	2.3	0.076	15.4	7.65	0.036	0.034	1.1	90	92	80	87	84	80	71	99
LE500	0	4.861	16.27	3.15	0.027	0.024	2	35	56	12	0	70	58	60	94
LE505	0	5.186	15.07	1.8	0.19	0.021	1.3	36	57	13	0	72	60	63	94
LE510	1.05	2.382	16.9	9.82	0.064	0.02	3.2	67	79	45	0	73	64	55	94
LE540	2.03	0.066	15.65	9.8	0.03	0.008	1.1	90	93	81	86	88	85	65	99
LE550	2.23	0.075	15.73	6.467	0.038	0.013	2.48	92	93	84	90	86	84	76	99

LE620	3.87	0.052	14.5	5.06	0.004	0.007	1.68	94	95	88	93	90	89	83	99
LE630	3.4	0.064	14.17	4.175	0.036	0.014	2	94	94	88	93	88	87	84	99
LE810	5.6	0.056	14.8	3.167	0.031	0.018	1.65	94	95	89	94	89	88	86	99
LE820	4.83	0.038	13.9	2.7	0.038	0.017	1.1	95	96	91	95	91	90	89	99

Table 4.S2 Monitored water quality parameters, concentration and calculated WQI values for different WQI models during the winter season in the Cork Harbour, Cork, Ireland (2019).

Monitoring sites	Water quality Parameters					Weighted WQI models				Unweighted WQI models			
	TON	DIN	pH	TRAN	DOX	NSF	WQM	SRDD	WJ	RMS	AM	Hanh	CCME
LE030	0	78.29	100	0	89.66	39	59	16	0	70	54	56	92
LE040	0	0	100	0	93.1	19	44	4	0	61	39	0	92
LE110	0	0	100	0	93.1	19	44	4	0	61	39	0	92
LE120	0	0	100	0	93.1	19	44	4	0	61	39	0	92
LE130	0	0	100	0	93.1	19	44	4	0	61	39	0	92
LE140	0	0	100	0	96.55	20	44	4	0	62	39	0	92
LE150	0	0	100	100	53.45	27	51	7	0	68	51	0	93
LE160	2	0	100	100	58.62	28	51	8	0	68	52	18	93
LE170	11	0	100	100	72.41	33	52	11	0	71	57	34	93
LE180	42.5	0	100	100	73.28	47	59	22	0	74	63	54	97
LE200	0	0	100	0	100	20	44	4	0	63	40	0	93
LE210	0	0	100	0	96.55	20	44	4	0	62	39	0	93
LE220	0	0	100	0	93.1	19	44	4	0	61	39	0	92
LE310	53	13.92	100	100	72.41	55	63	31	45	75	68	62	97
LE330	22.5	0	100	100	83.62	38	55	15	0	74	61	45	93
LE340	64	33.38	100	100	81.03	66	70	43	61	80	76	73	97
LE380	23	0	100	100	83.62	39	55	15	0	74	61	46	93
LE420	53	13.92	100	100	72.41	55	63	31	45	75	68	62	97
LE430	48.5	16.17	100	100	86.21	54	63	30	45	78	70	65	97
LE450	60.5	35.63	100	100	79.31	65	69	42	61	79	75	72	97
LE500	0	0	100	0	100	20	44	4	0	63	40	0	92
LE505	0	0	100	0	96.55	20	44	4	0	62	39	0	93
LE510	0	0	100	0	96.55	20	44	4	0	62	39	0	93
LE540	69.5	48.35	100	100	89.66	72	75	53	70	84	82	80	97
LE550	70.5	49.85	100	100	79.31	73	75	53	71	82	80	78	97

LE620	92	73.05	100	100	87.93	89	90	79	89	91	91	89	97
LE630	93	87.28	100	100	89.66	93	93	87	93	94	94	93	97
LE810	91	85.03	100	100	93.1	92	92	84	92	94	94	93	97
LE820	92.5	87.28	100	100	89.66	93	93	86	93	94	94	93	97

Table 4.S3 WQI model input indicators and their relative weight values used by Uddin et al., (2022)

Summer (2019)		Winter (2019)	
Indicators	Weight	Indicators	weight
Tran.	0.370	TON	0.457
DIN	0.228	DIN	0.257
Temp	0.156	pH	0.157
CHL	0.109	Tran.	0.090
AMN	0.073	DOX	0.040
MRP	0.044		
BOD5	0.020		

Table 4.S4 Binary conditions of respective indicators for calculating sub-index values by implying coastal water quality standard criteria (Uddin et al., 2022).

WQ indicators	Applying binary conditions	Sub-index functions
BOD, CHL, MRP, DIN, AMN, TON	-	Eq. (1)
DOX	(i) if DOX > 100 (ii) if, DOX < 100 (iii) if, DOX = 100	Eq. (2) Eq. (3) SI = 100
pH	(i) If, pH ≥ 5.0 and pH < 7.5 (ii) If, pH > 8.5 and pH ≤ 9.0 (iii) If, pH ≥ 7.5 and pH ≤ 8.5	Eq. (2) Eq. (3) 100
TEMP	(i) If, TEMP ≤ 25 (ii) If, TEMP > 25	100 0.0
TRAN	(i) If. TRAN < 1.0 (ii) If. TRAN ≥ 1.0	Eq. (3) 100

Table 4.S5 An overview of different WQI model aggregation functions and their components (Uddin et al., 2022).

Types of functions	WQIs Models	Aggregation functions
(i) Weighted	NSF index [Weighted Arithmetic Mean(WAM)]	$WQI = \sum_{i=1}^{n} s_i w_i$ (4)
	Weighted Quadratic Mean (WQM)	$WQM = \sqrt{\sum_{i=1}^{n} w_i\, s_i^2}$ (4.5)
	SRDD index (modified additive function)	$SRDD - WQI = \frac{1}{100}\left(\sum_{i=1}^{n} S_i W_i\right)^2$ (4.6)
	West Java WQI [Weighted Geometric Mean (WGM)]	$WQI = \prod_{i=1}^{n} {s_i}^{w_i}$ (4.7) where s_i is the SI value for parameter *i*; w_i is weight value of respective variables and *n* is the number of indicators.
(ii) Unweighted	Root Mean Squared (RMS)	$RMS = \sqrt{\frac{1}{n}\sum_{i=1}^{n} s_i^2}$ (4.8)
	Arithmetic Mean (AM)	$AM = \frac{1}{n}\sum_{i=1}^{n} s_i$ (4.9)
	CCME Index	$WQI = 100 - \left[\frac{\sqrt{{F_1}^2 + {F_2}^2 + {F_3}^2}}{1.732}\right]$ (4.10) Where, F1, F2 and F3 are the factors that are estimated using the separate equation. The CCME details are discussed in Uddin et al., 2020. The divisor 1.732 used as a normalizing factor to ensure the resultant WQI is in the range of 0 to 100.
	Hanh index	$WQI_b = \left[\frac{1}{n}\sum_{i=1}^{n} q_i \times \frac{1}{n} q_j \times q_k\right]^{1/3}$ (4.11) Where, WQI_b is the basic water quality index; q_i is the subindex value of the organic; q_j is the inorganic substance; q_k is the subindex value of the biological or bacterial groups components; n is the number of components each group

Table 4.S6 Calculated sub-index values using Eq. (4.1) –Eq. (4.3).

Monitoring sites	Sub-index (summer)							Sub-index (winter)				
	CHL	MRP	DIN	AMN	BOD5	TEMP	TRAN	DOX	DIN	pH	TON	TRAN
LE030	93	79	0	82.7	80	100	0	89.66	78.29	100	0	0
LE040	86.6	80.7	0	96	48.6	100	0	93.1	0	100	0	0
LE110	85.7	73.7	0	98	81.4	100	0	93.1	0	100	0	0
LE120	89.8	68.4	0	97.3	81.4	100	0	93.1	0	100	0	0
LE130	82.4	50.9	0	96	81.4	100	100	93.1	0	100	0	0
LE140	85.4	56.1	0	96	82.9	100	0	96.55	0	100	0	0
LE150	69.8	56.1	17.1	92.7	72.9	100	100	53.45	0	100	0	100
LE160	77.1	52.6	8.5	89.3	100	100	100	58.62	0	100	2	100
LE170	47.1	66.7	39.5	92	71.4	100	100	72.41	0	100	11	100
LE180	45.1	75.4	41.3	93.3	100	100	100	73.28	0	100	42.5	100
LE200	81.7	0	0	98.7	72.9	100	0	100	0	100	0	0
LE210	85.9	19.3	0	98.7	100	100	0	96.55	0	100	0	0
LE220	58	59.7	0	95.3	68.6	100	75	93.1	0	100	0	0
LE310	46.5	73.7	51.7	94	64.3	100	100	72.41	13.92	100	53	100
LE330	33.5	80.7	79.6	92.7	65.7	100	100	83.62	0	100	22.5	100
LE340	27.9	80.7	80.6	94	64.3	100	100	81.03	33.38	100	64	100
LE380	26.5	86	90.1	96	62.9	100	100	83.62	0	100	23	100
LE420	37.7	61.4	92.4	97.3	61.4	100	100	72.41	13.92	100	53	100
LE430	32.4	79	93.6	98	67.1	100	100	86.21	16.17	100	48.5	100
LE450	46.1	40.4	93.7	97.3	84.3	100	100	79.31	35.63	100	60.5	100
LE500	77.8	57.9	0	98	71.4	100	0	100	0	100	0	0
LE505	87.3	63.2	0	87.3	81.4	100	0	96.55	0	100	0	0
LE510	30.9	64.9	0	96	54.3	100	100	96.55	0	100	0	0
LE540	31	86	94.5	98	84.3	100	100	89.66	48.35	100	69.5	100
LE550	54.5	77.2	93.8	97.3	64.3	100	100	79.31	49.85	100	70.5	100
LE620	64.4	87.7	95.7	97.3	75.7	100	100	87.93	73.05	100	92	100
LE630	70.6	75.4	94.7	97.3	71.4	100	100	89.66	87.28	100	93	100
LE810	77.7	68.4	95.4	98	75.7	100	100	93.1	85.03	100	91	100
LE820	81	70.2	96.9	97.3	84.3	100	100	89.66	87.28	100	92.5	100

Table 4.S7 Classification scheme for assessing coastal water quality using WQI model (Uddin et al., 2022).

Classifications scheme	Range of score	Descriptions
(i) Good	80 - 100	Good waterbodies are those that meet the guidelines' values. Water quality is maintained and is suitable for all uses.
(ii) Fair	50 - 79	Waterbodies that a few indicators meet the guidelines values; water quality is usually protected with a minor degree of impairment.
(iii) Marginal	30 – 49	The majority of water quality indicators failed to meet the criteria; water quality is unprotected, which may be posing a risk for aquatic life.
(iv) Poor	0 - 29	Poor waterbodies are those that fail to meet all of the criteria. Water quality is completely unprotected and unsuitable for many specifics uses

Table 4.S8 Water quality status of monitoring sites in Cork Harbour during the summer period.

Monitoring Sites	NSF	WQM	SRDD	WJ	RMS	AM	Hanh	CCME
LE030	Marginal	Fair	poor	poor	Fair	Fair	Fair	Good
LE040	Marginal	Fair	poor	poor	Fair	Fair	Fair	Good
LE110	Marginal	Fair	poor	poor	Fair	Fair	Fair	Good
LE120	Marginal	Fair	poor	poor	Fair	Fair	Fair	Good
LE130	Fair	Good	Fair	poor	Good	Fair	Fair	Good
LE140	Marginal	Fair	poor	poor	Fair	Fair	Fair	Good
LE150	Fair	Good	Fair	Fair	Fair	Fair	Fair	Good
LE160	Fair	Good	Fair	Fair	Good	Fair	Fair	Good
LE170	Fair	Good	Fair	Fair	Fair	Fair	Fair	Good
LE180	Fair	Good	Fair	Fair	Good	Fair	Fair	Good
LE200	Marginal	Fair	poor	poor	Fair	Fair	Fair	Good
LE210	Marginal	Fair	poor	poor	Fair	Fair	Fair	Good
LE220	Fair	Fair	Marginal	poor	Fair	Fair	Fair	Good
LE310	Good	Good	Fair	Fair	Fair	Fair	Fair	Good
LE330	Good	Good	Fair	Good	Good	Fair	Fair	Good
LE340	Good	Good	Fair	Good	Good	Fair	Fair	Good
LE380	Good	Good	Fair	Good	Good	Good	Fair	Good
LE420	Good	Good	Fair	Good	Good	Fair	Fair	Good
LE430	Good	Good	Good	Good	Good	Good	Fair	Good
LE450	Good	Good	Good	Good	Good	Good	Fair	Good
LE500	Marginal	Fair	poor	poor	Fair	Fair	Fair	Good
LE505	Marginal	Fair	poor	poor	Fair	Fair	Fair	Good
LE510	Fair	Fair	Marginal	poor	Fair	Fair	Fair	Good
LE540	Good	Good	Good	Good	Good	Good	Fair	Good
LE550	Good	Good	Good	Good	Good	Good	Fair	Good
LE620	Good	Good	Good	Good	Good	Good	Good	Good
LE630	Good	Good	Good	Good	Good	Good	Good	Good
LE810	Good	Good	Good	Good	Good	Good	Good	Good
LE820	Good	Good	Good	Good	Good	Good	Good	Good

Table 4.S9 Water quality status of monitoring sites in Cork Harbour during the summer period.

Monitoring Sites	NSF	WQM	SRDD	WJ	RMS	AM	Hanh	CCME
LE030	Marginal	Fair	poor	poor	Fair	Fair	Fair	Good
LE040	poor	Marginal	poor	poor	Fair	Marginal	poor	Good
LE110	poor	Marginal	poor	poor	Fair	Marginal	poor	Good
LE120	poor	Marginal	poor	poor	Fair	Marginal	poor	Good
LE130	poor	Marginal	poor	poor	Fair	Marginal	poor	Good
LE140	poor	Marginal	poor	poor	Fair	Marginal	poor	Good
LE150	poor	Fair	poor	poor	Fair	Fair	poor	Good
LE160	poor	Fair	poor	poor	Fair	Fair	poor	Good
LE170	Marginal	Fair	poor	poor	Fair	Fair	Marginal	Good
LE180	Marginal	Fair	poor	poor	Fair	Fair	Fair	Good
LE200	poor	Marginal	poor	poor	Fair	Marginal	poor	Good
LE210	poor	Marginal	poor	poor	Fair	Marginal	poor	Good
LE220	poor	Marginal	poor	poor	Fair	Marginal	poor	Good
LE310	Fair	Fair	Marginal	Marginal	Fair	Fair	Fair	Good
LE330	Marginal	Fair	poor	poor	Fair	Fair	Marginal	Good
LE340	Fair	Fair	Marginal	Fair	Good	Fair	Fair	Good
LE380	Marginal	Fair	poor	poor	Fair	Fair	Marginal	Good
LE420	Fair	Fair	Marginal	Marginal	Fair	Fair	Fair	Good
LE430	Fair	Fair	Marginal	Marginal	Fair	Fair	Fair	Good
LE450	Fair	Fair	Marginal	Fair	Fair	Fair	Fair	Good
LE500	poor	Marginal	poor	poor	Fair	Marginal	poor	Good
LE505	poor	Marginal	poor	poor	Fair	Marginal	poor	Good
LE510	poor	Marginal	poor	poor	Fair	Marginal	poor	Good
LE540	Fair	Fair	Fair	Fair	Good	Good	Good	Good
LE550	Fair	Fair	Fair	Fair	Good	Good	Fair	Good
LE620	Good	Good	Fair	Good	Good	Good	Good	Good
LE630	Good	Good	Good	Good	Good	Good	Good	Good
LE810	Good	Good	Good	Good	Good	Good	Good	Good
LE820	Good	Good	Good	Good	Good	Good	Good	Good

Table 4.S10. MCS results for model input entities with 95% confidence interval at $p < 0.0001$, N= 29.

Input entities		*Summer (2019)*		Uncertainty interval	
(a)Water quality parameters	Eq.	Types of PDF	PDF parameters	Parametric	Nonparametric
CHL		Normal	Mean = 5.32; SD = 3.22	μ = 5.29 ± 6.41 (95%)	μ = 5.30 ± 6.43 (95%)
DIN		Normal	Mean = 1.54; SD = 1.78	μ = 1.54 ± 3.54 (95%)	μ = 1.53 ± 3.54 (95%)
AMN		Normal	Mean = 0.07; SD = 0.056	μ = 0.07 ± 0.112 (95%)	μ = 0.069 ± 0.111 (95%)
TEMP		Normal	Mean = 15.59; SD = 0.74	μ = 15.59 ± 1.47 (95%)	μ = 15.59 ± 1.48 (95%)
BOD		Normal	Mean = 1.73; SD = 0.87	μ = 1.72 ± 1.72 (95%)	μ = 1.73 ± 1.72 (95%)
MRP		Normal	Mean = 0.02; SD = 0.011	μ = 0.0264 ± 3.516 (95%)	μ = 0.02 ± 0.02 (95%)
TRAN		Logistic	location = 1.448; scale = 0.796	μ = 1.45 ± 2.87 (95%)	μ = 1.45 ± 2.87 (95%)
(b)Sub-index	Eq.				
CHL	(1)	Normal	Mean = 62.53; SD = 22.66	μ = 84.82± 57.26(95%)	μ = 84.91 ± 57.04 (95%)
DIN	(1)	Normal	Mean = 43.41; SD = 43.50	μ = 10.92 ± 48.32 (95%)	μ = 10.85 ± 48.09 (95%)
AMN	(1)	Triangular	Mean = 95.24; SD = 3.68	μ = 57.25 ± 47.50 (95%)	μ = 57.28 ± 47.52 (95%)
TEMP	(binary)	Uniform	Min. = 99.5; Max = 100.0	μ = 100 ± 0 (95%)	μ = 100 ± 0 (95%)
BOD	(1)	Normal	Mean = 74.97; SD = 12.57	μ = 72.9 ± 32.1 (95%)	μ = 72.9 ± 31.89 (95%)
MRP	(1)	Normal	Mean = 65.21; SD = 19.47	μ = 61.85 ± 40.82 (95%)	μ = 61.77 ± 40.82 (95%)
TRAN	(3 and binary)	Normal	Mean = 68.10; SD = 46.72	μ = 76.2 ± 77.0 (95%)	μ = 75.93 ± 76.09 (95%)
(c) Parameters weight		Normal	Mean = 0.142, SD = 0.123	μ = 0.142 ± 0.245(95%)	μ = 0.143 ± 0.245 (95%)
(a) Water quality parameters		*Winter (2019)*			
DIN		Normal	Mean = 2.51; SD = 2.07	μ = 95.94 ± 3.05 (95%)	μ = 95.94 ± 3.05 (95%)
TON		Normal	Mean = 2.64; SD = 2.208	μ = 2.64 ± 4.41 (95%)	μ = 2.65 ± 4.42 (95%)
pH		Normal	Mean = 7.78; SD = 0.149	μ = 7.78 ± 0.29 (95%)	μ = 7.78 ± 0.29 (95%)
DOX		Normal	Mean = 95.94; SD = 3.48	μ =2.51± 4.13 (95%)	μ = 2.52 ± 4.11 (95%)
TRAN		Normal	Mean = 1.47; SD = 1.52	μ = 1.46 ± 3.03 (95%)	μ = 1.46 ± 3.02 (95%)
(b) Sub-index	Eq.				
DIN	(1)	Normal	Mean = 21.45; SD = 31.87	μ = 85.45 ± 10.82 (95%)	μ = 85.45 ± 10.78 (95%)
TON	(1)	Normal	Mean = 30.64; SD = 35.46	μ = 11.86 ± 49.26 (95%)	μ = 12.02 ± 49.17 (95%)
pH	(binary)	Uniform	Min. = 99.5; Max. = 100	μ = 99.93 ± 1.04 (95%)	μ = 99.9 ± 1.04 (95%)
DOX	(2, 3 and binary)	Normal	Mean = 85.70; SD = 11.71	μ = 44.28 ± 37.23 (95%)	μ = 6.88 ± 39.38 (95%)
TRAN	(3 and binary)	Normal	Mean = 58.62; SD = 50.12	μ = 73.39 ± 79.61 (95%)	μ = 73.42 ± 79.82 (95%)
(c)Parameters weight		Normal	Mean = 0.202, SD = 0.1630	μ = 0.273 ± 0.187 (95%)	μ = 0.233 ± 0.184 (95%)

Table 4.S11. MCS results for model output entities with 95% confidence interval at p < 0.0001, N= 29.

Aggregation functions	Eq.	PDF	PDF parameters	Uncertainty interval	
		Summer (2019			
(a) Weighted				Parametric	Nonparametric
NSF	(4)	Normal	Mean = 68.83; SD = 23.53	µ = 63.53 ± 32.96 (95%)	µ = 63.56 ± 32.77 (95%)
WQM	(5)	Normal	Mean = 78.36; SD = 14.96	µ = 74.85 ± 24.02 (95%)	µ = 74.81 ± 23.28 (95%)
SRDD	(6)	Normal	Mean = 52.92; SD = 29.78	µ = 43.05 ± 39.32 (95%)	µ = 43.05 ± 39.63 (95%)
WJ	(7)	Normal	Mean = 48.04; SD = 41.25	µ = 15.03 ± 69.31 (95%)	µ = 15.05 ± 69.35 (95%)
(b) Unweighted					
RMS	(8)	Normal	Mean = 72.78; SD = 11.03	µ = 74.97 ± 13.15 (95%)	µ = 74.96 ± 13.18 (95%)
AM	(9)	Normal	Mean = 79.32; SD = 6.54	µ = 66.22 ± 19.12 (95%)	µ = 66.27 ± 19.13 (95%)
Hanh	(10)	Normal	Mean = 68.52; SD = 8.81	µ = 62.01 ± 33.1(95%)	µ = 62.0 ± 37.21 (95%)
CCME	(11)	Normal	Mean = 96.87; SD = 2.72	µ = 96.88± 5.45 (95%)	µ = 96.88 ± 5.45 (95%)
		Winter (2019)			
(a) weighted					
NSF	(4)	Normal	Mean = 44.92; SD = 25.87	µ = 33.0 ± 25.64 (95%)	µ = 32.9 ± 25.72 (95%)
WQM	(5)	Normal	Mean = 59.01; SD = 16.41	µ = 53.56 ± 17.12 (95%)	µ = 53.63 ± 17.09 (95%)
SRDD	(6)	Normal	Mean = 25.99; SD = 27.77	µ = 12.53 ± 22.37 (95%)	µ = 12.52 ± 22.33 (95%)
WJ	(7)	Normal	Mean = 26.38; SD = 35.72	µ = 1.66 ± 19.33 (95%)	µ = 1.66 ± 19.3 (95%)
(b) Unweighted					
RMS	(8)	Normal	Mean = 72.60; SD = 10.83	µ = 71.07 ± 14.32 (95%)	µ = 71.07 ± 14.38 (95%)
AM	(9)	Normal	Mean = 59.29; SD = 19.42	µ = 6.60 ± 5.0 (95%)	µ = 6.61 ± 5.13 (95%)
Hanh	(10)	Normal	Mean = 38.38; SD = 36.08	µ = 8.46 ± 37.93(95%)	µ = 8.47 ± 38.06 (95%)
CCME	(11)	Normal	Mean = 94.36; SD = 2.20	µ = 94.36 ± 4.37 (95%)	µ = 94.36 ± 4.39 (95%)

References

Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment. Water Res. 219, 118532. https://doi.org/10.1016/j.watres.2022.118532

Appendix 5. Performance analysis of the water quality index model for classification water state using machine learning techniques

Table 5.S1 Averaged concentrations in the Cork Harbour, Cork, Ireland (2019) and computed pollution status used for input to XGBoost model for selecting crucial indicators. The guideline values adopted for the research are included at the bottom and values in bold indicate compliance failures.

Monitoring sites	CHL (mg/m^3)	DOX (% sat)	MRP (μg/l as P)	DIN (mg/l)	AMN (mg/l)	BOD5 (mg/l)	pH -	Temp (^0C)	TON (mg/l as N)	Tran. (m/depth)	PS*
LE030	1	**69.333**	0.012	**3.423**	0.26	1.37	7.6	15	**3.17**	0	1
LE040	1.9	103.333	0.011	**2.258**	0.06	3.55	7.93	15.43	**2.2**	0	1
LE110	2.033	98	0.015	**1.992**	0.025	1.3	7.73	16.8	1.97	0	1
LE120	1.45	93.333	0.018	**2.64**	0.039	1.33	7.67	16.13	**2.6**	**0**	1
LE130	2.5	89.333	0.028	**2.394**	0.06	1.25	7.77	15.83	**2.3**	1.5	1
LE140	2.067	93.333	0.025	**2.357**	0.057	1.2	7.7	15.53	**2.3**	**0**	1
LE150	4.283	90.167	0.025	1.001	0.11	1.86	7.81	15.83	0.89	2.18	0
LE160	3.25	88.833	0.027	1.105	0.16	0	7.83	15.75	0.95	2.26	0
LE170	7.518	102	0.019	0.731	0.12	2	7.97	15.84	0.65	1.77	0
LE180	7.8	109.167	0.014	0.709	0.1	0	8.05	15.68	0.61	1.9	0
LE200	2.6	101.333	**0.064**	**6.021**	0.021	1.9	7.7	14.83	**6**	**0**	1
LE210	2	103	0.046	**4.587**	0.02	0	7.77	14.77	**4.57**	**0**	1
LE220	5.967	101	0.023	**1.351**	0.068	2.17	7.93	16.6	1.28	**0.75**	1
LE310	7.6	112.5	0.015	0.584	0.09	2.48	8.25	15.7	0.14	1.53	0
LE330	9.442	123.667	0.011	0.246	0.11	2.38	8.24	15.82	0.14	1.65	0
LE340	10.233	121.333	0.011	0.234	0.09	2.48	8.25	15.7	0.14	1.53	0
LE380	10.433	119.5	0.008	0.12	0.056	2.55	8.21	15.57	0.064	1.83	0
LE420	8.85	**136.167**	0.022	0.092	0.035	2.7	8.33	16.6	0.057	1.53	1
LE430	9.6	**130.833**	0.012	0.077	0.028	2.25	8.28	16.17	0.048	1.8	1
LE450	7.65	120.667	0.034	0.076	0.036	1.1	8.23	15.4	0.04	2.3	0
LE500	3.15	106.667	0.024	**4.861**	0.027	2	7.8	16.27	**4.83**	**0**	1
LE505	1.8	104.333	0.021	**5.186**	0.19	1.3	7.8	15.07	**5.17**	**0**	1
LE510	9.82	**133.2**	0.02	**2.382**	0.064	3.2	8.16	16.9	**2.318**	1.05	1
LE540	9.8	124	0.008	0.066	0.03	1.1	8.25	15.65	0.036	2.03	0
LE550	6.467	121.833	0.013	0.075	0.038	2.48	8.22	15.73	0.037	2.23	0

LE620	5.06	110.333	0.007	0.052	0.04	1.68	8.18	14.5	0.017	3.87	0
LE630	4.175	105.333	0.014	0.064	0.036	2	8.15	14.17	0.28	3.4	0
LE810	3.167	113.667	0.018	0.056	0.031	1.65	8.16	14.8	0.026	5.6	0
LE820	2.7	103	0.017	0.038	0.038	1.1	8.13	13.9	0	4.83	0
Criteria	**0 - 14.2**	**72 - 128**	**0 - 0.057**	**0 - 1.208**	**0 - 1.5**	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	

PS = Pollution Status; 0 = unpolluted; 1= polluted; bolded underline is breached the criteria

Table 5.S2 Calculated WQI values and determined water quality classes for different WQI models in the Cork Harbour, Cork, Ireland.

Monitoring	Weighted WQI models				Unweighted WQI models			Weighted WQI models				Unweighted WQI models		
sites	NSF	WQM	SRDD	WJ	RMS	AM	Hanh	NSF	WQM	SRDD	WJ	RMS	AM	Hanh
LE030	37	58	14	0	74	62	65	Marginal	Fair	poor	poor	Fair	Fair	Fair
LE040	37	58	13	0	71	59	62	Marginal	Fair	poor	poor	Fair	Fair	Fair
LE110	37	59	14	0	75	63	64	Marginal	Fair	poor	poor	Fair	Fair	Fair
LE120	37	59	14	0	74	62	65	Marginal	Fair	poor	poor	Fair	Fair	Fair
LE130	72	83	52	0	80	73	77	Fair	Good	Fair	poor	Good	Fair	Fair
LE140	36	57	13	0	72	60	63	Marginal	Fair	poor	poor	Fair	Fair	Fair
LE150	75	82	56	62	78	73	74	Fair	Good	Fair	Fair	Fair	Fair	Fair
LE160	74	83	54	53	82	75	78	Fair	Good	Fair	Fair	Good	Fair	Fair
LE170	78	82	61	72	77	74	68	Fair	Good	Fair	Fair	Fair	Fair	Fair
LE180	79	83	63	74	83	79	70	Fair	Good	Fair	Fair	Good	Fair	Fair
LE200	33	56	11	0	67	50	56	Marginal	Fair	poor	poor	Fair	Fair	Fair
LE210	35	57	12	0	73	58	61	Marginal	Fair	poor	poor	Fair	Fair	Fair
LE220	61	70	37	0	72	65	65	Fair	Fair	Marginal	poor	Fair	Fair	Fair
LE310	81	84	65	77	79	76	69	Good	Good	Fair	Fair	Fair	Fair	Fair
LE330	86	88	74	82	82	79	64	Good	Good	Fair	Good	Good	Fair	Fair
LE340	86	89	73	81	82	78	60	Good	Good	Fair	Good	Good	Fair	Fair
LE380	88	91	78	83	84	80	60	Good	Good	Fair	Good	Good	Good	Fair
LE420	89	91	79	85	82	79	66	Good	Good	Fair	Good	Good	Fair	Fair
LE430	89	92	80	85	85	81	65	Good	Good	Good	Good	Good	Good	Fair
LE450	90	92	80	87	84	80	71	Good	Good	Good	Good	Good	Good	Fair
LE500	35	56	12	0	70	58	60	Marginal	Fair	poor	poor	Fair	Fair	Fair
LE505	36	57	13	0	72	60	63	Marginal	Fair	poor	poor	Fair	Fair	Fair
LE510	67	79	45	0	73	64	55	Fair	Fair	Marginal	poor	Fair	Fair	Fair
LE540	90	93	81	86	88	85	65	Good	Good	Good	Good	Good	Good	Fair
LE550	92	93	84	90	86	84	76	Good	Good	Good	Good	Good	Good	Fair
LE620	94	95	88	93	90	89	83	Good	Good	Good	Good	Good	Good	Good
LE630	94	94	88	93	88	87	84	Good	Good	Good	Good	Good	Good	Good
LE810	94	95	89	94	89	88	86	Marginal	Fair	poor	poor	Fair	Fair	Fair
LE820	95	96	91	95	91	90	89	Marginal	Fair	poor	poor	Fair	Fair	Fair

Appendix 6. Assessing optimization techniques for improving water quality model

6.4.3.1 Different features selection (FS) algorithms

6.4.3.1.1 Supervised techniques

(a) Wrapper

(i) Recursive features elimination –support vector machine (RFE_SVM)

RFE technique is a popular feature-selecting algorithm in machine learning technique. It is an effective method to select most relevant subset of features from the given dataset. This technique widely used for classification problem (Lin et al., 2012); whereas the SVM algorithm allows hyperplane that divides between classes the most using linear kernel functions (Jeon and Oh, 2020). Recently, several studies have widely used the SVM-based RFE approach for selecting importance variables by evaluating their relative significant with response variable in a dataset (Adorada et al., 2018; Jeon and Oh, 2020; Lin et al., 2012). In order to select the crucial water quality indicators, RFE_SVM algorithm utilized according of Granitto et al., (2006) in this study. For instance, $D(x)$ is the function for the hyperplane of SVM, and n is the number of classes. Number of hyperplane can be defined as follows:

$$N = \frac{n(n-1)}{2} \qquad (6.1)$$

Where N is the number of hyperplane; while the decision function denotes for the binary classification as follows:

$$D(x) = sign(x * w) \qquad (6.2)$$

Where, $D(x)$ is the decision function; x is a vector with the water quality indicators of a given dataset, and w is a vector perpendicular to the hyperplane that provides a linear decision function.

Finally, weight values are obtained for each water quality indicator to evaluate its relative importance with response using equation (3) based on the RFE_SVM decision.

$$W_{svm} = \frac{1}{N}\sum_{i=1}^{N} w_i \qquad (6.3)$$

where w_i weight value of i^{th} *water quality indicators.*

(ii) Recursive features elimination (RFE) – random forest (RF)

Like RFE_SVM, RF-based RFE follows also similar process to identify the relevant features with the response variables in a dataset (Jeon and Oh, 2020). Many studies have used RF-based RFE algorithm for selecting water quality indicators (Bahl et al., 2019; Pullanagari et al., 2018). Commonly, the RFE_RF technique claculates the features important using two approaches including the mean decrese in accruarcy and the mean decrese in Gini. For the purposes of the this research, the the mean decrese in accruarcy technique was utilized to select the importance water quality using approach of Jeon and Oh, (2020). Details of the algorithm can be found in Granitto et al., (2006) and Jeon and Oh, (2020). It can be defined as follows :

$$W_{RF}(X_i) = \frac{\sum_{t\epsilon B} I^t(X_i)}{N} \qquad (6.4)$$

Where B is the out-of-bag observations of a tree t; I is the crucial indicators X_i in tree t; and N is number of tree.

(b) Embedded techniques

(i) Extreme gradient boosting (XGBoost) algorithm

XGBoost algorithm is widely used machine learning technique for selecting important variables based on their relative important (Islam Khan et al., 2021; Uddin et al., 2022a). Recently several studies have utilized this technique to select the crucial water quality indicators for assessing water quality (Islam Khan et al., 2021; Naghibi et al., 2020; Uddin et al., 2022a). For the purposes of identifying the important indicators, the present study was utilized the XGBoost algorithm according to the approach of Uddin et al., (2022a). Details of this technique can be found in Uddin et al., (2022a). Like most machine learning techniques, XGBoost uses decision trees to develop models that predict the value of a dependent variable (the model output) based on the values of input variables or features. XGBoost can therefore be used to identify the relative importance of features with respect to their influence on the dependent variable. In this application, we use the water quality parameter data as the XGBoost input and the water quality status as the dependent variable. Implementation of XGBoost for parameter selection involves the following five steps.

(ii) Random forest

Random forest (RF) is a common binary classification algorithm. This algorithm was developed using a decision tree (DT) model in combination. Recently, this approach is widely used in machine learning models for selecting important features from large data sets (Bagherzadeh et al., 2021; K. Chen et al., 2020; Jović et al., 2015; Mao et al., 2022; Speiser et al., 2019). Several studies have utilized this technique for identifying the crucial indicators to develop prediction (Alnahit et al., 2022; Hou et al., 2022; Malek et al., 2022; Sakaa et al., 2022). During the creation of a decision tree, the bootstrap aggregation method is used to improve classification accuracy and obtain samples for each tree at random (R. C. Chen et al., 2020). M leaves are used to build a DT along the respective regions of leaves $R_m, 1 \leq m \leq M$. For each tree, prediction function f(x) used to produce the GiNi score for each features individually and creates a new subset of the features (K. Chen et al., 2020). The prediction function is written as follows:

$$f(x) = \sum_{m=1}^{M} c_m \prod (x, R_m) \tag{6.5}$$

Where M denotes the number of regions in the features space, R_m is the region that corresponds to m, c_m is a constant that relates to m.

$$\prod (x, R_m) = \{ \begin{matrix} 1, & if\ x, R_m \\ 0, & otherwise \end{matrix} \tag{6.6}$$

The Gini scores are obtained by voting scores of each DT (Ali Khan et al., 2022). Finally, the important features are chosen from the new subset based on the Gini score of the features. The optimum features are typically sorted from highest to lower Gini ratings (Menze et al., 2009).

(iii) Extreme tree algorithm (ExT)

ExT is another tree-based ensemble algorithm that is widely used for classification and regression analysis. In machine learning models, it is used for extracting important features to minimize the computational cost and increase the model prediction performance (Deng and Runger, 2012; Khaire and Dhanalakshmi, 2022). Recently, several studies have used this technique for the selection of crucial water quality indicators (Asadollah et al., 2021; Hannan and Anmala, 2021a; Malek et al., 2021; Uddin et al., 2022a). In this research, the ExT classifier algorithm was utilized to select important water quality indicators for the assessment of water quality by following the approach of Asadollah et al., (2021) because, relatively, this algorithm is much faster than the RF method in terms of computational performance. Details methodology can be found in Asadollah et al., (2021). It allows all original observations to be predicted without any subsampling. In this study, this algorithm was performed following the approach described (Hannan and Anmala, 2021).

(iv) Boruta

Boruta is another widely used feature selection method that is an extended algorithm of the random forest (RF) (R. C. Chen et al., 2020). Commonly, features are ranked based on the statistical significance of the features. Detail of the algorithm and procedures can be found in Kursa et al., (2010). The present study, The model was run several times to ensure that all features were confirmed. Significant validation of all features was used to decide the best run. Then, for the validation of important features, maxRun was set to run 100 times. Boruta completed 99 iterations in 2.98117 seconds, confirming all features, nine of which were deemed significant and two of which were deemed unimportant.

(v) Linear Regression (LR)

Linear regression model widely used to analyse the relationship between two or multiple scalar variables. Recently several studies have utilized this technique for the selection of crucial features within a dataset (Chen et al., 2017; Hasan et al., 2015; Kuhn and Johnson, 2013; Şahin et al., 2021; Sharifzadeh et al., 2014). In this research, the LR model used to extract the crucial water quality indicators using classification algorithms according to the approach of Alnahit et al., (2022) . Detail of the procedure can be found in Alnahit et al., (2022).

(vi) Least Absolute Shrinkage and Selection Operator (LASSO)

The LASSO is widely used for regularization and feature selection approaches

(Bagherzadeh et al., 2021). It is a popular technique for extracting and sorting important features from a given dataset in the field of machine learning , or data science and engineering applications (Ghosh et al., 2021; Liu et al., 2022; Vasquez et al., 2016; Yan and Yao, 2015). For the purposes of developing a prediction model for assessing water quality, several studies have utilized this technique to select the crucial water quality indicators (Alnahit et al., 2022; Bagherzadeh et al., 2021; Narala et al., 2021). In this research, the LASSO algorithm was utilized to select the crucial water quality indicators because it optimizes the prediction errors and avoids the model over fitting problem with a number of covariates (Narala et al., 2021). Prior to performing the LASSO, it's required to standardize data to avoid the preferential elimination of water quality indicators. Once the absolute values were obtained for model parameters, a constraint value was generated by LASSO. The sum of model parameters must be smaller than the constant value (Alnahit et al., 2022; Gharari et al., 2014). During the processes, the regression coefficient tends to shrink to zero, whereas the model nonzero parameters could influence the model accuracy after the regularization process (Bagherzadeh et al., 2021; Bardsley et al., 2015). The linear LASSO for the feature selection can be defined as follows the equation (7):

$$Minimize, \quad \sum_{t=1}^{N} \left| y_t - \left(\alpha_o + \sum_{i=1}^{j} X_{it}\, \alpha_i \right) \right| + \partial \sum_{i=0}^{j} |\alpha_i| \qquad (6.7)$$

whereas, N is the number of indicators, y is the dependent water quality indicators, j is the independent water quality indicators, ∂ is the constant value, α_o is the coefficient value to zero, α_i is the preferentially forced to zero whereas X is the first standardized to dimensionless values.

(vii) Stepwise generalized linear regression model (SWGLM)

The SWGLM approach is a combined technique of forward selection and backward elimination methods. This technique is widely used for selecting the important features in a given dataset in the field of data science (Del Castillo et al., 2022; Kano and Harada, 2000; Zhang, 2016). A few studies have utilized this technique for extracting the crucial water quality indicators for forecasting water quality (Haque et al., 2018). The present study used the SWGLM with the forward selection method according to the approach of Zhang, (2016). Details of the methodology can be found in Zhang, (2016). Like the forward selection technique, the model is initialized without variables, whereas variables are added into the model one by one and checked for the statistical significant criteria of p (p <0.01) (Haque et al., 2018). This process continues up to the point of meeting the satisfaction level of the criteria. The best-fit model was developed and the key variables were suggested based on satisfactions criteria.

(c) Filter

(i) Mutual Information (MI)

MI is a statistical measure of the nonlinear relationship between two independent variables (predictors and response), which is not like the popular correlation coefficient (Bennasar et al., 2015; Zhou et al., 2022). It is widely used for selecting relevant features in an account to measure the amount of information that a random variable contains in another random variable (Liang et al., 2019; Lin et al., 2012; Zhou et al., 2022). This technique allows one to measure the uncertainty of random variables. The information content of random variables is measured using the entropy theory. The entropy of a discrete random variable X $= (X_1, X_2, \ldots \ldots X_N)$ can be denoted as follows:

$$H(X) = -\sum_{i=1}^{N} P(X_i)\, log\big(P(X_i)\big) \qquad (6.8)$$

where P(X_i) is the prior probabilities for all values of X. P(X_i) can be defined as

$$\mathrm{P}(X_i) = \frac{number\ of\ instants\ value\ of\ X_i}{toatal\ number\ of\ instants\ (N)}$$

For the entropy of two discrete random variables (joint entropy) X and Y $= (Y_1, Y_2, \ldots \ldots Y_M)$ can be defined as follows:

$$H(X,Y) = -\sum_{j=1}^{M}\sum_{i=1}^{N} P\big(X_i, Y_j\big) log(P\big(X_i, Y_j\big)) \qquad (6.9)$$

Where $P\big(X_i, Y_j\big)$ is the joint probability mass function of the X and Y. The conditional entropy of the variable X given Y is expressed as:

$$H(Y|X) = -\sum_{j=1}^{M}\sum_{i=1}^{N} P(X_i, Y_j) log(P(X_i, Y_j)) \quad (6.10)$$

The conditional entropy is the uncertainty level of random variables, whereas it should be less than or equal to the basic entropy of both variables (Bennasar et al., 2015; Vergara and Estévez, 2014). Usually, it is possible to equal the entropy if, and only if, the two variables are independent (Bennasar et al., 2015). The relationship between joint and conditional entropy is defined as equation (11) and equation (12), respectively.

$$H(X,Y) = H(X) + H(Y|X) \quad (6.11)$$

$$H(X,Y) = H(Y) + H(X|Y) \quad (6.12)$$

Once the joint and conditional entropy were obtained for both variables, and then the amount of information was calculated using equation (13).

$$I(X;Y) = H(X) - H(X|Y) = H(Y) - H(Y|X) \quad (6.13)$$

where I is the amount of mutual information between X and Y.

However, commonly higher I values indicate the more relevancy between variables [(water quality indicators (predictors) and status of water quality classes (response)] (Barraza et al., 2019; Bennasar et al., 2015; Yang et al., 2011) Details of the water quality indicators and classes can be found in Table S3. The higher I obtained when two variables are independent, the lower I obtained when the joint entropy drops down (Bagherzadeh et al., 2021).

(ii) Relief

The relief algorithm is a filter based algorithm for selecting relevant features. Recently, this technique is widely used because it is more effective than other filter methods in order to select important features from a given dataset (Eiras-Franco et al., 2021; Stief et al., 2020; Urbanowicz et al., 2018; Yang et al., 2011). Relief provides a proxy statistic for each water quality indicator that could be utilized to evaluate the indicators' relevance to the target (model response variable). Commonly, indicator statistics refer to the weight value of the indicators, it ranges from -1 (less relevant) to +1 (most relevant) (Urbanowicz et al., 2018). A number of studies have utilized this technique for selecting crucial water quality indicators to develop more accurate predicting models with the most relevant indicators (Gong et al., 2022; Nikitin et al., 2021; Rizal and Apriliani, 2021). The present study used this technique by following the approach of Urbanowicz et al., (2018). Details of the algorithm can be found in Urbanowicz et al., (2018).

6.4.3.1.2 Unsupervised techniques

(a) Univariate or filter methods

(i) Chi-squared test or χ^2 statistics

To determine the importance of variations between classes, the chi-square test is used. It also provides categorical information regarding features that differ between classes. Unlike other selection methods, the $\boldsymbol{\chi^2}$ a test can be used to perform a null hypothesis test based on differences between observed and expected frequency, rather than requiring data to have a normal distribution (Liu et al., 2020). Usually, χ^2 Statistics are used to estimate the importance of each feature individually by comparisons between classes (Chandra and Gupta, 2011). The score of χ^2 is calculated by the following equation:

$$\chi^2 = \sum_{x \in x_i} \sum_{c \in C} \frac{\left(\eta_{(x \epsilon x_{i\,\&} c \epsilon C)} - \delta_{(x \epsilon x_{i\,\&\,c \epsilon C})}\right)^2}{\delta_{(x \epsilon x_{i\,\&\,c \epsilon C})}} \qquad (6.14)$$

Where, $\eta_{(x \epsilon x_{i\,\&} c \epsilon C)}$ is the number of samples in x_i for class *C* whose value is *x*. The predicted frequency $\delta_{(x \epsilon x_{i\,\&\,c \epsilon C})}$ is defined as:

$$\delta_{(x \epsilon x_{i\,\&\,c \epsilon C})} = \frac{\eta_{x \in x_i} \times \eta_{c \epsilon C}}{\eta} \qquad (6.15)$$

Where $\eta_{x \in x_i}$ is the number of samples in x_i, $\eta_{c \epsilon C}$ is the number of samples of class *C*. η denotes the total number of samples (x_i and *C*). Impotence features are ranked based on the score of χ^2 statistics.

(iv) K_Best Score

K-best is a straightforward univariate feature selection technique widely used for selecting relevant features based on the highest average relevance scores of K (Rojas et al., 2015; Subasi, 2020). It yields an individual score for each feature, and the K score is employed to evaluate the relevance of the features (Zhou et al., 2012). Several studies have utilized this technique for selecting the most relevant features to develop efficient models in machine learning techniques. In this research, this technique was utilized by performing the SelectKBest function from the sklearn.feature_selection module in Python to select crucial water quality indicators for developing a WQI model (Subasi, 2020). Details of the procedures can be found in Subasi, (2020).

(v) F-test

The F-test is a one-way ANOVA based statistical test. It is widely used to test hypotheses. Recently, several studies have utilized this technique for selecting relevant features to develop more precise models in machine learning applications (Elssied et al., 2014; Lindsey and Sheather, 2010; Méndez et al., 2006). In this research, the F-test was used for selecting crucial water quality indicators for developing a WQI model focusing on coastal water quality (Leščešen et al., 2016; Samandar, 2010). For the purposes of selecting relevant indicators, the test was performed according to Méndez et al., (2006). Details of the procedures can be found in Méndez et al., (2006).

(vi) Laplacian Score (LAP)

LAP is another widely used unsupervised technique for selecting relevant features in a given dataset(George et al., 2020; Liu et al., 2009). It is evaluated the important features using its power of locality preserving or Laplacian score(He et al., 2005). Recently, many researchers have utilized this technique for identifying the most relevant indicators from unlabelled water quality dataset because it is difficult to extract important indicators using supervised technique (Liu et al., 2016; Zhang and Xin, 2017). The present study was performed this technique according of He et al., (2011). Details of the algorithm can be found in He et al., (2011).

(vii) Pearson Correlation analysis (PCOR)

PCOR is another popular dimensionality reduction technique that is widely used to leave-out less significant features or variables from the analysis in order to predict accurately (He et al., 2021; Jain et al., 2018; Kowshalya et al., 2019; Ning et al., 2018). Commonly, the analysis examines the correlation among the features within a dataset and removes the features that have high variance (Seo and Cho, 2020). In recent research, several researchers have utilized this technique for selecting crucial water quality indicators based on data variances among features (Alizadeh et al., 2018; Bonansea et al., 2015; Kothari et al., 2021; Kouadri et al., 2021; Kumar and Chong, 2018; Muhammad et al., 2021). In this research, this technique was used for selecting the most relevant water quality indicators in terms of assessing coastal water quality by following the approaches of Biesiada and Duch, (2007). Details of the methodology can be found in Biesiada and Duch, (2007). It is noted that setting a criterion for determining the correlation between features is required when choosing significant features using PCOR (Bagherzadeh et al., 2021). Therefore, Due to the possibility of overfitting problems, highly correlated features were therefore not taken into account in this study. The present study considered a correlation value of between + 0.75 and + 0.80 for selecting crucial water quality indicators. The relationship between the indicators of coastal water quality is shown in Figure S1.

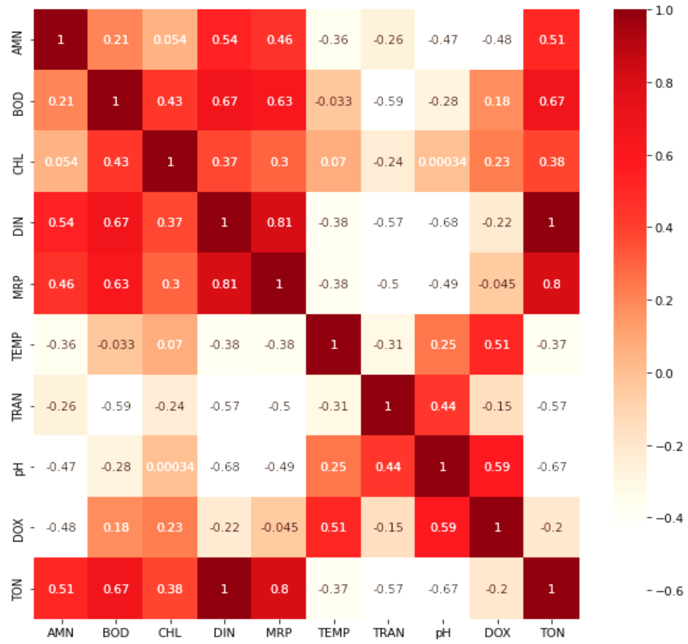


Fig. 6.S1 Pearson correlation between water quality indicators.

The correlation coefficient r_{ij} between a given feature X_i and all other features of the dataset X_j . It can be defined as follows:

$$r_{ij} = \frac{Cov(X, X_j)}{\sqrt{Var(X_i)Var(X_j)}} \quad (6.16)$$

(viii) Principal component analysis (PCA)

PCA technique is widely utilized in the field of computer science for transforming high dimensional data into low dimension (Song et al., 2010). It is a kind of vector transformation technique that allows the observe variables transform into a new uncorrelated variables vector position with loading linear combinations of the original data (Adhao and Pachghare, 2020; Parinet et al., 2004; Shrestha and Kazama, 2007). The new variables vector position composed with along the direction of the highest variance of original variables (Wang et al., 2013). Commonly, this technique used to extract the most important relative variables that are representing the characteristics of the entire data set, resulting in data reduction in terms of minimum loss of original data information (Shrestha and Kazama, 2007). Recently, several studies have used this technique for selecting important water quality indicators to assess water quality using minimal indicators with reducing uncertainty (Liou et al., 2004; Ma et al., 2020; Mahapatra et al., 2012; Mohammed Siraj Ansari and Saraswathi, 2022; Tripathi and Singal, 2019). The present study was used PCA analysis to identify the important monitoring sites based on the relative importance of water quality variables. It can be denoted as follows:

$$z_{in} = c_{f1}x_{1i} + c_{f2}x_{2i} + c_{f3}x_{3i} + \cdots + c_{fm}x_{mi} + e_{fi} \qquad (6.17)$$

where, z is the observed value of component score, c is the component loading, x is the observed value of variable, i is the number of variable, n is the sample number, f is the factor score, m is the total number of components, and e is the residual for considering errors or any variation of variables.

(b) Multivariate

(i) Minimum Redundancy Maximum Relevance (MRMR)

The MRMR algorithms can find an optimal set of features that is mutual and maximally dissimilar (Zhao et al., 2019). It can focus the response variable effectively in a data set. This algorithm quantifies the redundancy and relevance using the mutual information of variables based on the pairwise mutual information of features (Ding and Peng, 2005; Radovic et al., 2017). Commonly this algorithm used to solve classification problems. The highest relevance features selector defined as:

$$V_s = \frac{1}{|S|}\sum_{x \in S} I(x, y) \qquad (6.18)$$

where S is the optimal set of the features, V_s is the maximize relevance, x is the predictor variables, y is the response variable(s) and I is the mutual information of features.

Searching zero redundancy of selected optimal features defined as follows:

$$W_s = \frac{1}{|S|^2}\sum_{x,z \in S} I(x, z) \qquad (6.19)$$

Where, W_s is the minimizes redundancy of S, $|S|$ is the number of maximum relevance features in S, and z is the new response.

The MRMR algorithm selects the important features by using the mutual information quotient (MIQ) value. Details MRMR algorithms are presented in Ding and Peng, 2005. The MIQ value obtained from equation (20).

$$MIQ_x = \frac{V_x}{W_x} \qquad (6.20)$$

where, V_x and W_x are the relevance and redundancy of a feature, respectively.

6.5.1 Prediction approaches

6.5.1.1 Deep neural network (DNN) algorithm

DNN is a part of a machine learning method in artificial intelligence that processes data and computes the likelihood of a prediction, much like the human brain, to produce more accurate computational decisions (Ahmed et al., 2019; Choi et al., 2021; Ewuzie et al., 2022; Kim et al., 2020). The DNN model, unlike artificial neural networks, has more than one hidden layer, while it may vary depending on the data types or input quantities (Bagherzadeh et al., 2021; Tosun et al., 2016). For the last few decades, DNN applications have been reportedly increased for predicting and assessing water quality and assessment purposes. Recently, several studies have utilized this technique for predicting water quality index (Aldhyani et al., 2020; Bi et al., 2021; Choi et al., 2021). The present study was used to predict the WQM-WQI values for assessing coastal water quality in this research. The present study developed a DNN model using five fully connected hidden layers, including input and output layers. Figure S2 presents the details of the DNN model architecture that was used in this research.

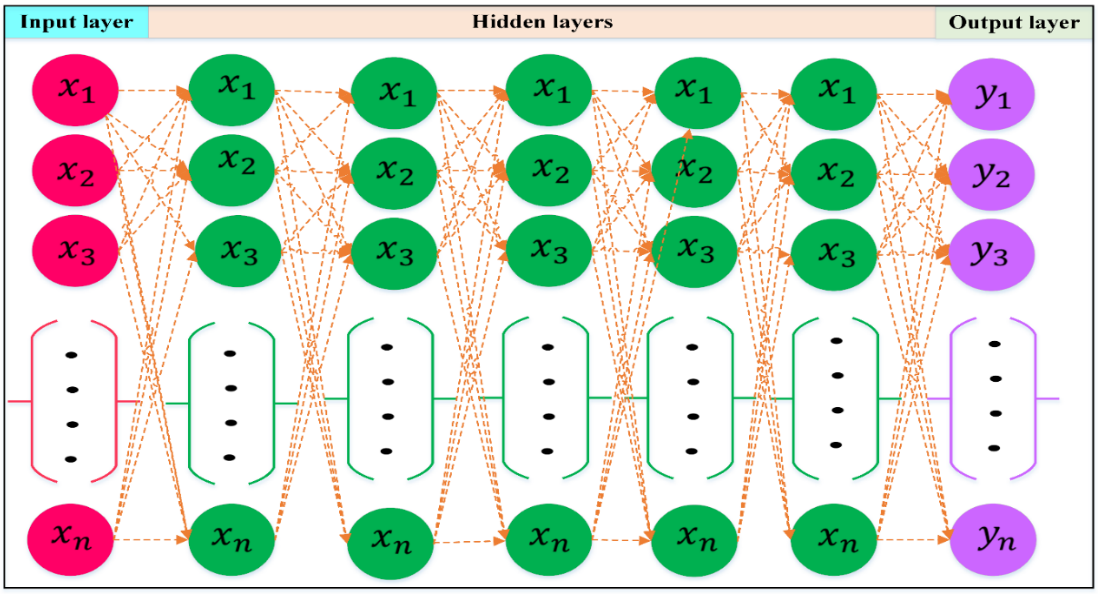


Fig. 6.S2 Fully connected deep neural network model architecture.

The number of input neurons was initialized based on the subsets of water quality indicators, whereas usually it is equal to the number of input indicators (details of the indicator subsets can be found in Table 2). The six neurons were used in the hidden layers with the ReLU activation function. For training purposes, the rest of the hyperparameters were optimized using the grid search optimization techniques. The details of this technique are described in detail in section 3. 3. Table 4 provides the details of the hyperparameters for the DNN model.

6.5.1.2 Machine learning algorithms

The present study was used eight algorithms for predicting the WQM-WQIs in order to assess coastal water quality. These algorithms were chosen for this study because, recently, several studies have reported that those algorithms have performed better than other existing algorithms in terms of predicting water quality as well as WQI values. Many researchers has revealed that those algorithms could be effective to predict water quality with and higher accuracy of prediction results (Bui et al., 2020; Hafeez et al., 2019; Islam Khan et al., 2021; Uddin et al., 2022a;2022b).

(i) Support Vector Machine (SVM) algorithm

SVM is the combination of various supervised learning techniques, which commonly used for the classification and regression purposes (Jalal and Ezzedine, 2019; Modaresi and Araghinejad, 2014). In 1992, this method was developed by Boser and Guyon, although the basic foundation was established by Vapnik in 1995 (Vapnik, 2000). Principally the SVM algorithm differ from the traditional neural networks (NN) algorithm; it uses the structural risk minimization technique for the regression model where the NN used empirical risk minimization functions (Modaresi and Araghinejad, 2014). In this study, the SVM was performed according to Li et al., (2013) approach. The SVM mathematical expression can be defined as follows:

$$Minimize: \qquad R_{sum}(\omega, \varepsilon^*) = \frac{1}{2}||\omega||^2 + C\sum_{i=1}^{n}(\varepsilon_i + \varepsilon_i^*) \qquad (6.21)$$

Subject:

$$d_i - \omega\varphi(x_i) + b_i \leq \epsilon + \varepsilon_i$$

$$\omega\varphi(x_i) + b_i - d_i \leq \epsilon + \varepsilon_i$$

$$\varepsilon_i, \varepsilon_i^* \geq 0, i = 1,2 \dots, n,$$

where ω is the normal vector, $\frac{1}{2}||\omega||^2$ refers to the regularization factor, C is the error penalty factor, b is the bias, $\varphi(x_i)$is the features space, ϵ is the error function, x_i is the input vector, $d_i$refers to the response variable, n is the number of features in the training dataset, ε_i and ε_i^* are the upper and lower excess deviation respectively (Haghiabi et al., 2018). Where radial basis function (RBF) kernel can be expressed as follows:

$$K(x_i, x_j) = exp(-\gamma|| x_i - x_j||)^2, \gamma > 0 \qquad (6.22)$$

where $x_i and\ x_j$ are inputs variables, K is the RBF kernel, and γ is the regularization indicator.

(ii) Least-Squares Boosting (LSBoost-ensemble) algorithm

Ensemble methods are widely used to predict or forecast more accurately (Isabona et al., 2022; Sun et al., 2017). Compared to the ensemble techniques, LSBoost is the most robust algorithm for regression and forecasting studies. It allows fitting a new learner at each step and aggregating the predicted results of all learners that have been grown previously. This technique can control the model overfitting problem (to reduce model training error) by adjusting weight values through the repeated training process (Barzegar et al., 2018). Commonly, the LGBoost regression model uses a sequence of regression trees (weak learners) in order to minimize the mean squared error (MSE) response variable and predict the results of the weak learners. Recently, a number of studies have used this technique for regression or forecasting water quality (Barzegar et al., 2018). In this research, the LSBoost algorithm was utilized according to the procedures of Isabona et al., (2022) for predicting coastal water quality index values using various combinations of indicators. Details of the algorithm can be found in Isabona et al., (2022).

(iii) Gaussian Process Regression (GPR)model

The GPR, which incorporates Bayesian theory and statistical learning theory, is an effective method for solving complex regression problems or forecasting such as high dimensionality and nonlinearity (Zhang et al., 2016, 2019). Compared to other traditional machine learning approaches, GPR is different; it automatically determines the prediction uncertainty when the model is fit (Rasmussen, 2003). In the literature, a number of studies have revealed that this algorithm for predicting or forecasting to achieve a higher predictive accuracy with probable uncertainty in prediction results (Abdar et al., 2021). Recently, many researches have utilized this algorithm for predicting water quality and uncertainty with a 95% confidence interval (Asadollah et al., 2021; Grbić et al., 2013). In this research, GPR was utilized successfully for predicting coastal water quality index in order to compare the model performance with other models (i.e. Asadollah et al., 2021; Tavazza et al., 2021). Details of the procedures of GPR can be found in Zhang et al., (2016).

(iv) Decision Tree (DT) algorithm

DT is another tree-based supervised algorithm that is widely utilized for both regression and classification studies in machine learning technique. It splits a large dataset into smaller homogenous datasets easily. In this study, the DT was used according to the approach of Chen et al., (2020). The DT model development process can be defined as follows:

$$DT_r = \sum_{n=1}^{n} \sum_{i \epsilon R_j} \left(y_i - \hat{y}_{R_j} \right)^2 \qquad (6.23)$$

Where DT_r refers to the decision tree model, *n* is the number of the observations, R_j is the observation region, y_i and $\hat{y}_{R_j}$ are the each individual response and mean response, respectively for the training observation with n^{th} data variables.

(v) Linear Regression (LR)

LR is one of the most widely and extensively used algorithm for the regression model, specially predicting water quality. To date, several studied have utilized this technique to predict water quality (Grbčić et al., 2021; Kadam et al., 2019). Details of the LR algorithm can be found in Grbčić et al., (2021). It is expressed as follows:

$$y = b_0 + b_1 x_1 + b_2 x_2 + \cdots b_n x_n \qquad (6.24)$$

where *y* is the MLR-predicted index score, b_0 is constant, x_n is the MLR inputs for the n^{th} WQ parameters, and b_n is the regression coefficient for the n^{th} input.

(vi) Extreme Gradient Boosting (XGBoost)

Recently, several studies have widely used boosting algorithm for the regression and classification analysis. The XGBoost algorithm constructs many weak learners' models (Bourel and Segura, 2018). Up to date now, several boosting approaches have been developed including LightGBM, AdaBoost.MH, GradientBoost, LogitBoost, XGBoost, CatBoost etc. In this study, the XGBoost algorithm was used for predicting the WQM-WQIs because recently, several studies has revealed that this technique is effective compare than other learning methods for regression analysis (Islam Khan et al., 2021; Tanha et al., 2020). The detail of the algorithm can be found in Huan et al., (2020).

(vii) K-Nearest Neighbors (KNN)

KNN is one of the commonly used algorithm that technique predicts a new observation uses of the distance measures. A number ofSeveral distance measures used in KNN algorithm. They can be Euclidean, Manhattan, Minkowski distance. In this study, we used Minkowski distances function for the determination of k-nearest neighbours because this algorithm efficient for the small datasets (32 observations were used for this study). Detail algorithm can be found in (Modaresi and Araghinejad, (2014). The Minkowski distances is given as follows:

$$D = \left(\sum_{i=1}^{n} |p_i - q_i|^p\right)^{1/p} \qquad (6.25)$$

where n is the number of dimensions, p_i , q_i are the data points and p refers to the order of the norm.

(viii) Random Forest (RF)

Currently, the RF algorithm is widely used in machine learning approaches for solving both regression and classification problems. It is one of the tree-based algorithms that applies multiple base models using subsets of the given data, whereas model decisions are made based on the average of each individual tree decision. Recently, several studies have used this technique for assessing water quality by predicting water quality indicators as well as water quality index values (Roguet et al., 2018; Sakaa et al., 2022; Tiyasha et al., 2021; Xu et al., 2021). The present study was performed the boosting algorithm for predicting the WQM-WQI values by following the methodology of Liaw and Wiener, (2002). The details algorithm are presented by Liaw and Wiener, (2002).

List of supplementary Table(s)

Table 6.S1. EPA’s water quality monitoring sites and WWTPs locations in Cork Harbour, Ireland.

Stations ID	User_ID	WFD water body name	geographical location Lat.	Lon.	site descriptions
(a) Monitoring sites					
LE030	1	Lee (Cork) Estuary Upper	51.892	-8.5062	R Curragheen, County Hall
LE040	2		51.8947	-8.5106	R. Lee, Lee Road Water Works Weir
LE110	3		51.8965	-8.4997	Upper Lee Est N Channel, Daly's Bridge
LE120	4		51.8934	-8.4946	Upper Lee Est S Channel, Donovan's Br
LE130	5		51.9002	-8.4663	Upper Lee Est N Channel, St. Patrick's Br
LE140	6		51.8953	-8.4692	Upper Lee Est S Channel, George's Quay
LE150	7	Lee (Cork) Estuary Lower	51.89946	-8.459071	Custom House Dock
LE160	8		51.90193	-8.446311	Tivoli Dock
LE170	9		51.90049	-8.423487	Balintemple
LE180	10		51.90137	-8.402429	Blackrock Castle
LE200	11	Glashaboy Estuary	51.92602	-8.395003	Glashaboy River d/s Butlerstown Confl.
LE210	12		51.91892	-8.396046	Glashaboy Estuary, Glanmire Bridge
LE220	13		51.90678	-8.396375	Glashaboy Estuary, Dunkettle Bridge
LE310	14	Lough Mahon	51.89827	-8.390053	Upper Lough Mahon (Lee Tunnel)
LE330	15		51.8867	-8.3565	Mid Lough Mahon (Buoy No 6)
LE340	16		51.8778	-8.3361	Lough Mahon, Marino Point
LE380	17	Cork Harbour	51.8378	-8.3126	Ringaskiddy
LE410	18		51.8895	-8.3036	
LE420	19	North Channel Great Island	51.8851	-8.2708	North Channel, Weir Island (Pylons)
LE430	20		51.8798	-8.2432	North Channel, Brick Island
LE450	21	Owenacurra Estuary	51.8817	-8.204	North Channel, Bagwells Hill
LE500	22		51.9168	-8.1766	Owenacurra north, Midleton
LE505	23		51.9111	-8.17401	Owenacurra north, Midleton
LE510	24		51.906	-8.1773	Owenacurra Est, New Road Br Midleton
LE520	25		51.8983	-8.1714	
LE530	26		51.8952	-8.1823	
LE540	27	North Channel Great Island	51.8826	-8.1895	Ballynacorra Est, Rathcoursey

LE550	28		51.8691	-8.204	East Ferry Quay, Rathcoursey West
LE620	29	Cork Harbour	51.8366	-8.2633	E Spike Island
LE630	30	Outer Cork Harbour	51.8105	-8.269	Adjacent to Carlisle Fort
LE810	31		51.7899	-8.2652	Roches Point
LE820	32		51.7746	-8.2745	Roches Point
(b) Wastewater Treatment Plants (WWTPs)					
1		Upper Cork	51.87124	-8.33597	Passage West
2		Lower Cork (river Owenboy, north)	51.81721	-8.33469	Carrigaline
3		Lower Cork (river Owenboy, south)	51.80363	-8.30054	Crosshaven
4		Lower Cork	51.83029	-8.32175	Ringaskiddy Village
5		Lower Cork (Pasagge East)	51.8505	-8.29467	Cobh
6		Lower Cork (Pasagge East)	51.83192	-8.2341	Whitegate
7		Lower Harbour	51.83689	-8.20918	Aghada
8		Upper Harbour	51.888818	-8.333839	Carrigrennan WWTP

Table 6.S2. Water quality indicators, units and standard threshold for coastal water quality.

Indicators	Unit	Standard threshold	
		Lower	Upper
CHL*(i)*	mg/m^3	0.0	13.6
DOX*(i)*	% sat	73	127
MRP*(i)*	mg/l as P	0.0	0.054
DIN*(i)*	mg/l	0.0	1.08
AMN*(ii)*	mg/l	0	1.5
BOD*(ii)*	mg/l	0	7
pH*(iii)*	-	5	9
TEMP*(ii)*	˚C	-	25
TON*(iv)*	mg/l as N	0.0	2
TRAN*(v)*	m/depth	> 1	-
SAL*(ii)*	psu	12	38

(xvi) ATSEBI standards, determine the standard values based on median value of Salinity. In this study, SAL median value was calculated 21.64 (see details in Table 6.S3.

(xvii) EPA, Ireland (2001), recommended values for the surface water/freshwater/river water/aquatic life.

(xviii) estuary Monitoring Manual for pH and Alkalinity, EPA,USA

(xix) the European Communities (Quality of surface water intended for the abstraction of drinking water) regulations, 1989 (S.I. No. 294/1989).

(xx)bathing Water Quality Regulations 2008, (S.I. No. 79/2008).

Table 6.S3 Averaged concentrations and estimated pollution status used for input to various FS algorithms. The guideline values used for the research are included at the last row and red-bold indicate compliance failures.

Monitoring sites	water quality indicators										
	AMN	BOD	CHL	DIN	MRP	TEMP	TRAN	pH	DOX	TON	Status
LE030	0.30	1.28	1.66	**4.48**	0.04	12.9	**0.10**	7.63	81.50	**4.18**	1
LE040	0.04	1.23	3.05	**2.10**	0.02	15.8	**0.03**	7.70	97.67	**2.07**	1
LE110	0.04	1.38	2.45	**1.66**	0.01	15.3	**0.25**	7.73	101.50	1.63	1
LE120	0.06	1.28	2.65	**1.96**	0.02	14.9	**0.05**	7.75	98.25	1.90	1
LE130	0.06	1.40	6.35	**1.79**	0.03	15.6	**0.13**	7.68	95.50	1.73	1
LE140	0.05	1.40	3.14	**1.69**	**0.07**	14.5	**0.18**	7.86	105.40	1.64	1
LE150	0.13	0.83	2.41	**1.23**	0.02	14.8	3.40	7.78	78.68	1.10	1
LE160	0.14	0.85	2.57	1.06	0.02	14.7	3.40	7.78	85.50	0.93	0
LE170	0.13	0.87	3.60	1.04	0.02	14.9	3.70	7.85	92.88	0.91	0
LE180	0.14	1.70	1.86	1.03	0.04	14.8	3.39	7.86	97.38	0.89	0
LE200	0.22	2.53	7.80	**4.90**	**0.08**	13.3	**0.05**	7.73	98.25	**4.68**	1
LE210	0.08	1.88	9.28	**4.73**	**0.06**	13.6	**0.08**	7.88	101.50	**4.65**	1
LE220	0.05	1.23	1.60	**1.69**	0.04	15.8	**0.03**	8.03	110.67	1.64	1
LE310	0.11	0.80	5.27	0.76	0.02	14.5	3.40	8.00	100.46	0.65	0
LE330	0.11	1.46	4.40	0.64	0.03	14.8	2.42	8.07	112.25	0.53	0
LE340	0.12	0.76	2.60	0.54	0.03	14.8	5.55	8.08	106.36	0.42	0
LE380	0.08	0.87	2.31	0.43	0.03	14.1	2.18	8.09	102.88	0.35	0
LE410	0.16	1.28	3.88	**1.66**	0.04	13.2	1.99	7.95	90.05	1.50	1
LE420	0.06	1.46	5.45	0.12	0.01	17.4	1.80	8.15	109.00	0.06	0
LE430	0.05	1.65	6.05	0.90	0.01	17.1	1.50	8.23	115.75	0.85	0
LE450	0.06	2.25	4.28	0.20	0.01	14.8	5.17	8.07	99.50	0.14	0
LE500	0.07	2.85	3.84	**3.72**	0.05	13.2	**0.08**	7.91	98.50	**3.65**	1
LE505	0.10	2.50	3.44	**3.95**	**0.08**	13.3	**0.10**	7.75	97.25	**3.85**	1
LE510	0.08	1.42	6.14	**1.32**	0.03	14.5	**0.90**	7.93	94.50	1.24	1
LE520	0.07	1.17	3.06	**1.22**	0.02	14.0	1.13	7.92	95.50	1.15	1
LE530	0.07	1.27	2.27	0.66	0.02	15.0	1.33	8.03	98.83	0.59	0
LE540	0.04	1.08	2.31	0.19	0.01	15.1	1.23	8.10	104.33	0.15	0
LE550	0.05	0.90	4.21	0.19	0.01	15.0	2.32	8.10	101.50	0.14	0
LE620	0.04	0.50	2.56	0.13	0.01	13.4	9.43	8.08	98.75	0.09	0
LE630	0.03	0.50	2.75	0.08	0.01	13.6	9.17	8.06	96.50	0.05	0
LE810	0.03	0.50	2.95	0.08	0.01	13.4	13.53	8.05	95.50	0.05	0
LE820	0.03	0.50	3.04	0.10	0.01	13.2	11.98	8.05	93.25	0.07	0
Guide values	**0 – 1.5**	**0 - 7**	**0 – 13.6**	**0 – 1.08**	**0 – 0.054**	**25**	**>1**	**5 – 7**	**73 – 127**	**0 - 2**	

0 = unpolluted, 1 = polluted, and red indicate exceed the guide values.

Table 6.S4 Estimated weight values for different subsets of water quality indicators.

Key indicators	Various FS techniques															
	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	Number of votes*
AMN	-	0.200	0.036	-	-	-	-	0.028	0.250	0.095	-	-	-	0.167	-	
BOD	-	-	0.143	0.083	0.107	-	0.048	0.139	0.036	0.143	-	-	-	-	-	
CHL	-	0.067	0.214	-	-	-	-	0.056	-	0.048	-	-	-	-	-	
DIN	0.267	-	0.250	0.194	0.250	0.400	0.238	0.222	0.179	0.286	0.238	-	-	-	0.240	13
MRP	0.333	-	0.107	0.111	0.071	-	0.095	-	0.071	0.190	0.143	-	-	-	0.095	11
TEMP	-	-	0.071	0.056	0.036	-	-	0.111	-	-	0.095	-	-	-	-	
TRAN	0.133	0.333	-	0.167	0.179	0.200	0.190	0.194	0.214	-	0.190	0.300	0.167	-	0.143	14
pH	-	0.267	-	0.139	0.143	0.300	0.143	0.167	0.143	-	0.048	0.200	0.333	0.333	0.190	14
DOX	0.200	0.133	0.179	0.028	-	-	-	0.083	0.107	-	-	0.100	-	-	0.047	7
TON	0.067	-	-	0.222	0.214	0.100	0.286	-	-	0.238	0.286	0.400	0.500	0.500	0.285	13
SUM	1	**1**	**1**	**1**	**1**	**1**	1	**1**	**1**	1	1	**1**	1	1	**1**	

**S15 (MAXVOT) subset of indicators selected based on the majority votes of the FS techniques.*

Table 6.S5 Calculated SI for various water quality indicators and ambiguity of SI functions at each monitoring sites in Cork harbour.

Monitoring sites	water quality indicators									
	AMN	DOX	DIN	CHL	BOD	TEMP	TON	TRAN	pH	MRP
LE030	80	31.48	**0**	87.79	81.79	100	**0**	10	100	24.07
LE040	97.67	91.36	**0**	77.57	82.39	100	**0**	3.3	100	62.96
LE110	97.67	94.44	**0**	81.99	80.36	100	18.75	25	100	74.07
LE120	96	93.52	**0**	80.51	81.79	100	5	5	100	61.11
LE130	95.8	83.33	**0**	53.35	80	100	13.75	12.5	100	48.15
LE140	96.8	80	**0**	76.91	80	100	18	18	100	**0**
LE150	91.2	21.02	**0**	82.28	88.19	100	45	100	100	57.41
LE160	90.87	46.3	1.39	81.08	87.87	100	53.6	100	100	55.56
LE170	91.53	73.61	3.7	73.5	87.56	100	54.35	100	100	57.41
LE180	90.6	90.28	5	86.36	75.74	100	55.75	100	100	31.48
LE200	85.2	93.52	**0**	42.68	63.93	100	**0**	5	100	**0**
LE210	94.33	94.44	**0**	31.8	73.16	100	**0**	7.5	100	**0**
LE220	96.73	60.52	**0**	88.24	82.39	100	17.95	3.3	100	18.52
LE310	92.53	98.3	29.72	61.25	88.57	100	67.7	100	100	59.26
LE330	92.73	54.63	40.93	67.63	79.14	100	73.55	100	100	51.85
LE340	92.2	76.44	49.91	80.86	89.2	100	78.8	100	100	51.85
LE380	94.73	89.33	60.28	82.99	87.56	100	82.45	100	100	53.7
LE410	89.53	63.15	**0**	71.46	81.79	100	25	100	100	20.37
LE420	96.07	66.67	89.26	59.93	79.1	100	97.15	100	100	77.78
LE430	96.73	41.67	16.3	55.51	76.43	100	57.25	100	100	87.04
LE450	96.13	98.15	81.85	68.51	67.86	100	93.1	100	100	81.48
LE500	95.4	**94.44**	**0**	71.8	59.29	100	**0**	7.5	100	12.96
LE505	93.2	89.81	**0**	74.71	64.29	100	**0**	10	100	**0**
LE510	94.53	79.63	**0**	54.88	79.76	100	37.9	90	100	50
LE520	95.47	83.33	**0**	77.5	83.33	100	42.4	100	100	57.41
LE530	95.13	95.68	39.07	83.33	81.9	100	70.75	100	100	61.11
LE540	97.13	83.96	82.41	82.99	84.53	100	92.65	100	100	83.33
LE550	96.4	94.44	82.04	69.07	87.14	100	92.95	100	100	81.48
LE620	97.07	95.37	87.5	81.19	92.86	100	95.45	100	100	85.19
LE630	97.87	87.04	92.78	79.82	92.86	100	97.75	100	100	87.04
LE810	97.93	83.33	92.22	78.32	92.86	100	97.35	100	100	88.89
LE820	97.67	75	90.37	77.68	92.86	100	96.55	100	100	79.63

* Bold underline SI values were smaller because indicators exceeded the guide value at these monitoring sites. In terms of ambiguity rules, there were no ambiguity issues in SI functions. Details of the ambiguity evaluation methodology can be found in Uddin et al., (2022a).

Table 6.S6 Measured WQM-WQIs for various subsets of water quality indicators in Cork Harbour.

SL No.	Different subsets of water quality indicators														
	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15
1	20	68	62	51	51	55	43	67	59	46	39	46	58	66	45
2	55	78	72	56	53	55	46	71	72	55	45	53	58	70	48
3	61	80	75	59	55	56	50	72	74	58	49	57	60	71	51
4	55	78	73	56	53	55	46	71	72	54	44	54	58	70	48
5	47	75	64	55	52	55	45	69	70	50	43	53	59	70	47
6	37	77	66	53	51	56	43	70	69	47	40	54	60	71	46
7	51	90	63	71	71	72	68	80	79	58	66	77	78	76	65
8	55	92	65	73	72	73	69	81	80	60	68	80	80	78	67
9	61	94	68	74	73	73	70	82	82	60	68	82	80	79	67
10	59	96	71	72	70	73	68	83	82	55	66	84	81	79	67
11	42	74	59	50	47	55	40	66	66	37	38	54	58	67	45
12	42	76	60	52	49	55	41	68	69	41	38	54	58	69	45
13	29	75	66	52	51	55	43	69	67	49	40	50	59	71	46
14	71	96	73	78	77	76	75	85	86	66	73	88	85	84	73
15	60	92	64	78	78	79	76	82	82	67	75	86	88	86	76
16	67	94	74	81	81	81	80	86	85	72	78	90	90	89	79
17	73	97	79	84	83	84	82	89	88	75	81	92	92	91	82
18	48	92	62	67	67	71	62	81	79	47	60	75	73	71	60
19	84	93	78	93	93	96	94	90	92	88	94	96	99	98	95
20	67	91	61	76	74	74	73	79	83	66	74	81	81	81	71
21	89	97	83	91	90	92	91	90	94	84	91	97	97	96	92
22	8	70	52	48	47	55	40	62	62	41	38	45	58	70	45
23	40	77	65	50	47	55	41	68	68	41	38	53	58	69	45
24	57	91	63	68	66	69	63	79	81	53	61	75	73	74	61
25	63	96	70	72	70	72	67	83	84	57	66	80	77	76	64
26	72	97	77	79	78	78	76	86	87	69	75	89	87	86	75
27	86	96	85	92	92	93	92	92	93	88	92	96	96	96	92
28	88	97	85	92	92	93	92	92	94	87	91	97	97	96	92
29	91	98	90	94	94	95	94	95	95	91	94	98	98	97	94
30	91	97	89	96	96	97	96	95	96	93	96	98	99	99	97
31	91	96	88	96	96	97	96	95	95	93	96	97	99	98	96
32	86	95	85	94	95	96	95	94	94	91	94	96	98	98	95

Table 6.S7 Optimized hyper-parameters of various ML models.

Model parameters	Predictive models							
	SVM	Ensemble	GPR	Tree	LR	XGBoost	KNN	RF
n_estimators	100	100	50	100	100	100	-	100
learning_rate	-	0.405	-	-	-	0.2	-	-
max.depth	-	-	-	10		10		10
gamma	auto	-	-	-	-	0	-	-
booster		LSBoost		-	-	gbtree	-	-
Kernel	linear	-	nonisotrophic rational quardatic	-	-	-	-	-
Kernel_scale	-	-	0.5796	-	-	-	-	-
Sigma	-	-	0.1176	-	-	-	-	-
Basic function	-	-	zero	-	-	-	-	-
subsample	-	-	-	-	-	1		
colsample_bytree	-	-	-	-	-	1	-	-
base_score	-	-	-	-	-	0.5	-	-
reg_lamda	-	-	-	-	-	1	-	-
bootstrap	-	-	-	-	-	True	-	True
cv.folds	10	10	10	10	10	10	10	10
random_state	-	-	-	-	-	1	-	1
Objective	-	-	-	-	-	reg.linear	-	-
criterion								*Squared_error*
max_leaf_nodes	-	1	-	10	-		30	5
min_samples_leaf	-	-	-	2	-		-	1
epsilon	0.1	-	-	-	-	-	-	-
shrinking	True	-	-	-	-	-	-	-
fit_intercept	-	-	-	-	TRUE	-	-	-
n_neighbors	-	-	-	-	-	-	5	-
weight	-	-	-	-	-	-	uniform	-
metrics							minkowski	
power_parameters	-	-	-	-	-	-	2	-
Number of learners	-	11						
ensemble method	-	Bag						

Table 6.S8: 10-fold cross validation results of various ML and AI models for different scenarios

(a) SVM

Scenarios	Training					Testing				
	MSE	MAE	RMSE	Bic	AIC	MSE	MAE	RMSE	BIC	AIC
S1	56.95	4.34	7.54	146.67	139.35	24.53	2.73	4.95	119.73	112.40
S2	22.41	3.28	4.73	116.82	109.50	5.37	1.13	2.38	71.15	63.78
S3	27.70	3.71	5.26	130.55	120.29	4.32	1.92	2.07	70.41	60.15
S4	12.88	2.62	3.58	109.51	97.78	0.38	0.60	0.62	-3.24	-14.96
S5	10.29	2.10	3.21	98.86	88.60	0.72	0.82	0.84	13.75	3.49
S6	7.82	2.13	2.79	79.67	73.81	3.93	1.12	1.98	57.66	51.80
S7	17.72	2.90	4.21	112.78	103.99	7.85	1.83	2.80	86.73	77.94
S8	16.23	3.12	4.02	116.91	105.18	10.78	3.12	3.28	103.81	92.10
S9	10.45	2.14	3.23	99.35	89.09	0.10	0.25	0.33	-49.42	-59.68
S10	7.65	2.09	2.76	85.91	77.11	1.81	0.62	1.34	39.78	30.98
S11	9.78	2.39	3.13	93.76	84.97	1.63	0.75	1.28	36.42	27.64
S12	24.53	2.97	4.95	116.26	110.34	15.28	1.94	3.91	101.11	95.25
S13	5.73	1.78	2.39	66.26	61.86	0.02	0.15	0.15	-114.78	-119.19
S14	3.62	1.19	1.90	51.56	47.17	1.24	0.49	1.12	21.62	17.22
S15	3.63	1.52	1.90	81.33	72.50	0.32	0.25	0.57	-15.67	-24.46

(b) LSBoost

Scenarios	Training					Testing				
	MSE	MAE	RMSE	BIC	AIC	MSE	MAE	RMSE	BIC	AIC
S1	78.07	6.46	8.84	156.70	149.44	39.30	4.36	6.24	134.81	127.48
S2	7.18	2.00	2.68	80.41	73.08	2.86	1.25	1.68	50.96	43.63
S3	26.86	4.02	5.18	129.56	119.30	8.64	2.09	2.93	93.27	83.00
S4	7.66	2.21	2.77	92.88	81.15	2.20	1.18	1.49	164.68	152.94
S5	6.12	1.78	2.47	82.23	71.97	2.05	1.19	1.43	47.23	36.97
S6	4.92	1.51	2.22	64.85	58.98	1.59	0.86	1.26	28.70	22.84
S7	8.28	2.35	2.87	88.44	79.64	1.63	1.02	1.27	36.43	27.64
S8	8.14	2.05	2.85	94.82	83.10	3.02	1.29	1.74	63.01	51.39
S9	11.85	2.47	3.44	103.38	93.11	0.10	0.27	0.32	-48.47	-58.74
S10	8.58	2.23	2.93	89.58	80.78	3.08	1.29	1.76	56.79	48.00
S11	7.22	2.08	2.68	73.66	69.26	2.63	1.34	1.62	41.34	36.94
S12	7.74	2.23	2.78	79.35	73.49	1.51	1.15	1.23	27.05	21.20
S13	2.04	0.85	1.43	33.21	28.81	0.02	0.10	0.15	-114.78	-119.18
S14	5.09	1.52	2.26	62.47	58.07	1.28	0.88	1.13	18.29	13.90
S15	6.15	1.79	2.48	78.92	70.13	0.00	0.00	0.00	-200.25	-209.05

(c) GPR

Scenarios	Training					Testing				
	MSE	MAE	RMSE	BIC	AIC	MSE	MAE	RMSE	BIC	AIC
S1	19.98	3.33	4.47	113.16	105.83	0.00	0.02	0.04	-203.72	-211.05
S2	10.06	2.33	3.17	91.20	83.87	0.00	0.00	0.00	-203.72	-211.05
S3	20.15	2.22	4.48	120.37	110.11	0.00	0.00	0.01	-196.78	-207.05
S4	9.82	2.18	3.13	100.83	89.10	0.00	0.01	0.02	-193.32	-205.05
S5	6.78	1.32	2.60	85.51	75.25	0.00	0.00	0.04	-196.78	-207.05
S6	5.56	1.46	2.36	68.76	62.89	0.00	0.05	0.06	-207.19	-213.05
S7	10.15	1.52	3.16	94.95	86.16	0.00	0.00	0.00	-200.25	-209.05
S8	8.21	2.09	2.86	95.09	83.37	0.00	0.00	0.00	-193.32	-205.05
S9	12.82	2.52	3.59	105.89	95.63	0.00	0.01	0.00	-196.78	-207.05
S10	1.49	0.67	1.22	33.56	24.76	0.00	0.00	0.08	-200.25	-209.05
S11	17.90	2.85	4.23	113.11	104.31	0.04	0.14	0.19	-200.25	-209.05
S12	23.14	3.01	4.81	114.39	108.53	0.32	0.39	0.56	-22.56	-28.46
S13	3.55	0.84	1.88	50.94	46.54	0.00	0.03	0.04	-200.25	-209.05
S14	0.00	0.02	0.02	-210.65	-215.05	0.00	0.02	0.02	-210.65	-215.05
S15	9.92	2.30	3.15	94.22	85.43	0.34	0.45	0.58	-13.73	-22.52

(d) Tree

Scenarios	Training					Testing				
	MSE	MAE	RMSE	BIC	AIC	MSE	MAE	RMSE	BIC	AIC
S1	108.00	7.27	10.41	167.16	159.83	48.70	4.89	6.98	141.67	134.34
S2	7.76	2.12	2.79	82.89	75.56	3.23	1.33	1.80	54.84	47.52
S3	38.88	5.03	6.23	141.40	131.14	12.02	2.68	3.46	103.83	93.60
S4	35.68	3.78	5.97	142.11	130.38	3.96	1.62	1.99	71.76	60.04
S5	18.99	3.61	4.35	118.46	108.21	23.17	3.17	4.81	124.83	114.57
S6	19.13	2.25	4.37	108.30	102.44	2.52	1.09	1.59	43.44	37.58
S7	9.35	2.33	3.05	92.33	83.53	3.64	1.59	1.91	62.14	53.34
S8	11.19	2.38	3.38	105.00	93.30	3.37	1.59	1.84	66.60	54.87
S9	9.71	2.56	3.12	97.00	86.70	5.45	1.76	2.34	78.52	68.26
S10	39.04	4.88	6.25	138.06	129.30	10.96	2.61	3.31	97.41	88.62
S11	14.69	3.16	3.83	106.78	97.90	5.05	1.65	2.25	72.62	63.82
S12	26.85	3.17	5.18	126.10	117.30	6.26	1.92	2.60	79.48	70.70
S13	12.74	2.42	3.57	91.83	87.43	4.07	1.24	2.02	55.31	50.92
S14	4.34	1.64	2.08	57.37	52.98	2.17	1.12	1.47	35.20	30.80
S15	41.98	3.72	6.47	1410.38	131.56	5.25	1.84	2.29	73.86	65.06

(e) LR

Scenarios	Training					Testing				
	MSE	MAE	RMSE	BIC	AIC	MSE	MAE	RMSE	BIC	AIC
S1	219	10.88	14.81	189.8	182.5	111.6	8.07	10.56	168.21	160.87
S2	52.21	5.06	7.23	143.89	136.6	31.03	4.02	5.57	127.25	119.9
S3	70.04	6.63	8.36	160.23	149.97	31.14	4.61	5.58	134.29	124.03
S4	47.35	4.99	6.88	151.2	139.4	22.89	3.56	4.78	127.91	116.18
S5	47.86	5.16	6.92	148.05	137.78	23.99	3.77	4.89	125.95	115.68
S6	39.271	4.75	6.27	131.3	125.45	29.83	4.1	5.46	122.52	116.66
S7	59.81	6.06	7.73	151.71	142.92	33.95	4.55	7.73	133.59	124.79
S8	20.83	3.81	4.56	124.89	113.16	9.03	2.59	3	98.14	86.42
S9	32.92	4.17	5.74	136.07	125.8	13.81	2.92	3.71	108.273	98.01
S10	146	10.69	12.08	180.27	171.48	80.47	8.23	8.97	161.21	152.41
S11	66.52	6.15	8.15	155.11	146.32	38.78	4.68	6.22	137.85	129.05
S12	57.17	6.074	7.56	143.64	137.78	44.657	5.24	6.68	135.43	129.6
S13	45.19	5.48	6.72	132.35	127.95	33.93	4.71	5.83	123.17	118.78
S14	37.8	4.97	6.15	126.63	122.23	30.93	4.49	5.56	120.21	115.82
S15	72.26	6.56	8.5	157.97	149.17	38.18	4.65	6.17	137.35	128.55

f) XGBoost

Scenarios	Training					Testing				
	MSE	MAE	RMSE	BIC	AIC	MSE	MAE	RMSE	BIC	AIC
S1	0.00	0.02	0.14	-203.72	-211.05	0.00	0.02	0.10	-203.72	-211.05
S2	0.00	0.01	0.10	-203.72	-211.05	0.00	0.01	0.10	-203.72	-211.05
S3	0.00	0.02	0.14	-196.79	-207.05	0.00	0.02	0.10	-196.79	-207.05
S4	0.00	0.02	0.14	-193.32	-205.05	0.00	0.02	0.14	-193.32	-205.05
S5	0.00	0.01	0.10	-196.79	-207.05	0.00	0.01	0.10	-196.79	-207.05
S6	0.00	0.01	0.10	-207.19	-213.05	0.00	0.01	0.10	-207.19	-213.05
S7	0.00	0.01	0.10	-200.25	-209.50	0.00	0.01	0.10	-200.25	-209.50
S8	0.00	0.02	0.14	-193.32	-205.05	0.00	0.02	0.14	-193.32	-205.05
S9	0.00	0.01	0.10	-196.79	-207.05	0.00	0.01	0.10	-196.79	-207.05
S10	0.00	0.01	0.10	-207.19	-213.05	0.00	0.01	0.10	-207.19	-213.05
S11	0.00	0.02	0.14	-200.25	-209.50	0.00	0.02	0.14	-200.25	-209.50
S12	0.00	0.02	0.14	-207.19	-213.05	0.00	0.02	0.14	-207.19	-213.05
S13	0.00	0.01	0.10	-210.65	-215.05	0.00	0.01	0.10	-210.65	-215.05
S14	0.00	0.01	0.10	-210.65	-215.05	0.00	0.01	0.10	-210.65	-215.05
S15	0.00	0.02	0.14	-200.25	-209.50	0.00	0.02	0.14	-200.25	-209.50

(g) KNN

Scenarios	Training					Testing				
	MSE	MAE	RMSE	BIC	AIC	MSE	MAE	RMSE	BIC	AIC
S1	151.92	9.04	3.01	105.89	98.56	71.94	6.07	2.46	154.16	146.83
S2	41.44	4.51	2.12	136.51	129.20	35.67	4.01	2.00	131.71	124.40
S3	95.46	8.00	2.83	170.14	160.00	26.17	3.91	1.98	1283.73	118.47
S4	53.76	6.50	2.55	155.23	143.51	26.30	3.76	1.94	132.35	120.63
S5	57.79	6.78	2.60	154.10	143.80	29.54	3.84	1.96	132.56	122.30
S6	27.89	4.19	2.05	120.00	368.00	18.83	3.00	1.73	107.80	101.90
S7	47.49	5.74	2.40	144.33	135.54	31.06	3.85	1.96	130.74	121.95
S8	49.85	5.75	2.40	152.80	141.10	18.18	3.08	1.75	120.54	108.80
S9	21.28	4.16	2.04	122.10	11.85	18.25	2.76	1.66	117.20	107.00
S10	63.88	5.97	2.44	153.80	145.02	27.09	4.22	2.05	126.40	117.60
S11	68.90	6.74	2.60	156.23	147.44	41.90	4.19	2.05	66.64	57.85
S12	58.08	6.26	2.50	143.80	138.00	32.29	3.38	1.84	125.05	119.19
S13	12.99	2.75	1.66	92.45	88.05	20.26	3.05	1.75	106.67	102.27
S14	32.82	3.67	1.92	122.10	117.71	9.94	1.93	1.39	83.88	79.49
S15	38.66	5.32	2.31	137.75	128.95	29.09	3.69	1.92	128.65	119.85

(h) RF

Scenarios	Training					Testing				
	MSE	MAE	RMSE	BIC	AIC	MSE	MAE	RMSE	BIC	AIC
S1	69.31	6.04	2.46	152.96	145.64	37.49	3.40	1.84	133.30	125.97
S2	11.91	2.94	1.71	96.61	89.28	4.03	1.23	1.11	61.93	54.60
S3	42.29	5.19	2.28	144.08	133.83	13.87	2.18	1.48	108.41	98.15
S4	7.51	2.35	1.53	88.78	78.52	2.81	1.22	1.10	57.32	47.06
S5	12.39	2.92	1.71	104.80	94.54	4.26	1.31	1.14	70.64	60.38
S6	9.50	2.17	1.47	85.90	80.04	3.23	0.96	0.98	51.38	45.51
S7	7.85	2.73	1.65	86.73	77.94	3.01	1.25	1.12	56.06	47.26
S8	15.84	3.18	1.78	116.18	104.40	5.15	1.30	1.14	80.17	68.45
S9	11.82	2.52	1.59	103.93	93.03	5.04	1.44	1.20	76.02	65.76
S10	8.99	2.36	1.54	91.07	82.30	3.91	1.46	1.21	64.45	55.63
S11	7.11	1.98	1.41	83.56	74.80	2.73	1.09	1.04	52.93	44.12
S12	22.47	3.54	1.88	113.45	107.59	7.60	1.57	1.25	78.76	72.90
S13	7.74	2.12	1.46	75.88	71.50	2.67	0.99	0.99	41.82	37.43
S14	1.85	1.05	1.02	30.08	25.67	0.97	0.65	0.81	9.42	5.03
S15	6.44	2.01	1.42	80.40	71.60	2.82	1.21	1.10	54.00	45.20

Table 6.S9. Predicted WQM-WQIs for various subsets of water quality indicators in Cork Harbour.

SL. no	Different subsets of water quality indicators														
	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15
1	36	75	40	41	58	34	54	105	59	46	37	43	58	58	48
2	53	73	72	50	52	53	54	71	57	54	40	54	60	61	52
3	58	73	75	57	55	57	62	72	60	63	50	56	60	68	54
4	53	78	69	50	54	53	55	66	59	56	44	54	60	63	51
5	49	73	70	56	52	55	52	68	60	53	44	54	61	65	55
6	50	77	66	52	50	56	39	67	64	37	51	58	60	69	55
7	52	91	70	73	71	63	69	98	94	59	63	75	79	73	77
8	55	91	69	75	73	65	70	92	89	61	68	76	83	76	76
9	58	84	68	74	72	68	71	82	82	58	67	76	82	78	72
10	55	90	59	72	49	65	47	68	77	49	65	75	83	78	69
11	42	100	57	58	54	49	43	65	59	37	38	51	55	50	59
12	42	76	60	51	49	47	41	68	60	41	33	50	52	41	50
13	55	86	66	52	52	51	44	87	67	50	41	62	59	71	47
14	66	83	72	78	82	76	78	77	82	62	74	84	86	84	73
15	72	84	64	76	67	79	65	82	76	61	75	85	88	87	69
16	68	83	70	80	82	82	79	90	83	60	77	88	90	89	73
17	73	90	77	84	87	78	80	91	88	74	83	92	92	91	79
18	42	92	57	60	57	55	44	81	79	47	59	68	65	68	61
19	86	93	78	95	83	91	84	88	91	73	71	99	98	98	84
20	77	98	77	76	74	86	73	94	83	65	54	82	80	86	63
21	80	97	82	92	59	92	64	60	94	53	85	96	97	96	88
22	39	82	57	48	47	55	40	59	62	41	37	49	54	42	44
23	40	82	57	56	53	55	41	59	61	32	43	51	56	47	57
24	56	81	71	68	60	62	57	61	75	57	60	72	73	75	66
25	59	83	75	69	70	64	66	69	76	62	65	73	76	77	67
26	70	89	76	82	74	76	73	79	85	72	74	87	87	87	78
27	85	96	85	92	89	88	91	92	91	88	85	97	96	96	86
28	82	96	84	92	92	88	93	83	94	80	85	97	96	96	88
29	88	97	90	94	98	94	97	95	95	62	94	96	98	97	93
30	89	99	93	96	99	94	99	93	98	64	94	98	99	98	95
31	95	96	94	96	96	99	95	94	99	49	94	98	98	98	98
32	91	97	94	95	95	95	93	94	98	50	95	98	98	98	97

Table 6.S10. Classification scheme for assessing coastal water quality using WQI model according to Uddin et al., (2022a).

Classes	WQI score	definition
Good	80-100	Good waterbodies that meet the standard values and thus water quality is suitable for all use.
Fair	50-79	Waterbodies that a few indicators meet the standard values and the water quality is usually protected with a minor degree of impairment.
Marginal	30-49	The majority of the water quality indicators failed to meet the criteria; water quality in unprotected, which may be posing a risk for aquatic life.
Poor	0-29	Poor waterbodies are those that failed to meet all the criteria; water quality is completely unprotected and unsuitable for many specific usages.

Table 6.S11. Assessment of monitoring sites in Cork Harbour.

Monitoring sites	Different subsets of water quality indicators														
	S1	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**	**S10**	**S11**	**S12**	**S13**	**S14**	**S15**
LE030	P	F	F	F	F	F	M	F	F	M	M	M	F	F	M
LE040	F	F	F	F	F	F	M	F	F	F	M	F	F	F	M
LE110	F	G	F	F	F	F	M	F	F	F	M	F	F	F	F
LE120	F	F	F	F	F	F	M	F	F	F	M	F	F	F	M
LE130	M	F	F	F	F	F	M	F	F	M	M	F	F	F	M
LE140	M	F	F	F	F	F	M	F	F	M	M	F	F	F	M
LE150	F	G	F	F	F	F	F	G	F	F	F	F	F	F	F
LE160	F	G	F	F	F	F	F	G	F	F	F	F	G	F	F
LE170	F	G	F	F	F	F	F	G	G	F	F	G	G	F	F
LE180	F	G	F	F	F	F	F	G	G	F	F	G	G	F	F
LE200	M	F	F	F	M	F	M	F	F	M	M	F	F	F	M
LE210	M	F	F	F	M	F	M	F	F	M	M	F	F	F	M
LE220	P	F	F	F	F	F	M	F	F	M	M	M	F	F	M
LE310	F	G	F	F	F	F	F	G	G	F	F	G	G	G	F
LE330	F	G	F	F	F	F	F	G	G	F	F	G	G	G	F
LE340	F	G	F	G	G	G	F	G	G	F	F	G	G	G	F
LE380	F	G	F	G	G	G	G	G	G	F	G	G	G	G	G
LE410	M	G	F	F	F	F	F	G	F	M	F	F	F	F	F
LE420	G	G	F	G	G	G	G	G	G	G	G	G	G	G	G
LE430	F	G	F	F	F	F	F	F	G	F	F	G	G	G	F
LE450	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
LE500	P	F	F	M	M	F	M	F	F	M	M	M	F	F	M
LE505	M	F	F	F	M	F	M	F	F	M	M	F	F	F	M
LE510	F	G	F	F	F	F	F	F	G	F	F	F	F	F	F
LE520	F	G	F	F	F	F	F	G	G	F	F	G	F	F	F
LE530	F	G	F	F	F	F	F	G	G	F	F	G	G	G	F
LE540	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
LE550	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
LE620	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
LE630	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
LE810	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G
LE820	G	G	G	G	G	G	G	G	G	G	G	G	G	G	G

G= Good F= Fair M = Marginal P = Poor

List of supplementary Figure(s)

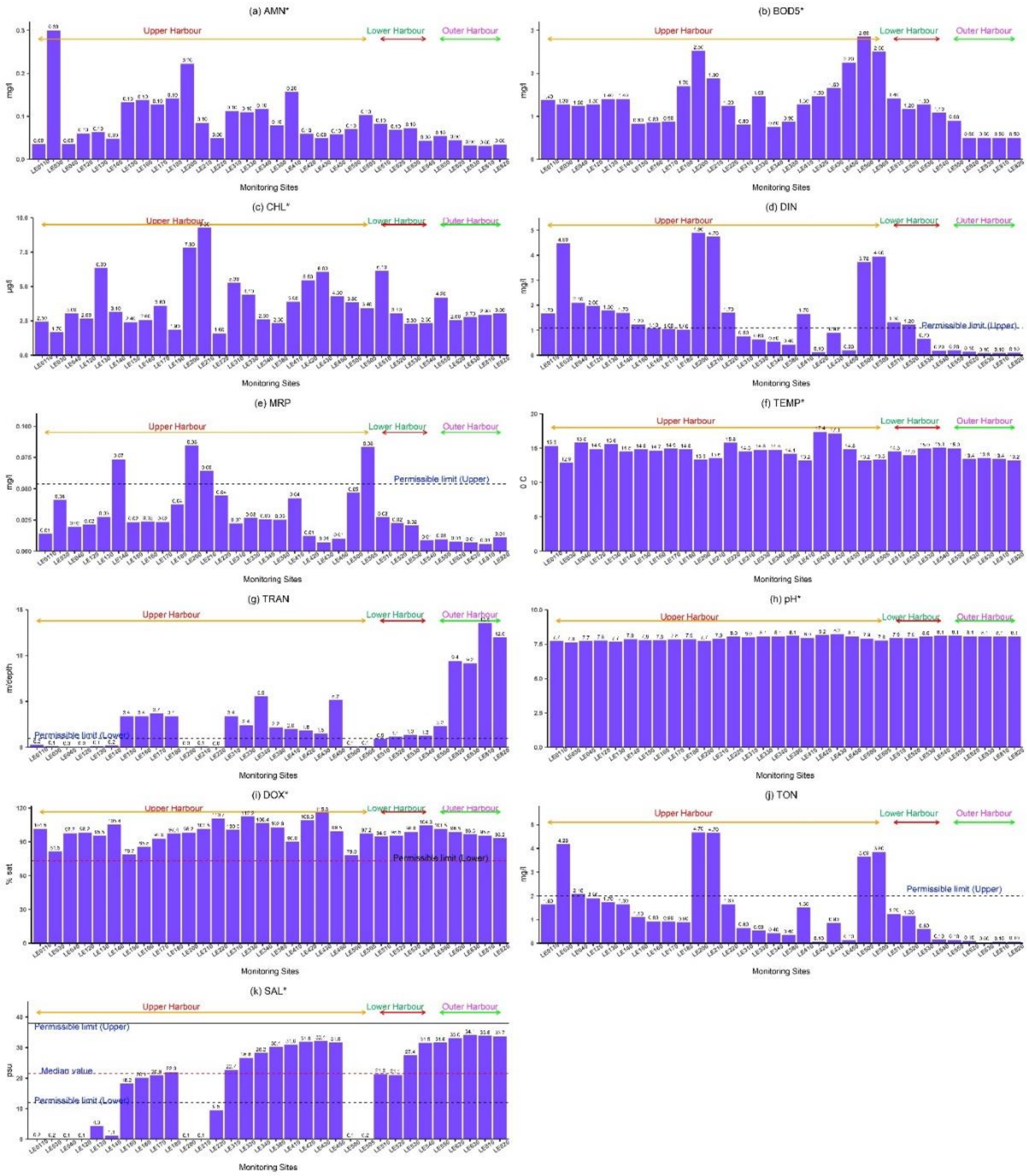


Fig 6.S3 Water quality indicators at each monitoring site in Cork Harbour.

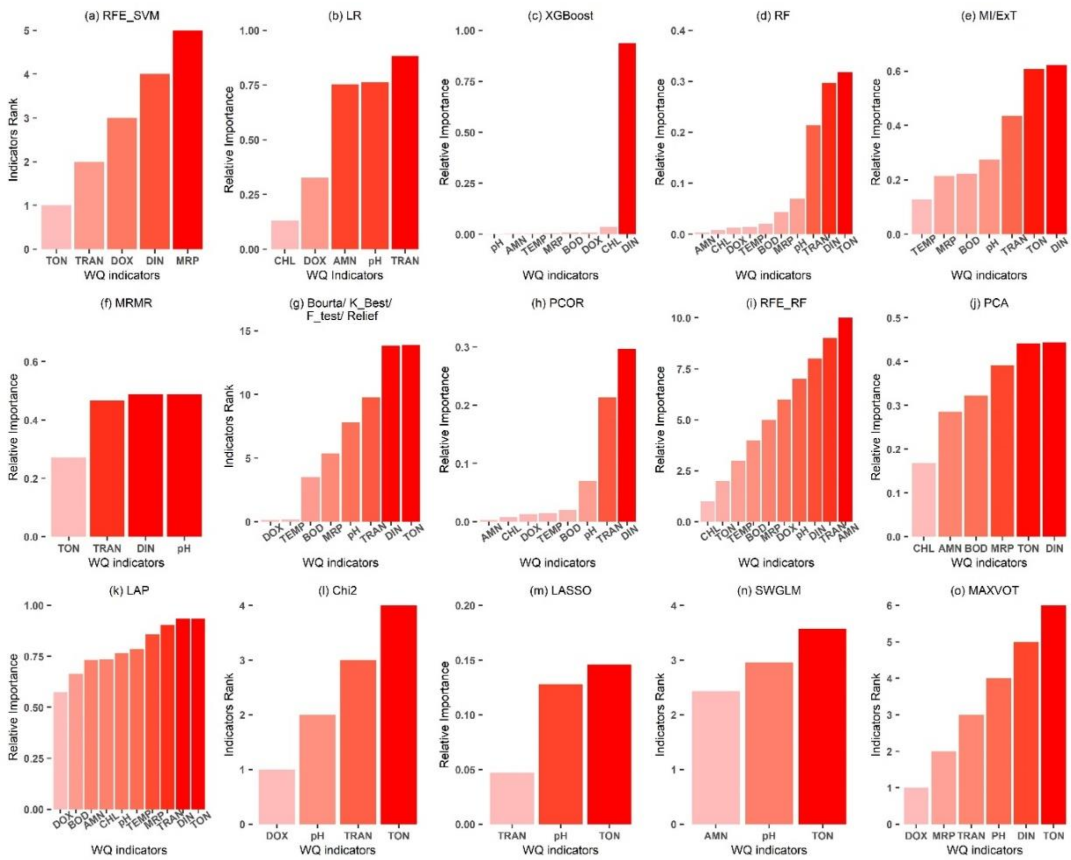


Fig. 6.S4 Indicators rank and relative importance based on various FS algorithms.

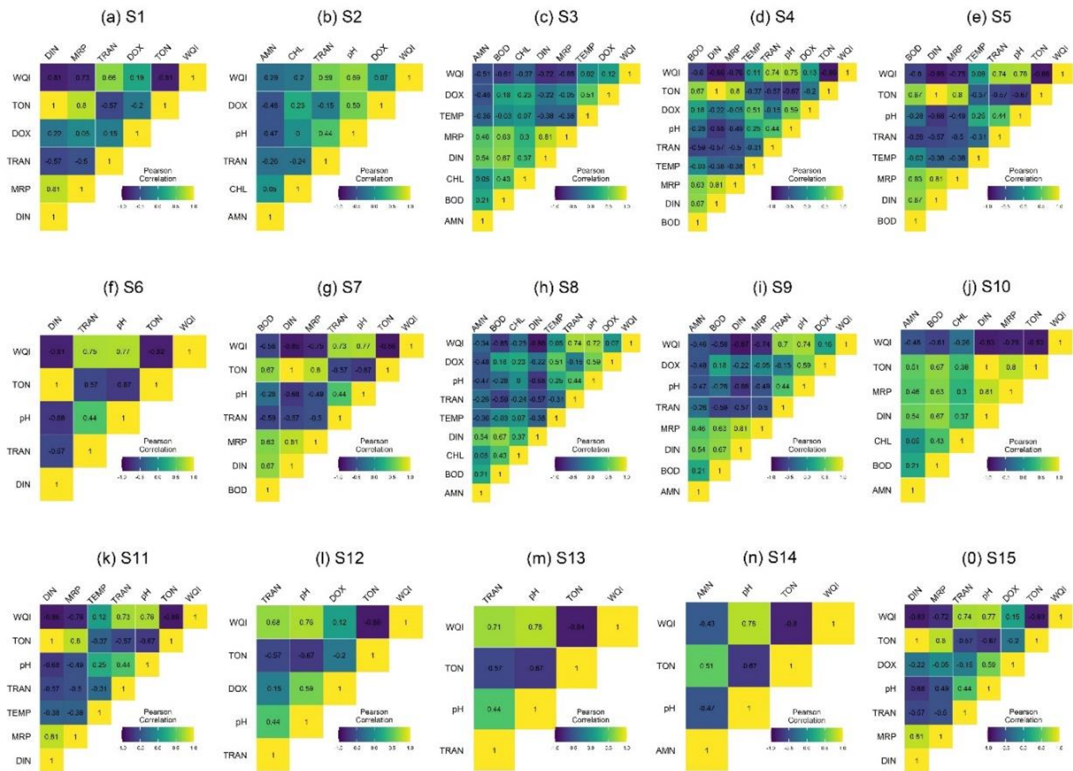


Fig. 6.S5 Pearson correlation results between various quality indicators scenarios and WQM-WQI in Cork Harbour.

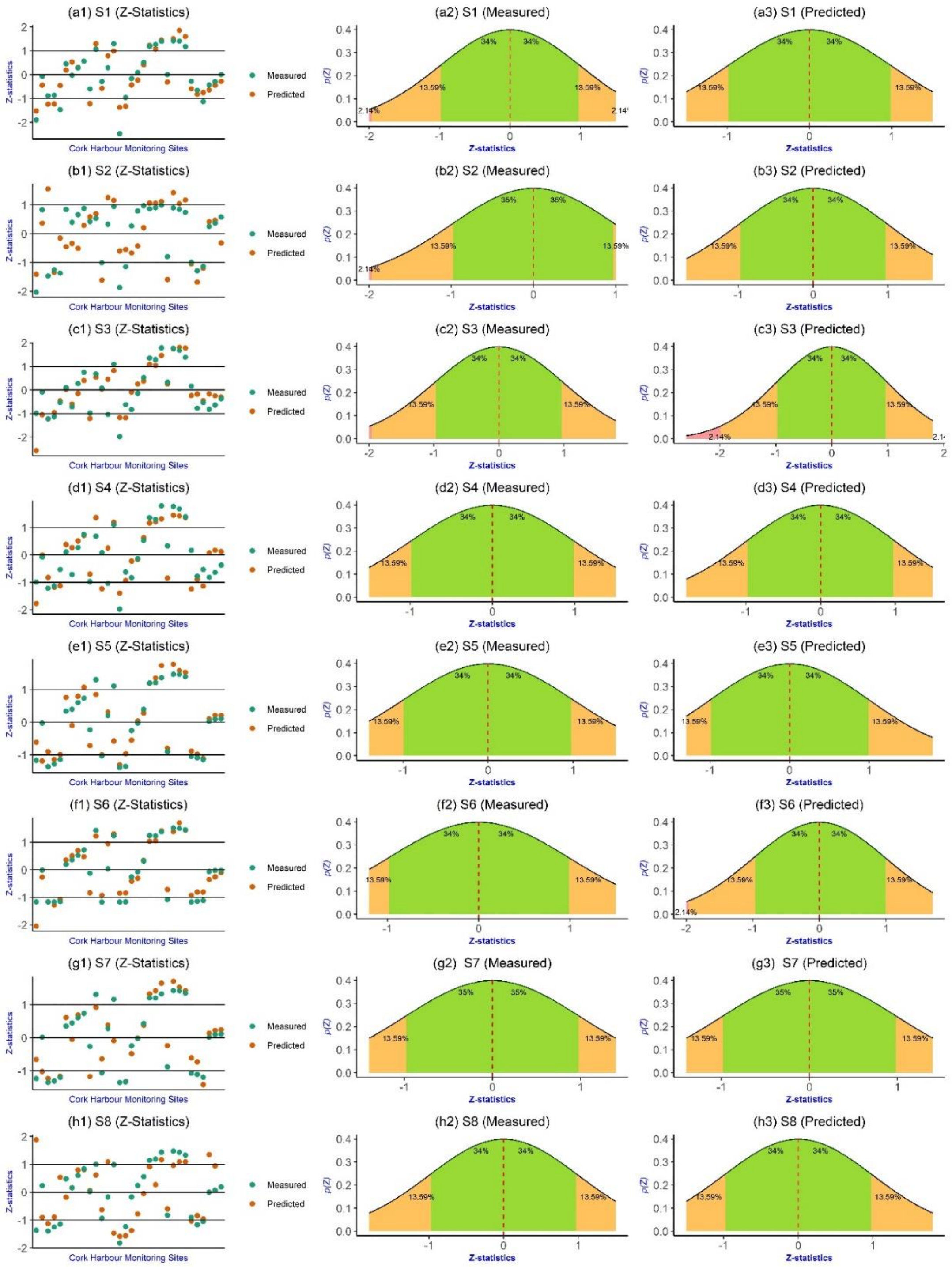


Fig. 6.S6.1. Results of the hypothesis test for different WQM-WQIs scenarios: Z-statistic, the probability curve for measured and predicted WQIs, respectively from left to right.

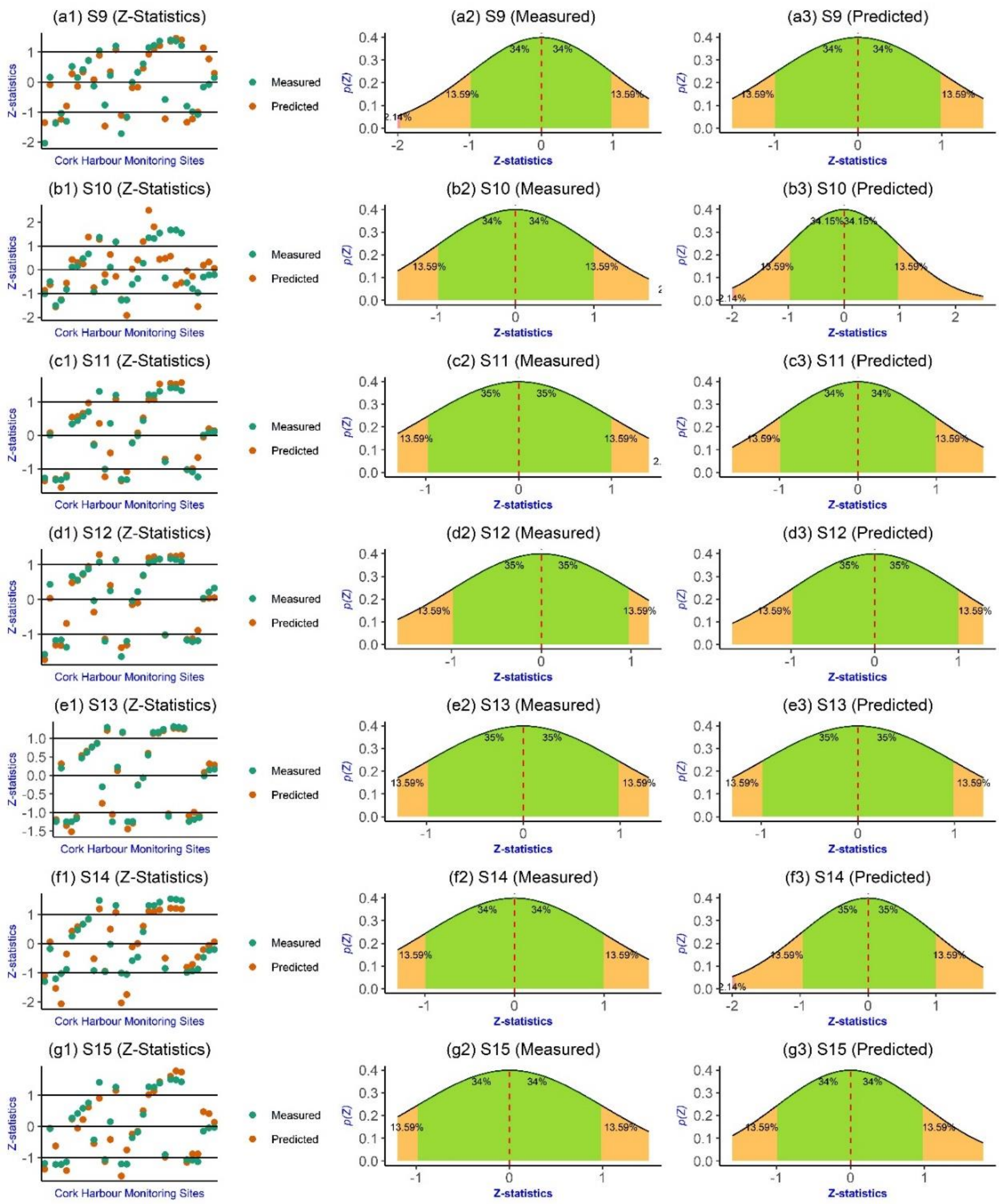


Fig. 6.S6.2. Results of the hypothesis test for different WQM-WQIs scenarios: Z-statistic, the probability curve for measured and predicted WQIs, respectively from left to right.

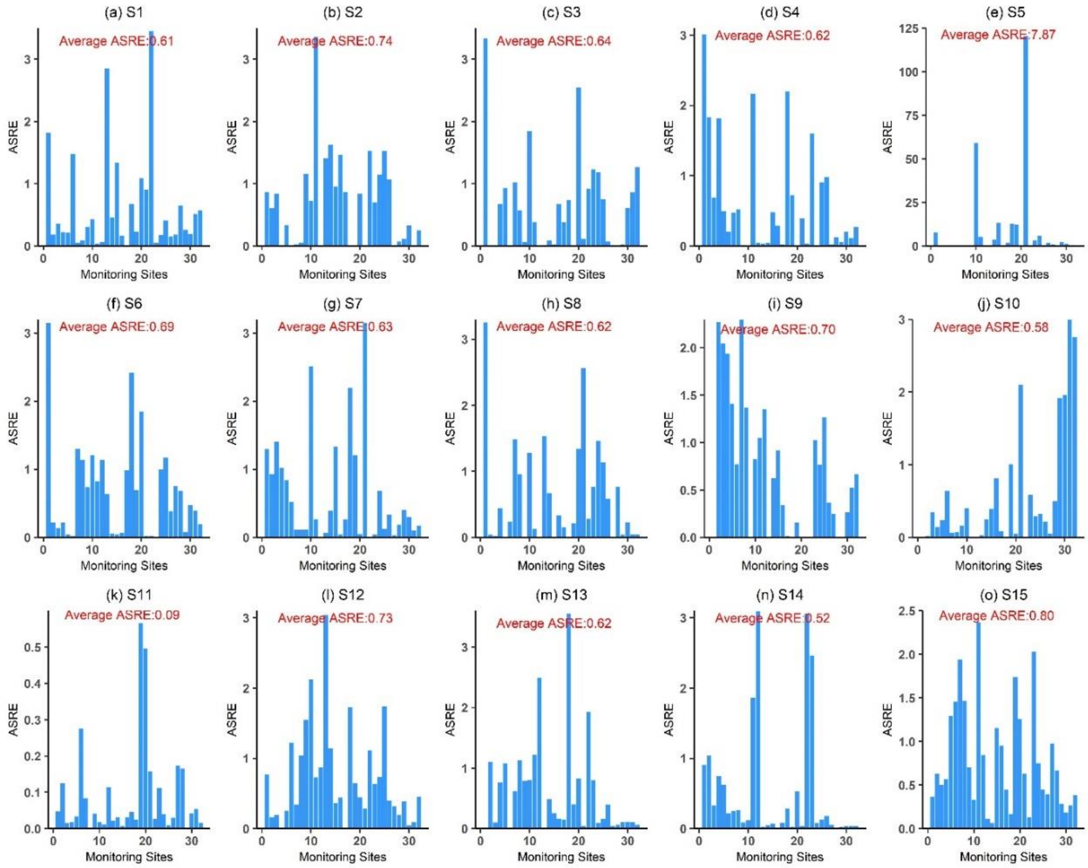


Fig 6.S7. Results of absolute standardized residual estimate (ASRE) for WQM-WQIs scenarios obtained from various FS methods.

References

Abdar, M., Pourpanah, F., Hussain, S., Rezazadegan, D., Liu, L., Ghavamzadeh, M., Fieguth, P., Cao, X., Khosravi, A., Acharya, U. R., Makarenkov, V., & Nahavandi, S. (2021). A review of uncertainty quantification in deep learning: Techniques, applications and challenges. Information Fusion, 76, 243–297. https://doi.org/10.1016/j.inffus.2021.05.008

Adhao, R., Pachghare, V., 2020. Feature selection using principal component analysis and genetic algorithm. J. Discret. Math. Sci. Cryptogr. 23, 595–602. https://doi.org/10.1080/09720529.2020.1729507

Adorada, A., Permatasari, R., Wirawan, P.W., Wibowo, A., Sujiwo, A., 2018. Support Vector Machine - Recursive Feature Elimination (SVM - RFE) for Selection of MicroRNA Expression Features of Breast Cancer. 2018 2nd Int. Conf. Informatics Comput. Sci. ICICoS 2018 165–168. https://doi.org/10.1109/ICICOS.2018.8621708

Ahmed, U., Mumtaz, R., Anwar, H., Shah, A.A., Irfan, R., 2019. E ffi cient Water Quality Prediction Using Supervised. Water 11, 1–14.

Aldhyani, T.H.H., Al-Yaari, M., Alkahtani, H., Maashi, M., 2020. Water Quality Prediction Using Artificial Intelligence Algorithms. Appl. Bionics Biomech. 2020. https://doi.org/10.1155/2020/6659314

Ali Khan, M., Izhar Shah, M., Faisal Javed, M., Ijaz Khan, M., Rasheed, S., El-Shorbagy, M.A., Roshdy El-Zahar, E., Malik, M.Y., 2022. Application of random forest for modelling of surface water salinity. Ain Shams Eng. J. 13, 101635. https://doi.org/10.1016/j.asej.2021.11.004

Alizadeh, M.J., Kavianpour, M.R., Danesh, M., Adolf, J., Shamshirband, S., Chau, K.W., 2018. Effect of river flow on the quality of estuarine and coastal waters using machine learning models. Eng. Appl. Comput. Fluid Mech. 12, 810–823. https://doi.org/10.1080/19942060.2018.1528480

Alnahit, A.O., Mishra, A.K., Khan, A.A., 2022. Stream water quality prediction using boosted regression tree and random forest models. Stoch. Environ. Res. Risk Assess. 4. https://doi.org/10.1007/s00477-021-02152-4

Asadollah, S.B.H.S., Sharafati, A., Motta, D., Yaseen, Z.M., 2021. River water quality index prediction and uncertainty analysis: A comparative study of machine learning models. J. Environ. Chem. Eng. 9, 104599. https://doi.org/10.1016/j.jece.2020.104599

Bagherzadeh, F., Mehrani, M.-J., Basirifard, M., Roostaei, J., 2021. Comparative study on total nitrogen prediction in wastewater treatment plant and effect of various feature selection methods on machine learning algorithms performance. J. Water Process Eng. 41, 102033. https://doi.org/10.1016/j.jwpe.2021.102033

Bahl, A., Hellack, B., Balas, M., Dinischiotu, A., Wiemann, M., Brinkmann, J., Luch, A., Renard, B.Y., Haase, A., 2019. Recursive feature elimination in random forest classification supports nanomaterial grouping. NanoImpact 15, 100179. https://doi.org/10.1016/j.impact.2019.100179

Bardsley, W.E., Vetrova, V., Liu, S., 2015. Toward creating simpler hydrological models: A LASSO subset selection approach. Environ. Model. Softw. 72, 33–43. https://doi.org/10.1016/j.envsoft.2015.06.008

Barraza, N., Moro, S., Ferreyra, M., de la Peña, A., 2019. Mutual information and sensitivity analysis for feature selection in customer targeting: A comparative study. J. Inf. Sci. 45, 53–67. https://doi.org/10.1177/0165551518770967

Barzegar, R., Asghari Moghaddam, A., Adamowski, J., Ozga-Zielinski, B., 2018. Multi-step water quality forecasting using a boosting ensemble multi-wavelet extreme learning machine model. Stoch. Environ. Res. Risk Assess. 32, 799–813. https://doi.org/10.1007/s00477-017-1394-z

Bennasar, M., Hicks, Y., Setchi, R., 2015. Feature selection using Joint Mutual Information Maximisation. Expert Syst. Appl. 42, 8520–8532. https://doi.org/10.1016/j.eswa.2015.07.007

Bi, J., Lin, Y., Dong, Q., Yuan, H., Zhou, M.C., 2021. Large-scale water quality prediction with integrated deep neural network. Inf. Sci. (Ny). 571, 191–205. https://doi.org/10.1016/j.ins.2021.04.057

Biesiada, J., Duch, W., 2007. Feature selection for high-dimensional data - A pearson redundancy based filter. Adv. Soft Comput. 45, 242–249. https://doi.org/10.1007/978-3-540-75175-5_30

Bonansea, M., Rodriguez, M.C., Pinotti, L., Ferrero, S., 2015. Using multi-temporal Landsat imagery and linear mixed models for assessing water quality parameters in Río Tercero reservoir (Argentina). Remote Sens. Environ. 158, 28–41. https://doi.org/10.1016/j.rse.2014.10.032

Bourel, M., Segura, A.M., 2018. Multiclass classification methods in ecology. Ecol. Indic. 85, 1012–1021. https://doi.org/10.1016/j.ecolind.2017.11.031

Bui, D.T., Khosravi, K., Tiefenbacher, J., Nguyen, H., Kazakis, N., 2020. Improving prediction of water quality indices using novel hybrid machine-learning algorithms. Sci. Total Environ. 721, 137612. https://doi.org/10.1016/j.scitotenv.2020.137612

Chandra, B., Gupta, M., 2011. An efficient statistical feature selection approach for classification of gene expression data. J. Biomed. Inform. 44, 529–535. https://doi.org/10.1016/j.jbi.2011.01.001

Chen, K., Chen, H., Zhou, C., Huang, Y., Qi, X., Shen, R., Liu, F., Zuo, M., Zou, X., Wang, J., Zhang, Y., Chen, D., Chen, X., Deng, Y., Ren, H., 2020. Comparative analysis of surface water quality prediction performance and identification of key water parameters using different machine learning models based on big data. Water Res. 171, 115454. https://doi.org/10.1016/j.watres.2019.115454

Chen, R.C., Dewi, C., Huang, S.W., Caraka, R.E., 2020. Selecting critical features for data classification based on machine learning methods. J. Big Data 7. https://doi.org/10.1186/s40537-020-00327-4

Chen, X., Nie, F., Yuan, G., Huang, J.Z., 2017. Semi-supervised feature selection via rescaled linear regression. IJCAI Int. Jt. Conf. Artif. Intell. 0, 1525–1531. https://doi.org/10.24963/ijcai.2017/211

Choi, H., Suh, S.I., Kim, S.H., Han, E.J., Ki, S.J., 2021. Assessing the performance of deep learning algorithms for short-term surface water quality prediction. Sustain. 13. https://doi.org/10.3390/su131910690

Del Castillo, A.F., Yebra-Montes, C., Garibay, M.V., de Anda, J., Garcia-Gonzalez, A., Gradilla-Hernández, M.S., 2022. Simple Prediction of an Ecosystem-Specific Water Quality Index and the Water Quality Classification of a Highly Polluted River through Supervised Machine Learning. Water (Switzerland) 14. https://doi.org/10.3390/w14081235

Deng, H., Runger, G., 2012. Feature selection via regularized trees. Proc. Int. Jt. Conf. Neural Networks. https://doi.org/10.1109/IJCNN.2012.6252640

Ding, C., Peng, H., 2005. Minimum redundancy feature selection from microarray gene expression data. J. Bioinform. Comput. Biol. 3. https://doi.org/10.1142/S0219720005001004

Eiras-Franco, C., Guijarro-Berdiñas, B., Alonso-Betanzos, A., Bahamonde, A., 2021. Scalable feature selection using ReliefF aided by locality-sensitive hashing. Int. J. Intell. Syst. 36, 6161–6179. https://doi.org/10.1002/int.22546

Elssied, N.O.F., Ibrahim, O., Osman, A.H., 2014. A novel feature selection based on one-way ANOVA F-test for e-mail spam classification. Res. J. Appl. Sci. Eng. Technol. 7, 625–638. https://doi.org/10.19026/rjaset.7.299

Ewuzie, U., Bolade, O.P., Egbedina, A.O., 2022. Application of deep learning and machine learning methods in water quality modeling and prediction: a review, Current Trends and Advances in Computer-Aided Intelligent Environmental Data Engineering. INC. https://doi.org/10.1016/b978-0-323-85597-6.00020-3

George, A., Purnaprajna, M., Athri, P., 2020. Laplacian score and genetic algorithm based automatic feature selection for Markov State Models in adaptive sampling based molecular dynamics. PeerJ Phys. Chem. 2, e9. https://doi.org/10.7717/peerj-pchem.9

Gharari, S., Hrachowitz, M., Fenicia, F., Gao, H., Savenije, H.H.G., 2014. Using expert knowledge to increase realism in environmental system models can dramatically reduce the need for calibration. Hydrol. Earth Syst. Sci. 18, 4839–4859. https://doi.org/10.5194/hess-18-4839-2014

Ghosh, P., Azam, S., Jonkman, M., Karim, A., Shamrat, F.M.J.M., Ignatious, E., Shultana, S., Beeravolu, A.R., De Boer, F., 2021. Efficient prediction of cardiovascular disease using machine learning algorithms with relief and lasso feature selection techniques. IEEE Access 9, 19304–19326. https://doi.org/10.1109/ACCESS.2021.3053759

Gong, Y.L., Hu, M.J., Yang, H.F., Han, B., 2022. Research on application of ReliefF and improved RVM in water quality grade evaluation. Water Sci. Technol. 85, 799–810. https://doi.org/10.2166/wst.2022.005

Granitto, P.M., Furlanello, C., Biasioli, F., Gasperi, F., 2006. Recursive feature elimination with random forest for PTR-MS analysis of agroindustrial products. Chemom. Intell. Lab. Syst. 83, 83–90. https://doi.org/10.1016/j.chemolab.2006.01.007

Grbčić, L., Družeta, S., Mauša, G., Lipić, T., Lušić, D.V., Alvir, M., Lučin, I., Sikirica, A., Davidović, D., Travaš, V., Kalafatović, D., Pikelj, K., Fajković, H., Holjević, T., Kranjčević, L., 2021. Coastal water quality prediction based on machine learning with feature interpretation and spatio-temporal analysis.

Grbić, R., Kurtagić, D., Slišković, D., 2013. Stream water temperature prediction based on Gaussian process regression. Expert Syst. Appl. 40, 7407–7414. https://doi.org/10.1016/j.eswa.2013.06.077

Hafeez, S., Sing Wong, M., Chak Ho, H., Nazeer, M., Nichol, J., Abbas, S., Tang, D., Ho Lee, K., Pun, L., 2019. Comparison of machine learning algorithms for retrieval of water quality indicators in case-II waters: a case study of Hong Kong Comparison of machine learning algorithms for retrieval of water quality indicators in case-II waters: a case study of Hong Kong.

Haghiabi, A.H., Nasrolahi, A.H., Parsaie, A., 2018. Water quality prediction using machine learning methods. Water Qual. Res. J. 53, 3–13. https://doi.org/10.2166/wqrj.2018.025

Hannan, A., Anmala, J., 2021. Classification and Prediction of Fecal Coliform in Stream Waters Using Decision Trees (DTs) for Upper Green River Watershed, Kentucky, USA. Water 2021, Vol. 13, Page 2790 13, 2790. https://doi.org/10.3390/W13192790

Haque, M.M., Rahman, A., Hagare, D., Chowdhury, R.K., 2018. A comparative assessment of variable selection methods in urban water demand forecasting. Water (Switzerland) 10, 1–15. https://doi.org/10.3390/w10040419

Hasan, M.A., Hasan, M.K., Mottalib, M.A., 2015. Linear regression-based feature selection for microarray data classification. Int. J. Data Min. Bioinform. 11, 167–179. https://doi.org/10.1504/IJDMB.2015.066776

He, X., Cai, D., Niyogi, P., 2005. Laplacian Score for feature selection. Adv. Neural Inf. Process. Syst. 507–514.

He, X., Ji, M., Zhang, C., Bao, H., 2011. A variance minimization criterion to feature selection using laplacian regularization. IEEE Trans. Pattern Anal. Mach. Intell. 33, 2013–2025. https://doi.org/10.1109/TPAMI.2011.44

He, Y., Yu, H., Yu, R., Song, J., Lian, H., He, J., Yuan, J., 2021. A Correlation-Based Feature Selection Algorithm for Operating Data of Nuclear Power Plants. Sci. Technol. Nucl. Install. 2021. https://doi.org/10.1155/2021/9994340

Hou, Y., Zhang, A., Lv, R., Zhao, S., Ma, J., Zhang, H., Li, Z., 2022. A study on water quality parameters estimation for urban rivers based on ground hyperspectral remote sensing technology. Environ. Sci. Pollut. Res. https://doi.org/10.1007/s11356-022-20293-z

Huan, J., Li, H., Li, M., Chen, B., 2020. Prediction of dissolved oxygen in aquaculture based on gradient

boosting decision tree and long short-term memory network: A study of Chang Zhou fishery demonstration base, China. Comput. Electron. Agric. 175, 105530. https://doi.org/10.1016/j.compag.2020.105530
Isabona, J., Imoize, A.L., Kim, Y., 2022. Machine Learning-Based Boosted Regression Ensemble Combined with Hyperparameter Tuning for Optimal Adaptive Learning. Sensors 22, 3776. https://doi.org/10.3390/s22103776
Islam Khan, M.S., Islam, N., Uddin, J., Islam, S., Nasir, M.K., 2021. Water quality prediction and classification based on principal component regression and gradient boosting classifier approach. J. King Saud Univ. - Comput. Inf. Sci. https://doi.org/10.1016/j.jksuci.2021.06.003
Jain, I., Jain, V.K., Jain, R., 2018. Correlation feature selection based improved-Binary Particle Swarm Optimization for gene selection and cancer classification. Appl. Soft Comput. https://doi.org/10.1016/j.asoc.2017.09.038
Jalal, D., Ezzedine, T., 2019. Performance analysis of machine learning algorithms for water quality monitoring system. 2019 Int. Conf. Internet Things, Embed. Syst. Commun. IINTEC 2019 - Proc. 86–89. https://doi.org/10.1109/IINTEC48298.2019.9112096
Jeon, H., Oh, S., 2020. applied sciences Hybrid-Recursive Feature Elimination for E ffi cient Feature Selection 1–8.
Jović, A., Brkić, K., Bogunović, N., 2015. A review of feature selection methods with applications. 2015 38th Int. Conv. Inf. Commun. Technol. Electron. Microelectron. MIPRO 2015 - Proc. 1200–1205. https://doi.org/10.1109/MIPRO.2015.7160458
Kadam, A.K., Wagh, V.M., Muley, A.A., Umrikar, B.N., Sankhua, R.N., 2019. Prediction of water quality index using artificial neural network and multiple linear regression modelling approach in Shivganga River basin, India. Model. Earth Syst. Environ. 5, 951–962. https://doi.org/10.1007/s40808-019-00581-3
Kano, Y., Harada, A., 2000. Stepwise variable selection in factor analysis. Psychometrika 65, 7–22. https://doi.org/10.1007/BF02294182
Khaire, U.M., Dhanalakshmi, R., 2022. Stability of feature selection algorithm: A review. J. King Saud Univ. - Comput. Inf. Sci. 34, 1060–1073. https://doi.org/10.1016/j.jksuci.2019.06.012
Kim, M., Lee, S., Kim, J., 2020. A wide & Deep learning sharing input data for regression analysis. Proc. - 2020 IEEE Int. Conf. Big Data Smart Comput. BigComp 2020 8–12. https://doi.org/10.1109/BigComp48618.2020.0-108
Kothari, V., Vij, S., Sharma, S.K., Gupta, N., 2021. Correlation of various water quality parameters and water quality index of districts of Uttarakhand. Environ. Sustain. Indic. 9, 100093. https://doi.org/10.1016/j.indic.2020.100093
Kouadri, S., Elbeltagi, A., Islam, A.R.M.T., Kateb, S., 2021. Performance of machine learning methods in predicting water quality index based on irregular data set: application on Illizi region (Algerian southeast). Appl. Water Sci. 11. https://doi.org/10.1007/s13201-021-01528-9
Kowshalya, A.M., Madhumathi, R., Gopika, N., 2019. Correlation Based Feature Selection Algorithms for Varying Datasets of Different Dimensionality. Wirel. Pers. Commun. 108, 1977–1993. https://doi.org/10.1007/s11277-019-06504-w
Kuhn, M., Johnson, K., 2013. Applied predictive modeling, Applied Predictive Modeling. https://doi.org/10.1007/978-1-4614-6849-3
Kumar, S., Chong, I., 2018. Correlation analysis to identify the effective data in machine learning: Prediction of depressive disorder and emotion states. Int. J. Environ. Res. Public Health 15. https://doi.org/10.3390/ijerph15122907
Kursa, M.B., Jankowski, A., Rudnicki, W.R., 2010. Boruta - A system for feature selection. Fundam. Informaticae 101, 271–285. https://doi.org/10.3233/FI-2010-288
Leščešen, I., Pantelić, M., Dolinaj, D., Stojanović, V., Miloševič, D., 2016. Statistical analysis of water quality parameters of the Drina river (West Serbia), 2004-11. Polish J. Environ. Stud. 24, 555–561. https://doi.org/10.15244/pjoes/29684
Li, W., Yang, M., Liang, Z., Zhu, Y., Mao, W., Shi, J., Chen, Y., 2013. Assessment for surface water quality in Lake Taihu Tiaoxi River Basin China based on support vector machine. Stoch. Environ. Res. Risk Assess. 27, 1861–1870. https://doi.org/10.1007/s00477-013-0720-3
Liang, J., Hou, L., Luan, Z., Huang, W., 2019. Feature Selection with Conditional Mutual Information Considering Feature Interaction. Symmetry (Basel). 11, 858. https://doi.org/10.3390/sym11070858
Liaw, A., Wiener, M., 2002. Classification and Regression by randomForest 2.
Lin, X., Yang, F., Zhou, L., Yin, P., Kong, H., Xing, W., Lu, X., Jia, L., Wang, Q., Xu, G., 2012. A support vector machine-recursive feature elimination feature selection method based on artificial contrast variables and mutual information. J. Chromatogr. B Anal. Technol. Biomed. Life Sci.

910, 149–155. https://doi.org/10.1016/j.jchromb.2012.05.020
Lindsey, C., Sheather, S., 2010. Variable selection in linear regression. Stata J. 10, 650–669. https://doi.org/10.1177/1536867x1101000407
Liou, S.M., Lo, S.L., Wang, S.H., 2004. A generalized water quality index for Taiwan. Environ. Monit. Assess. 96, 35–52. https://doi.org/10.1023/B:EMAS.0000031715.83752.a1
Liu, R., Yang, N., Ding, X., Ma, L., 2009. An unsupervised feature selection algorithm: Laplacian score combined with distance-based entropy measure. 3rd Int. Symp. Intell. Inf. Technol. Appl. IITA 2009 3, 65–68. https://doi.org/10.1109/IITA.2009.390
Liu, Y., Ju, S., Wang, J., Su, C., 2020. A New Feature Selection Method for Text Classification Based on Independent Feature Space Search. Math. Probl. Eng. 2020, 1–14. https://doi.org/10.1155/2020/6076272
Liu, Y., Yu, Z., Yuxuan, L., Liu, S., Rosenblum, D.S., 2016. Urban water quality prediction based on multi-task multi-view learning. IJCAI Int. Jt. Conf. Artif. Intell. 2016-Janua, 2576–2582.
Liu, Z., Wang, Y., Huang, X., Qi, X., Qian, C., Zhao, S., 2022. Development and Validation of a Diagnostic Nomogram to Predict the Anthracycline-Induced Early Cardiotoxicity in Children with Hematological Tumors. Cardiovasc. Toxicol. https://doi.org/10.1007/s12012-022-09755-5
Ma, X., Wang, L., Yang, H., Li, N., Gong, C., 2020. Spatiotemporal analysis of water quality using multivariate statistical techniques and the water quality identification index for the qinhuai river basin, east china. Water (Switzerland) 12. https://doi.org/10.3390/w12102764
Mahapatra, S.S., Sahu, M., Patel, R.K., Panda, B.N., 2012. Prediction of Water Quality Using Principal Component Analysis. Water Qual. Expo. Heal. https://doi.org/10.1007/s12403-012-0068-9
Malek, N.H.A., Wan Yaacob, W.F., Nasir, S.A.M., Shaadan, N., 2021. The effect of chemical parameters on water quality index in machine learning studies: A meta-analysis. J. Phys. Conf. Ser. 2084. https://doi.org/10.1088/1742-6596/2084/1/012007
Malek, N.H.A., Yaacob, W.F.W., Nasir, S.A.M., Shaadan, N., 2022. Prediction of Water Quality Classification of the Kelantan River Basin, Malaysia, Using Machine Learning Techniques. Water (Switzerland) 14. https://doi.org/10.3390/w14071067
Mao, X., Peng, L., Wang, Z., 2022. Nonparametric feature selection by random forests and deep neural networks. Comput. Stat. Data Anal. 170, 107436. https://doi.org/10.1016/j.csda.2022.107436
Méndez, J.R., Fdez-Riverola, F., Díaz, F., Iglesias, E.L., Corchado, J.M., 2006. A Comparative Performance Study of Feature Selection Methods for the Anti-spam Filtering Domain, in: Lecture Notes in Computer Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics). pp. 106–120. https://doi.org/10.1007/11790853_9
Menze, B. H., Kelm, B. M., Masuch, R., Himmelreich, U., Bachert, P., Petrich, W., & Hamprecht, F. A. (2009). A comparison of random forest and its Gini importance with standard chemometric methods for the feature selection and classification of spectral data. BMC Bioinformatics, 10, 1–16. https://doi.org/10.1186/1471-2105-10-213
Modaresi, F., Araghinejad, S., 2014. A comparative assessment of support vector machines, probabilistic neural networks, and K-nearest neighbor algorithms for water quality classification. Water Resour. Manag. 28, 4095–4111. https://doi.org/10.1007/s11269-014-0730-z
Mohammed Siraj Ansari, A., Saraswathi, R., 2022. use of Principal Component Analysis for Parameter Selection to Compute Water Quality Index and Assessment of Groundwater Quality Status: A Case Study of Sanganur Stream, Coimbatore City. J. Geol. Soc. India 98, 417–422. https://doi.org/10.1007/s12594-022-1994-1
Muhammad, L.J., Algehyne, E.A., Usman, S.S., Ahmad, A., Chakraborty, C., Mohammed, I.A., 2021. Supervised Machine Learning Models for Prediction of COVID-19 Infection using Epidemiology Dataset. SN Comput. Sci. 2, 1–13. https://doi.org/10.1007/s42979-020-00394-7
Naghibi, S.A., Hashemi, H., Berndtsson, R., Lee, S., 2020. Application of extreme gradient boosting and parallel random forest algorithms for assessing groundwater spring potential using DEM-derived factors. J. Hydrol. 589, 125197. https://doi.org/10.1016/j.jhydrol.2020.125197
Narala, S., Li, S.Q., Klimas, N.K., Patel, A.B., 2021. Application of least absolute shrinkage and selection operator logistic regression for the histopathological comparison of chondrodermatitis nodularis helicis and hyperplastic actinic keratosis. J. Cutan. Pathol. 48, 739–744. https://doi.org/10.1111/cup.13931
Nikitin, A., Tregubova, P., Shadrin, D., Matveev, S., Oseledets, I., Pukalchik, M., 2021. Regulation-based probabilistic substance quality index and automated geo-spatial modeling for water quality assessment. Sci. Rep. 11, 1–14. https://doi.org/10.1038/s41598-021-02564-w
Ning, Y., Wang, G., Yu, J., Jiang, H., 2018. A Feature Selection Algorithm Based on Variable Correlation and Time Correlation for Predicting Remaining Useful Life of Equipment Using RNN. 2018 Cond. Monit. Diagnosis, C. 2018 - Proc. 17–22.

https://doi.org/10.1109/CMD.2018.8535843
Parinet, B., Lhote, A., Legube, B., 2004. Principal component analysis: An appropriate tool for water quality evaluation and management - Application to a tropical lake system. Ecol. Modell. 178, 295–311. https://doi.org/10.1016/j.ecolmodel.2004.03.007
Pullanagari, R.R., Kereszturi, G., Yule, I., 2018. Integrating airborne hyperspectral, topographic, and soil data for estimating pasture quality using recursive feature elimination with random forest regression. Remote Sens. 10. https://doi.org/10.3390/rs10071117
Rasmussen, C.E., 2004. Gaussian Processes in Machine Learning. In: Bousquet, O., von Luxburg, U., Rätsch, G. (eds) Advanced Lectures on Machine Learning. ML 2003. Lecture Notes in Computer Science(), vol 3176. Springer, Berlin, Heidelberg. https://doi.org/10.1007/978-3-540-28650-9_4
Radovic, M., Ghalwash, M., Filipovic, N., Obradovic, Z., 2017. Minimum redundancy maximum relevance feature selection approach for temporal gene expression data. BMC Bioinformatics 18, 1–14. https://doi.org/10.1186/s12859-016-1423-9
Rizal, A., Apriliani, I.M., 2021. Analysis of Several Water Environment Parameters Affecting the Accumulation of Heavy Metal Lead in the Body of Blood Shells in the Coastal Waters of Muara Gembong Sub-District 153, 65–79.
Roguet, A., Eren, A.M., Newton, R.J., McLellan, S.L., 2018. Fecal source identification using random forest. Microbiome 6, 1–15. https://doi.org/10.1186/s40168-018-0568-3
Rojas, I., Rojas, F., Eds, F.O., Myers, E., 2015. Bioinformatics and Biomedical Engineering: New Advances, Bioinformatics and Biomedical Engineering: New Advances. https://doi.org/10.1201/b19238
Şahin, D.Ö., Kural, O.E., Akleylek, S., Kılıç, E., 2021. A novel permission-based Android malware detection system using feature selection based on linear regression. Neural Comput. Appl. 1. https://doi.org/10.1007/s00521-021-05875-1
Sakaa, B., Elbeltagi, A., Boudibi, S., Chaffaï, H., Islam, A.R.M.T., Kulimushi, L.C., Choudhari, P., Hani, A., Brouziyne, Y., Wong, Y.J., 2022. Water quality index modeling using random forest and improved SMO algorithm for support vector machine in Saf-Saf river basin. Environ. Sci. Pollut. Res. 48491–48508. https://doi.org/10.1007/s11356-022-18644-x
Samandar, A., 2010. Ranking water quality variables using feature selection algorithms to improve generalization capability of artificial neural networks. Sci. Res. Essays 5, 1254–1259.
Seo, H., Cho, D.H., 2020. Feature selection algorithm based on dual correlation filters for cancer-associated somatic variants. BMC Bioinformatics 21, 1–19. https://doi.org/10.1186/s12859-020-03767-0
Sharifzadeh, S., Clemmensen, L.H., Borggaard, C., Støier, S., Ersbøll, B.K., 2014. Supervised feature selection for linear and non-linear regression of L*a*b* color from multispectral images of meat. Eng. Appl. Artif. Intell. 27, 211–227. https://doi.org/10.1016/j.engappai.2013.09.004
Shrestha, S., Kazama, F., 2007. Assessment of surface water quality using multivariate statistical techniques: A case study of the Fuji river basin, Japan. Environ. Model. Softw. https://doi.org/10.1016/j.envsoft.2006.02.001
Song, F., Guo, Z., Mei, D., 2010. Feature selection using principal component analysis. Proc. - 2010 Int. Conf. Syst. Sci. Eng. Des. Manuf. Informatiz. ICSEM 2010 1, 27–30. https://doi.org/10.1109/ICSEM.2010.14
Speiser, J.L., Miller, M.E., Tooze, J., Ip, E., 2019. A comparison of random forest variable selection methods for classification prediction modeling. Expert Syst. Appl. 134, 93–101. https://doi.org/10.1016/j.eswa.2019.05.028
Stief, A., Ottewill, J.R., Baranowski, J., 2020. ReliefF-based feature ranking and feature selection for monitoring induction motors 171–176.
Subasi, A., 2020. Practical Machine Learning for Data Analysis Using Python, Practical Machine Learning for Data Analysis Using Python. https://doi.org/10.1016/B978-0-12-821379-7.00008-4
Sun, J., Yang, J., Shi, S., Chen, B., Du, L., Gong, W., Song, S., 2017. Estimating rice leaf nitrogen concentration: Influence of regression algorithms based on passive and active leaf reflectance. Remote Sens. 9. https://doi.org/10.3390/rs9090951
Tanha, J., Abdi, Y., Samadi, N., Razzaghi, N., Asadpour, M., 2020. Boosting methods for multi-class imbalanced data classification: an experimental review. J. Big Data 7. https://doi.org/10.1186/s40537-020-00349-y
Tavazza, F., Decost, B., Choudhary, K., 2021. Uncertainty prediction for machine learning models of material properties. ACS Omega 6, 32431–32440. https://doi.org/10.1021/acsomega.1c03752
Tiyasha, Tung, T.M., Yaseen, Z.M., 2021. Deep Learning for Prediction of Water Quality Index Classification: Tropical Catchment Environmental Assessment. Nat. Resour. Res. 30, 4235–4254. https://doi.org/10.1007/s11053-021-09922-5

Tosun, E., Aydin, K., Bilgili, M., 2016. Comparison of linear regression and artificial neural network model of a diesel engine fueled with biodiesel-alcohol mixtures. Alexandria Eng. J. 55, 3081–3089. https://doi.org/10.1016/j.aej.2016.08.011

Tripathi, M., Singal, S.K., 2019. Use of Principal Component Analysis for parameter selection for development of a novel Water Quality Index: A case study of river Ganga India. Ecol. Indic. 96, 430–436. https://doi.org/10.1016/j.ecolind.2018.09.025

Uddin, M.G., Nash, S., Rahman, A., Olbert, A.I., 2022a. A comprehensive method for improvement of water quality index (WQI) models for coastal water quality assessment. Water Res. 219, 118532. https://doi.org/10.1016/j.watres.2022.118532

Uddin, M.G., Nash, S., Talas, M., Diganta, M., Rahman, A., Olbert, A.I., 2022b. Robust machine learning algorithms for predicting coastal water quality index. J. Environ. Manage. https://doi.org/https://doi.org/10.1016/j.jenvman.2022.115923

Urbanowicz, R.J., Meeker, M., La Cava, W., Olson, R.S., Moore, J.H., 2018. Relief-based feature selection: Introduction and review. J. Biomed. Inform. 85, 189–203. https://doi.org/10.1016/j.jbi.2018.07.014

Vapnik, V.N., 2000. The Nature of Statistical Learning Theory. Nat. Stat. Learn. Theory. https://doi.org/10.1007/978-1-4757-3264-1

Vasquez, M.M., Hu, C., Roe, D.J., Chen, Z., Halonen, M., Guerra, S., 2016. Least absolute shrinkage and selection operator type methods for the identification of serum biomarkers of overweight and obesity: simulation and application. BMC Med. Res. Methodol. 16, 1–19. https://doi.org/10.1186/s12874-016-0254-8

Vergara, J.R., Estévez, P.A., 2014. A review of feature selection methods based on mutual information. Neural Comput. Appl. 24, 175–186. https://doi.org/10.1007/s00521-013-1368-0

Wang, Y., Wang, P., Bai, Y., Tian, Z., Li, J., Shao, X., Mustavich, L.F., Li, B.L., 2013. Assessment of surface water quality via multivariate statistical techniques: A case study of the Songhua River Harbin region, China. J. Hydro-Environment Res. 7. https://doi.org/10.1016/j.jher.2012.10.003

Xu, J., Xu, Z., Kuang, J., Lin, C., Xiao, L., Huang, X., Zhang, Y., 2021. An alternative to laboratory testing: Random forest-based water quality prediction framework for inland and nearshore water bodies. Water (Switzerland) 13. https://doi.org/10.3390/w13223262

Yan, Z., Yao, Y., 2015. Variable selection method for fault isolation using least absolute shrinkage and selection operator (LASSO). Chemom. Intell. Lab. Syst. 146, 136–146. https://doi.org/10.1016/j.chemolab.2015.05.019

Yang, F., Cheng, W., Dou, R., Zhou, N., 2011. An improved feature selection approach based on ReliefF and Mutual Information. 2011 Int. Conf. Inf. Sci. Technol. ICIST 2011 246–250. https://doi.org/10.1109/ICIST.2011.5765246

Zhang, C., Wei, H., Zhao, X., Liu, T., Zhang, K., 2016. A Gaussian process regression based hybrid approach for short-term wind speed prediction. Energy Convers. Manag. 126, 1084–1092. https://doi.org/10.1016/j.enconman.2016.08.086

Zhang, S., Xin, X., 2017. Pollutant source identification model for water pollution incidents in small straight rivers based on genetic algorithm. Appl. Water Sci. 7, 1955–1963. https://doi.org/10.1007/s13201-015-0374-z

Zhang, Z., 2016. Variable selection with stepwise and best subset approaches. Ann. Transl. Med. 4, 1–6. https://doi.org/10.21037/atm.2016.03.35

Zhang, Z., Ye, L., Qin, H., Liu, Y., Wang, C., Yu, X., Yin, X., Li, J., 2019. Wind speed prediction method using Shared Weight Long Short-Term Memory Network and Gaussian Process Regression. Appl. Energy 247, 270–284. https://doi.org/10.1016/j.apenergy.2019.04.047

Zhao, Z., Anand, R., Wang, M., 2019. Maximum relevance and minimum redundancy feature selection methods for a marketing machine learning platform. Proc. - 2019 IEEE Int. Conf. Data Sci. Adv. Anal. DSAA 2019 442–452. https://doi.org/10.1109/DSAA.2019.00059

Zhou, H., Wang, X., Zhu, R., 2022. Feature selection based on mutual information with correlation coefficient. Appl. Intell. 52, 5457–5474. https://doi.org/10.1007/s10489-021-02524-x

Zhou, S., Zhang, S., Karypis, G., 2012. Advanced Data Mining and Applications, International Conference,ADMA, Lecture Notes in Computer Science. Springer Berlin Heidelberg, Berlin, Heidelberg. https://doi.org/10.1007/978-3-642-35527-1

Appendix 7. A sophisticated model for rating water quality

Table 7.S1 EPA's water quality monitoring sites descriptions for selected four domains in Ireland.

Application domains	EPA' monitoring ID	Geographical location (Irish National grid)		Site descriptions and physical location	Types of domain
		Easting	Northing		
(a) Dublin Bay	DB010	313762.8	234363.12	Liffey at Heuston Bridge	Tra.
	DB015	314999.71	234155.32	Liffey at Wood quay	Tra.
	DB020	316413.82	234487.97	Liffey at Matt Talbot Bridge	Tra.
	DB210	318204.94	234275.8	East Link Toll Bridge	Tra.
	DB120	317892.3	234109.21	Dodder / Grand Canal Basin	Tra.
	DB300	316639.04	236407.81	DS Drumcondra Bridge	Tra.
	DB310	317307.69	235929.41	Tolka Estuary at Annesley Rd Br	Tra.
	DB320	317897.35	235754.07	Tolka Estuary at Eastpoint Business Park Br	Tra.
	DB330	319134.29	235625.09	Tolka Estuary, Castle Avenue	Tra.
	DB340	320434.07	235224.79	Tolka Estuary, Clontarf Boat Club	Tra.
	DB350	321174.53	235898.28	Tolka Est/ S Lagoon at Bull Wall Wooden Br	Tra.
	DB420	323264.98	234124.11	Poolbeg Lighthouse	Tra.
	DB410	321589.92	234089.9	Ringsend Cascade	Tra.
	DB220	320193.64	234136.3	RO RO Ramp No 5 (Old TW Outfall)	Tra.
	DB510	325780.4	235161.66	2.5km ENE Poolbeg Lighthouse	C
	DB560	328039.08	235755.59	Drumleck Point: 5 km ENE Poolbeg Lighthouse	C
	DB730	329989.16	241654.13	Ireland's Eye,Howth Head NE	C
	DB610	330095.34	235833.51	Bailey	C
	DB570	327875.04	232227.57	5 km ESE Poolbeg Lighthouse	C
	DB540	325481.13	232924.26	2.5km SSE Poolbeg Lighthouse	C
	DB450	324092.7	233067.57	South Bull Buoy: 1km SE Poolbeg Lighthouse, Sandymount	C
	DB550	324022.01	231417.79	No 4 Buoy: 2.5km E of S Poolbeg Lighthouse	C
	DB580	325631.38	229768.59	D-Ã€n Laoghaire: 5 km E of S Poolbeg Lighthouse	C
	DB740	325792	245627.51	Portmarnock N	C
(b) Cork Harbour	LE040	165283.8	71503.53	Lee road water works	Tra.
	LE030	165537.7	71188.46	Curragheen Stream	Tra.
	LE110	165619.5	71642.57	Upper Lee Est N Channel, Daly's Bridge	Tra.
	LE120	165954.2	71348.12	Upper Lee Est S Channel, Donovan's Br	Tra.
	LE140	167703.9	71548.13	Upper Lee Est S Channel, George's Quay	Tra.

	LE130	167906.7	72089.94	Upper Lee Est N Channel, St. Patrick's Br	Tra.
	LE150	168404	72006.06	Custom House Dock	Tra.
	LE160	169284.2	72275.87	Tivoli Dock	Tra.
	Tivoli	170241.7	72195.08	Tivoli	Tra.
	LE170	170854	72106.03	Balintemple	Tra.
	LE180	172303.6	72196.25	Blackrock Castle	Tra.
	BLKC*	172537.1	72182.08	Blackrock Castle (BLKC)	Tra.
	LE220	172723.4	72796.18	Glashaboy Estuary, Dunkettle Bridge	Tra.
	LE210	172764.8	74145.53	Glashaboy Estuary, Glanmire Bridge	Tra.
	LE310	173153.3	71845.98	Upper Lough Mahon (Lee Tunnel)	Tra.
	LE330	175456.5	70547.26	Mid Lough Mahon (Buoy No 6)	Tra.
	LE340	176856.6	69550.31	Lough Mahon, Marino Point	Tra.
	LE410	179127.2	70773.28	Belvelly Bridge	Tra.
	LE420	181355.9	70343.93	North Channel, Weir Island (Pylons)	Tra.
	LE430	183254	69747.97	North Channel, Brick Island	Tra.
	LE440	184552.1	69948.4	North Channel, Red Shed	Tra.
	LE450	185953.6	69950.87	North Channel, Bagwells Hill	Tra.
	LE540	186952.4	70048.01	Ballynacorra Est, Rathcoursey	Tra.
	LE500	187960.7	73222.03	Owenacurra River 0.5km d/s Cork Bridge	Tra.
	LE550	185949.6	68549.06	East Ferry Quay, Rathcoursey West	Tra.
	HBLIN*	178089.8	65386.12	Haulbowline (HBLIN)	C
	LE380	178455.7	65093.02	Ringaskiddy	C
	LE620	181852.6	64945.99	E Spike Island	C
	LE610	183315.2	65375.21	Adjacent to Aghada	C
	RLD*	186941.9	65949.86	Rostellan Lake Downstream (RLD)	Tra.
	LE630	181449	62043.9	Adjacent to Carlisle Fort	C
	LE810	181702.9	59751.51	Roches Point	C
	LE820	181054.7	58051.61	Myrtleville	C
	LE505	188305.4	73290.64	Dungourney River Br Midleton (Main Street)	Tra.
	LE510	187904.6	72600.54	Owenacurra Est, New Road Br Midleton	Tra.
	LE520	188202.7	71791.63	Ballynacorra Est, Ballynacorra	Tra.
	LE530	187451.2	71448.66	Ballynacorra Est, Ballyannan (Pylons)	Tra.
(c) Galway Bay	GY250	121015.08	215849.43	Center of Galway Bay	C
	GY210	122942.59	220865.01	Galway Bay (S of Barna Quay)	C
	GY200	126132.02	221137.09	Black Rock Buoy CIL	C
	GY220	118892.7	221674.9	Furbo	C
	GY260	124989	217429.94	6km S Barna	C
	GY150	127844.87	222691.65	SW of Mutton Island	C
	GY180	130968.96	221287.31	Galway Bay (S of Galway Docks)	C
	GY160	132347	222892.73	SE of Hare Island	C

	GY170	135305.93	223508.16	Oranmore Bay	C
	GY130	130681.67	223127.81	E of Mutton Island	Tra.
	GY140	129955.98	222760.28	Mutton Island Buoy CIL	Tra.
	GY120	130759.42	223872.68	SE of Galway Docks	Tra.
	GY110	130256.82	224636.27	Outside Galway Docks	Tra.
	KA050	135436.21	213907.14	Parkmore Quay	Tra.
	KA060	135744	214427.31	Doorus Point	Tra.
	KA070	136835.5	213288.7	Tarrea Quay	Tra.
	KA040	136035.35	213324.32	Long Rock	Tra.
	KA080	135483.44	212745.58	Calf Islands	Tra.
	KA030	136597.2	212398.56	Gormeen Rock	Tra.
	KA025	137100.51	211280.32	Illauncullin	Tra.
	KA020	137411.91	210408.36	Kinvarra Pier	Tra.
	GY190	129218.1	221179.58	Tawin Shoal Buoy CIL	C
(d) Mulroy Bay	MB140	214498	445496.82	Mouth of Mulroy Bay	C
	MB130	214129.1	444587.66	Ballyhoorisky island	C
	MB120	213908.2	442339.14	Gortnalughoge Bay	C
	MB110	212875.3	441395.67	Inverbeg Bay	C
	MB100	212362.2	439854.4	Crannoge Point	C
	MB090	214142.4	437975.38	Carraigart	C
	MB080	215485.1	438160.19	Millstone Bay	C
	MB070	216503.8	437330.31	Marks Point	C
	MB060	218241.2	435746.23	The Narrows	C
	MB050	219189.9	435134.45	Scalpmore	C
	MB040	220171.7	434083.59	Deegagh Point	C
	MB030	219802.7	431397.24	Beacon at Ranny Rocks	C
	MB020	219100.1	429773.93	Cratlagh Island	C
	MB010	219797.5	428705.28	Millford	C

Tra. = Transitional water, C = Coastal water

*user defined monitoring ID, BLKC = Blackrock Castle, HBLIN = Haulbowline, and RLD = Rostellan Lake Downstrea.

Table 7.S2. Averaged winter concentrations of water quality indicators and eclipsing impacts on the WQM aggregation process by comparing actual water quality parameters and qualitative status in **Dublin Bay, 2021**. The guideline values (thresholds) adopted for the Dublin Bay during **summer** are included at the bottom and values in bold indicate compliance failures.

Monitoring sites	SAL (psu)	Common water quality indicators					nutrient enrichment indicators				
		BOD5 (mg/l)	pH -	TEMP (^{0}C)	TON (mg/l as N)	TRAN (m/depth)	DIN (mg/l)	MRP (mg/l as P)	DOX (% sat)	WQI score	Water quality status
DB010	5.10	0.00	8.2	17.8	1.50	1.50	**1.54**	0.010	89.50	73	Fair
DB015	17.08	0.00	8.0	16.8	0.86	1.10	**0.92**	0.027	89.00	74	Fair
DB020	11.09	0.00	8.1	17.3	1.18	1.30	**1.23**	0.018	89.25	73	Fair
DB210	27.63	1.20	8.1	16.6	0.62	1.50	**0.68**	0.019	96.20	76	Fair
DB120	24.43	1.75	8.0	16.4	**0.29**	1.00	0.36	0.025	94.90	79	Fair
DB300	0.30	3.10	8.4	17.1	1.05	1.00	**1.09**	**0.047**	104.50	67	Fair
DB310	2.30	3.80	8.4	17.4	0.99	1.00	**1.06**	**0.064**	101.00	68	Fair
DB320	20.11	3.97	8.2	18.3	0.82	1.00	**1.01**	**0.127**	91.38	68	Fair
DB330	30.03	3.00	8.0	16.9	0.13	**0.80**	0.22	**0.054**	99.57	78	Fair
DB340	30.80	1.75	8.1	16.4	0.10	1.10	0.17	0.036	112.48	84	Good
DB350	30.18	3.00	8.1	16.8	0.11	1.00	0.18	**0.048**	104.29	83	Good
DB420	30.33	2.00	8.0	16.5	0.12	1.25	0.26	**0.075**	101.82	82	Good
DB410	31.14	2.60	7.9	17.2	0.25	1.13	**0.88**	**0.296**	97.00	77	Fair
DB220	32.55	2.00	8.1	16.3	0.14	1.40	0.19	0.014	100.38	87	Good
DB510	31.50	0.00	8.1	13.8	0.02	2.00	0.05	0.043	104.33	92	Good
DB560	32.13	0.00	8.1	14.1	0.01	2.10	0.04	0.006	104.83	96	Good
DB730	33.90	0.00	8.0	7.2	0.17	1.00	0.19	0.022	99.00	87	Good
DB610	33.60	0.00	8.0	7.3	0.12	1.20	0.16	0.014	98.00	90	Good
DB570	32.20	0.00	8.1	13.8	0.00	2.67	0.02	0.002	103.67	98	Good
DB540	32.20	0.00	8.1	13.9	0.00	2.17	0.02	0.001	105.00	98	Good
DB450	31.38	1.20	8.1	13.9	0.12	1.84	0.26	0.045	105.40	82	Good
DB550	32.00	0.00	8.1	14.0	0.04	1.96	0.08	0.010	105.17	94	Good
DB580	32.36	0.00	8.1	13.4	0.04	2.20	0.06	0.001	106.00	96	Good
DB740	33.60	0.00	8.0	6.9	0.17	1.20	0.19	0.014	99.00	89	Good
Criteria	**Median = 30.97**	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	**0 - 0.51**	**0- 0.044**	**78 - 122**		

Underestimate eclipsing

Table 7.S3. Averaged winter concentrations of water quality indicators and eclipsing impacts on the WQM aggregation process by comparing actual water quality parameters and qualitative status in **Dublin Bay, 2021**. The guideline values (thresholds) adopted for the Dublin Bay during **winter** are included at the bottom and values in bold indicate compliance failures.

Monitoring sites	SAL (psu)	Common water quality indicators					nutrient enrichment indicators				
		BOD5 (mg/l)	pH -	TEMP (^{0}C)	TON (mg/l as N)	TRAN (m/depth)	DIN (mg/l)	MRP (mg/l as P)	DOX (% sat)	WQI score	WQ Status
DB010	5.10	1.00	8.2	10.4	**2.43**	1.20	**2.48**	0.018	89.50	70	Fair
DB015	17.08	0.00	8.2	10.3	1.67	1.20	**1.75**	0.027	89.00	70	Fair
DB020	11.09	0.00	8.1	10.3	1.63	**0.73**	**1.77**	**0.060**	89.25	62	Fair
DB210	27.63	0.00	8.0	8.1	0.99	1.20	**1.06**	0.043	96.20	72	Fair
DB120	0.30	0.73	8.0	7.8	0.61	1.00	**0.67**	0.033	104.50	75	Fair
DB300	2.30	0.00	8.3	11.6	1.30	1.00	**1.35**	**0.052**	101.00	71	Fair
DB310	20.11	0.00	8.0	8.9	0.69	1.00	**0.79**	**0.071**	91.38	75	Fair
DB320	30.03	0.00	8.0	8.5	1.10	1.00	**1.16**	**0.049**	99.57	72	Fair
DB330	30.80	0.00	8.0	8.9	0.69	1.00	**0.79**	**0.071**	112.48	75	Fair
DB340	30.18	0.00	7.9	7.8	0.42	**0.80**	0.47	**0.054**	104.29	75	Fair
DB350	31.14	0.00	7.9	7.9	0.43	**0.80**	**1.01**	**0.061**	97.00	74	Fair
DB420	32.55	0.73	7.9	7.8	0.30	1.00	0.49	**0.075**	100.38	78	Fair
DB410	31.50	1.45	7.8	7.8	0.53	1.00	**1.29**	**0.300**	104.33	74	Fair
DB220	33.90	0.00	7.9	9.2	0.35	1.00	0.42	0.042	99.00	80	Good
DB510	33.60	0.00	8.0	11.3	0.12	2.20	0.16	0.032	98.00	88	Good
DB560	31.38	0.00	8.0	7.2	0.17	1.00	0.19	0.022	105.40	88	Good
DB730	32.00	0.00	8.0	7.3	0.12	1.20	0.16	0.014	105.17	91	Good
DB610	31.73	0.00	8.0	11.2	0.11	2.00	0.17	0.036	77.80	88	Good
DB570	30.70	0.00	8.0	11.4	0.10	2.20	0.14	0.026	106.00	90	Good
DB540	31.20	0.00	8.0	11.4	0.10	2.20	0.13	0.024	120.00	90	Good
DB450	31.60	0.00	8.0	11.3	0.09	2.50	0.12	0.020	110.22	91	Good
DB550	32.05	0.00	8.0	11.4	0.10	2.20	0.13	0.021	114.00	91	Good
DB580	32.20	0.00	8.0	11.4	0.08	2.20	0.11	0.022	125.50	91	Good
DB740	0.10	0.00	8.0	6.9	0.17	1.20	0.19	0.014	102.50	90	Good
Criteria	**Median = 29.15**	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	**0 - 0.633**	**0 - 0.047**	**77 - 123**		

	Breached criteria		Underestimate eclipsing		Overestimate eclipsing

Table 7.S4. Averaged winter concentrations of water quality indicators and eclipsing impacts on the WQM aggregation process by comparing actual water quality parameters and qualitative status in **Cork Harbour, 2021**. The guideline values (thresholds) adopted for the Cork Harbour during **summer** are included at the bottom and values in bold indicate compliance failures.

Monitoring sites	SAL (psu)	Common water quality indicators					nutrient enrichment indicators				
		BOD5 (mg/l)	pH -	TEMP (^{0}C)	TON (mg/l as N)	TRAN (m/depth)	DIN (mg/l)	MRP (mg/l as P)	DOX (% sat)	WQI scores	Water quality status
LE040	5.10	0.00	8.2	17.8	1.50	1.50	**1.54**	0.010	89.50	73	Fair
LE030	17.08	0.00	8.0	16.8	0.86	1.10	**0.92**	0.030	89.00	73	Fair
LE110	11.09	0.00	8.1	17.3	1.18	1.30	**1.23**	0.020	89.25	72	Fair
LE120	27.63	1.20	8.1	16.6	0.62	1.50	**0.68**	0.020	96.20	76	Fair
LE140	0.30	3.10	8.4	17.1	1.05	1.00	**1.09**	**0.050**	104.50	67	Fair
LE130	2.30	3.80	8.4	17.4	0.99	1.00	**1.06**	**0.060**	101.00	68	Fair
LE150	20.11	3.97	8.2	18.3	0.82	1.00	**1.01**	**0.130**	91.38	68	Fair
LE160	30.03	3.00	8.0	16.9	0.13	**0.80**	0.22	**0.050**	99.57	78	Fair
Tivoli	30.80	1.75	8.1	16.4	0.10	1.10	0.17	0.040	112.48	84	Good
LE170	30.18	3.00	8.1	16.8	0.11	1.00	0.18	**0.050**	104.29	83	Good
LE180	31.14	2.60	7.9	17.2	0.25	1.13	**0.88**	**0.300**	97.00	77	Fair
BLKC*	32.55	2.00	8.1	16.3	0.14	1.40	0.19	0.010	100.38	88	Good
LE220	31.50	0.00	8.1	13.8	0.02	2.00	0.05	0.040	104.33	92	Good
LE210	33.90	0.00	8.0	7.2	0.17	1.00	0.19	0.020	99.00	88	Good
LE310	33.60	0.00	8.0	7.3	0.12	1.20	0.16	0.010	98.00	91	Good
LE330	31.38	1.20	8.1	13.9	0.12	1.84	0.26	**0.050**	105.40	82	Good
LE340	32.00	1.48	8.1	14.0	0.04	1.96	0.08	0.010	105.17	92	Good
LE410	31.73	1.10	8.0	17.4	0.26	**0.65**	0.37	**0.050**	77.80	71	Fair
LE420	30.70	0.95	8.1	18.2	0.03	**0.50**	0.12	0.020	106.00	82	Good
LE430	31.20	2.00	8.2	17.9	0.03	**0.80**	0.1	0.010	120.00	87	Good
LE440	31.60	1.44	8.1	17.3	0.65	**0.99**	**0.71**	**0.070**	110.22	72	Fair
LE450	32.05	1.10	8.1	16.9	0.03	1.50	0.07	0.010	114.00	92	Good
LE540	32.20	1.15	8.2	17.6	0.01	**0.65**	0.04	0.020	125.50	86	Good
LE500	0.10	1.80	8.1	16.2	**4.10**	1.00	4.12	0.040	102.50	66	Fair
LE550	31.85	1.70	8.2	17.2	0.06	1.80	0.12	0.010	118.00	89	Good
HBLIN*	31.96	1.98	8.2	15.8	0.11	2.00	0.17	0.010	78.94	87	Good

LE380	32.20	1.10	8.2	16.2	0.10	2.00	0.16	0.010	105.25	89	Good
LE620	33.83	0.00	8.1	15.4	0.03	3.00	0.07	0.010	101.25	95	Good
LE610	32.20	1.10	8.15	15.82	0.10	2.00	0.16	0.01	101.25	90	Good
RLD*	4.30	2.10	8.2	18.2	0.08	1.13	0.16	**0.05**	100.10	85	Good
LE630	34.03	0.00	8.1	15.38	0.02	3.40	0.07	0.01	101.50	95	Good
LE810	34.05	1.54	8.1	15.4	0.00	3.50	0.04	0	99.50	97	Good
LE820	34.20	1.65	8.1	15.1	0.02	3.75	0.05	0.01	96.00	93	Good
LE505	0.30	1.00	8	16.2	**4.60**	1.00	**4.63**	0.03	107.00	67	Fair
LE510	22.80	1.88	7.98	16.25	1.62	1.00	**1.69**	0.03	97.50	67	Fair
LE520	23.75	1.50	7.98	16.45	1.43	1.00	**1.49**	0.02	100.25	70	Fair
LE530	27.80	1.65	8.1	16.65	0.58	1.10	**0.64**	0.02	106.00	76	Fair
Criteria	**Median = 31**	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	**0 - 0.51**	**0 - 0.044**	**78 - 122**		

Breached criteria — Underestimate eclipsing — Overestimate eclipsing

Table 7.S5 Averaged winter concentrations of water quality indicators and eclipsing impacts on the WQM aggregation process by comparing actual water quality parameters and qualitative status in **Cork Harbour, 2021**. The guideline values (thresholds) adopted for the Cork Harbour during **winter** are included at the bottom and values in bold indicate compliance failures.

		Common water quality indicators					nutrient enrichment indicators				
Monitoring sites	SAL (psu)	BOD5 (mg/l)	pH -	TEMP (^{0}C)	TON (mg/l as N)	TRAN (m/depth)	DIN (mg/l)	MRP (mg/l as P)	DOX (% sat)	WQI scores	Water quality status
LE040	0.10	1.00	7.4	11.6	2.20	1.00	**2.25**	0.030	94.00	68	Fair
LE030	0.20	0.80	7.6	10.2	5.70	**0.50**	**5.92**	0.050	91.00	57	Fair
LE110	0.10	1.20	7.5	11.6	1.60	1.00	**1.66**	0.020	97.00	70	Fair
LE120	0.10	1.40	7.5	11.4	2.40	**0.50**	**2.46**	0.030	95.00	58	Fair
LE140	0.20	1.20	7.6	10.0	2.50	**0.20**	**2.55**	0.030	98.00	55	Fair
LE130	0.20	1.20	7.6	10.8	2.60	**0.20**	**2.64**	**0.060**	97.00	53	Fair
LE150	14.40	1.23	7.8	12.6	1.16	1.35	1.31	0.030	81.85	71	Fair
LE160	16.30	1.09	7.7	12.7	1.02	1.35	1.17	0.030	84.00	72	Fair
Tivoli	18.45	0.90	8.0	10.2	1.36	1.00	**1.51**	0.020	77.35	70	Fair
LE170	20.57	1.23	7.8	12.6	1.08	1.29	1.23	0.020	89.86	72	Fair
LE180	17.83	1.07	7.8	12.6	1.02	1.25	1.18	0.030	93.75	72	Fair

BLKC*	24.70	1.11	8.0	10.2	0.90	1.29	1.03	0.020	75.31	74	Fair
LE220	0.10	8.60	7.6	12.4	4.20	**0.50**	**4.62**	**0.120**	94.00	50	Fair
LE210	0.10	7.90	7.7	10.3	4.25	**0.45**	**4.27**	**0.120**	95.00	50	Fair
LE310	15.50	0.50	7.5	12.1	2.00	1.50	**2.14**	0.040	80.00	67	Fair
LE330	16.78	0.80	7.8	11.9	1.37	1.50	**1.52**	0.040	86.50	69	Fair
LE340	20.60	0.00	7.8	12.0	0.94	1.50	1.09	0.030	83.50	74	Fair
LE410	25.70	0.82	7.9	8.7	0.93	1.00	1.02	0.030	95.00	74	Fair
LE420	25.50	0.50	8.0	7.7	1.30	1.00	**1.39**	0.040	96.00	71	Fair
LE430	25.70	0.82	8.0	7.8	1.30	1.00	**1.39**	0.030	95.00	71	Fair
LE440	27.20	0.73	8.0	8.3	1.40	1.00	**1.49**	0.030	94.00	70	Fair
LE450	29.00	0.80	8.0	8.6	0.93	1.20	1	0.030	96.00	75	Fair
LE540	28.90	0.77	7.9	8.6	0.70	1.20	0.77	0.030	95.00	78	Fair
LE500	0.10	0.72	7.6	9.8	4.50	1.00	**4.51**	**0.480**	99.00	67	Fair
LE550	0.10	0.85	7.6	9.8	4.40	1.00	**4.42**	**0.080**	92.00	66	Fair
HBLIN*	18.25	1.20	7.9	11.0	0.49	1.00	0.6	0.030	88.50	81	Good
LE380	15.65	1.30	7.8	9.1	0.59	1.00	0.68	0.030	86.00	78	Fair
LE620	26.70	0.95	7.9	11.6	0.61	1.00	0.69	0.020	84.50	79	Fair
LE610	30.00	0.95	7.9	8.7	0.52	2.50	0.58	0.050	95.00	79	Fair
RLD*	29.43	0.87	8.1	9.5	0.47	1.00	0.52	0.020	81.10	82	Good
LE630	28.08	1.20	8.0	12.1	0.61	2.00	0.7	0.040	100.50	78	Fair
LE810	32.78	0.50	8.0	12.1	0.15	2.65	0.19	0.020	96.25	91	Good
LE820	29.43	0.87	8.0	12.1	0.47	2.00	0.52	0.020	96.25	83	Good
LE505	9.00	1.50	8.1	15.1	1.81	1.00	1.06	0.030	100.50	69	Fair
LE510	34.13	0.00	8.0	11.8	0.10	2.40	0.12	0.020	91.50	93	Good
LE520	33.50	0.00	8.0	11.4	0.18	4.00	0.21	0.020	91.50	92	Good
LE530	33.20	0.00	8.0	11.3	0.25	3.00	0.28	0.030	90.50	89	Good
Criteria	**Median = 18.45**	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	**0 - 1.336**	**0 - 0.059**	**71 - 129**		

Breached criteria | Underestimate eclipsing | Overestimate eclipsing

Table 7.S6 Averaged winter concentrations of water quality indicators and eclipsing impacts on the WQM aggregation process by comparing actual water quality parameters and qualitative status in **Galway Bay, 2021**. The guideline values (thresholds) adopted for the Galway Bay during **summer** are included at the bottom and values in bold indicate compliance failures.

Monitoring sites	SAL (psu)	Common water quality indicators					nutrient enrichment indicators				
		BOD5 (mg/l)	pH -	TEMP (^{0}C)	TON (mg/l as N)	TRAN (m/depth)	DIN (mg/l)	MRP (mg/l as P)	DOX (% sat)	IEWQI scores	WQ status
GY250		1.58	8.2	17.0	0.12	8.25	0.146	0.015	106.50	89	Good
GY210	30.85	1.60	8.2	16.5	0.12	3.84	0.145	0.015	101.40	89	Good
GY200	30.54	1.43	8.2	16.1	0.12	3.96	0.134	0.008	103.00	91	Good
GY220	29.48	0.97	8.2	15.0	0.10	5.25	0.119	0.014	96.50	91	Good
GY260	31.35	0.75	8.1	16.7	0.12	6.80	0.14	0.016	108.00	90	Good
GY150	30.60	0.87	8.2	17.0	0.12	3.67	0.135	0.015	106.75	90	Good
GY180	28.57	1.27	8.2	16.4	0.12	3.60	0.133	0.016	101.00	90	Good
GY160	29.02	0.87	8.2	16.6	0.06	2.70	0.075	0.015	102.80	92	Good
GY170	27.98	1.55	8.2	16.5	0.12	2.56	0.133	0.015	100.83	90	Good
GY130	28.43	1.52	8.2	16.1	0.15	3.33	0.174	0.015	101.75	88	Good
GY140	27.63	1.49	8.2	16.1	0.12	3.18	0.135	0.014	100.41	90	Good
GY120	27.95	1.35	8.2	16.3	0.02	3.22	0.034	0.014	103.90	94	Good
GY110	25.80	1.43	8.3	16.7	0.01	2.80	0.039	0.012	103.00	94	Good
KA050	19.08	1.26	8.2	17.0	0.15	3.60	0.19	0.013	103.75	88	Good
KA060	29.86	1.49	8.2	17.5	0.12	5.25	0.158	0.015	99.50	89	Good
KA070	30.10	1.47	8.2	17.3	0.05	3.64	0.093	0.017	104.30	91	Good
KA040	29.18	1.43	8.1	17.2	0.12	3.28	0.156	0.013	104.00	89	Good
KA080	29.56	1.29	8.1	17.3	0.09	3.25	0.12	0.014	102.71	91	Good
KA030	29.00	1.15	8.1	17.1	0.16	2.84	0.203	0.016	103.83	88	Good
KA025	28.83	2.57	8.0	10.9	0.15	2.45	0.182	**0.043**	102.50	84	Good
KA020	25.60	2.06	7.9	16.7	0.15	2.00	0.173	0.018	101.91	87	Good
GY190	23.90	2.06	8.2	16.1	0.10	4.06	0.115	0.015	101.83	90	Good
Criteria	28.50	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	**0 - 0.380**	**0 - 0.042**	**77 - 123**		

Breached criteria — Underestimate eclipsing — Overestimate eclipsing

Table 7.S7 Averaged winter concentrations of water quality indicators and eclipsing impacts on the WQM aggregation process by comparing actual water quality parameters and qualitative status in **Galway Bay, 2021**. The guideline values (thresholds) adopted for the Galway Bay during **winter** are included at the bottom and values in bold indicate compliance failures.

Monitoring sites	SAL (psu)	Common water quality indicators					nutrient enrichment indicators				
		BOD5 (mg/l)	pH -	TEMP (^{0}C)	TON (mg/l as N)	TRAN (m/depth)	DIN (mg/l)	MRP (mg/l as P)	DOX (% sat)	IEWQI scores	Status
GY250	25.58	0.63	8.0	9.5	0.12	8.25	0.289	0.015	93.38	87	Good
GY210	26.45	0.84	8.0	9.3	0.12	3.84	0.253	0.021	89.05	86	Good
GY200	27.20	1.24	8.0	10.0	0.12	3.96	0.113	0.011	93.50	92	Good
GY220	31.80	1.10	8.0	11.1	0.10	5.25	0.115	0.020	93.00	90	Good
GY260	29.50	1.50	8.0	10.5	0.12	6.80	0.114	0.016	93.25	91	Good
GY150	26.60	1.43	8.0	9.8	0.12	3.67	0.104	0.011	95.00	92	Good
GY180	25.85	0.84	8.0	9.7	0.12	3.60	0.108	0.021	93.50	91	Good
GY160	27.15	0.68	8.0	9.9	0.06	2.70	0.392	0.015	92.00	84	Good
GY170	26.25	1.43	8.0	9.6	0.12	2.56	0.167	0.015	91.00	89	Good
GY130	23.65	1.52	8.0	9.9	0.15	3.33	0.116	0.016	91.00	90	Good
GY140	25.50	1.15	8.0	10.2	0.12	3.18	0.148	0.022	92.75	89	Good
GY120	23.05	1.25	8.1	9.5	0.02	3.22	0.117	0.025	90.50	89	Good
GY110	15.25	1.25	8.1	8.5	0.01	2.80	0.228	0.017	94.50	87	Good
KA050	26.00	0.98	7.9	8.5	0.15	3.60	0.281	0.006	95.50	89	Good
KA060	26.75	1.20	8.0	8.3	0.12	5.25	0.287	0.008	97.00	88	Good
KA070	25.35	1.17	7.9	8.4	0.05	3.64	0.343	0.011	95.00	86	Good
KA040	26.80	1.20	8.0	8.3	0.12	3.28	0.265	0.007	95.50	89	Good
KA080	28.60	1.14	7.9	8.3	0.09	3.25	0.202	0.008	93.00	90	Good
KA030	26.45	1.25	8.0	8.6	0.16	2.84	0.301	0.020	96.00	85	Good
KA025	26.45	1.10	7.9	9.5	0.15	2.45	**1.185**	0.010	99.37	76	Fair
KA020	15.80	1.16	7.8	8.4	0.15	2.00	0.42	0.020	89.50	81	Good
GY190	27.50	1.15	8.0	10.0	0.10	4.06	**0.807**	**0.131**	94.50	77	Fair
Criteria	**Median = 26.45**	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	**0 - 0.57**	**0 - 0.046**	**75 - 125**		

Breached criteria   Underestimate eclipsing   Overestimate eclipsing

Table 7.S8 Averaged winter concentrations of water quality indicators and eclipsing impacts on the WQM aggregation process by comparing actual water quality parameters and qualitative status in **Mulroy Bay, 2021**. The guideline values (thresholds) adopted for the Mulroy Bay during **summer** are included at the bottom and values in bold indicate compliance failures.

Monitoring sites	**SAL (psu)**	Common water quality indicators					nutrient enrichment indicators				
		BOD5 (mg/l)	pH -	TEMP (^{0}C)	TON (mg/l as N)	TRAN (m/depth)	DIN (mg/l)	MRP (mg/l as P)	DOX (% sat)	WQI scores	Status
MB140	**35.03**	0.83	8.1	14.2	0.03	8.00	0.05	0.000	103.25	96	Good
MB130	**33.25**	0.90	8.1	14.5	0.00	7.50	0.02	0.000	106.50	97	Good
MB120	**32.95**	2.30	8.1	16.0	0.00	7.75	0.02	0.000	109.50	96	Good
MB110	**33.00**	0.72	8.2	16.2	0.00	7.00	0.02	0.000	110.50	97	Good
MB100	**32.95**	0.92	8.2	16.4	0.00	7.50	0.02	0.000	111.50	97	Good
MB090	**32.80**	0.68	8.2	16.7	0.00	6.25	0.02	0.000	113.00	97	Good
MB080	**32.75**	0.42	8.2	16.7	0.00	6.50	0.02	0.000	113.75	97	Good
MB070	**32.70**	0.48	8.2	16.7	0.00	5.58	0.02	0.000	113.50	97	Good
MB060	**32.75**	0.45	8.2	16.7	0.00	7.25	0.02	0.000	112.50	97	Good
MB050	**32.78**	0.98	8.1	16.4	0.00	5.75	0.02	0.000	105.00	97	Good
MB040	**32.75**	0.91	8.2	16.3	0.00	5.65	0.02	0.000	112.50	97	Good
MB030	**32.60**	0.66	8.2	18.3	0.00	4.80	0.01	0.005	109.50	96	Good
MB020	**31.55**	0.83	8.2	18.4	0.00	6.00	0.02	0.076	105.00	92	Good
MB010	**32.45**	0.95	8.3	16.1	0.00	5.15	0.02	0.008	113.50	95	Good
Criteria	**Median = 32.77**	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	**0 - 0.380**	**0 - 0.042**	**79 - 121**		

	Breached criteria		Underestimate eclipsing		Overestimate eclipsing

Table 7.S9 Averaged winter concentrations of water quality indicators and eclipsing impacts on the WQM aggregation process by comparing actual water quality parameters and qualitative status in **Mulroy Bay, 2021**. The guideline values (thresholds) adopted for the Mulroy Bay during **summer** are included at the bottom and values in bold indicate compliance failures.

Monitoring sites	SAL (psu)	Common water quality indicators					nutrient enrichment indicators			IEWQI	WQ Status
		BOD5 (mg/l)	pH -	TEMP (^{0}C)	TON (mg/l as N)	TRAN (m/depth)	DIN (mg/l)	MRP (mg/l as P)	DOX (% sat)		
MB140	32.40	1.94	8.1	7.15	0.11	7.50	0.12	0.020	99.50	89	Good
MB130	32.15	2.01	8.05	6.1	0.13	7.50	0.14	**0.220**	99.50	86	Good
MB120	31.50	1.9	8	5.6	0.31	7.20	0.37	**0.140**	98.00	78	Fair
MB110	31.20	2.05	8	5.4	0.12	7.20	0.14	**0.052**	98.50	86	Good
MB100	31.20	1.94	8	5.4	0.11	7.00	0.12	0.022	98.00	88	Good
MB090	30.10	1.96	8	4	0.12	6.50	0.14	0.024	97.00	87	Good
MB080	30.40	2.25	8	5	0.11	6.50	0.13	0.030	97.50	87	Good
MB070	29.90	2.01	8	4.8	0.12	5.40	0.14	0.032	97.00	86	Good
MB060	29.90	1.98	8	4.9	0.12	6.10	0.14	0.026	97.00	87	Good
MB050	30.05	1.94	8	5	0.13	6.50	0.15	0.032	97.00	86	Good
MB040	30.20	2.1	8	5.2	0.13	6.20	0.16	**0.058**	96.50	85	Good
MB030	29.70	1.98	8	5	0.13	6.20	0.16	0.046	95.50	85	Good
MB020	28.90	1.85	7.9	4.65	0.14	5.50	0.19	0.037	91.50	84	Good
MB010	28.95	1.9	7.9	4.9	0.15	6.50	0.19	0.032	90.00	84	Good
Criteria	**Median = 30.15**	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	**0 - 0.57**	**0 - 0.046**	**77 - 123**		

	Breached criteria		Underestimate eclipsing		Overestimate eclipsing

Table 7.S10 Determining the moving thresholds (guideline) values for the nutrient indicators based on the entire range of salinities using the ATSEBI system.

Salinity Median (psu)	DIN Median (mg/l N)	MRP Median (µg/l P)	Chlorophyll Median (µg/l)	Chlorophyll 95 %ile (µg/l)	Dissolved Oxygen 5 %ile (% Saturation)	Dissolved Oxygen 95 %ile (% Saturation)
0	2.600	60	15.0	30.0	70	130
1	2.529	60	15.0	30.0	70	130
2	2.459	60	15.0	30.0	70	130
3	2.388	60	15.0	30.0	70	130
4	2.318	60	15.0	30.0	70	130
5	2.247	60	15.0	30.0	70	130
6	2.176	60	15.0	30.0	70	130
7	2.106	60	15.0	30.0	70	130
8	2.035	60	15.0	30.0	70	130
9	1.965	60	15.0	30.0	70	130
10	1.894	60	15.0	30.0	70	130
11	1.824	60	15.0	30.0	70	130
12	1.753	60	15.0	30.0	70	130
13	1.682	60	15.0	30.0	70	130
14	1.612	60	15.0	30.0	70	130
15	1.541	60	15.0	30.0	70	130
16	1.471	60	15.0	30.0	70	130
17	1.400	60	15.0	30.0	70	130
18	**1.336**	**59**	**14.7**	**29.4**	**71**	**129**
19	1.272	58	14.4	28.9	71	129
20	1.208	57	14.2	28.3	72	128
21	1.144	56	13.9	27.8	72	128
22	1.081	54	13.6	27.2	73	127
23	1.017	53	13.3	26.7	73	127
24	0.953	52	13.1	26.1	74	126
25	0.889	51	12.8	25.6	74	126
26	**0.825**	**50**	**12.5**	**25.0**	**75**	**125**
27	0.761	49	12.2	24.4	76	124
28	0.697	48	11.9	23.9	76	124
29	**0.633**	**47**	**11.7**	**23.3**	**77**	**123**
30	**0.569**	**46**	**11.4**	**22.8**	**77**	**123**
31	**0.506**	**44**	**11.1**	**22.2**	**78**	**122**
32	0.442	43	10.8	21.7	78	122
33	**0.378**	**42**	**10.6**	**21.1**	**79**	**121**
34	0.314	41	10.3	20.6	79	121
35	0.250	40	10.0	20.0	80	120

**Red and bold indicated that the median SAL values were used for the determination of the moving threshold in the present study across the four application domains through the study year.*

Table 7.S11 Calculated sub-index, IEWQI values and impact of ambiguity on final score for various water quality indicators at different monitoring sites in Dublin Bay through the summer season.

Monitoring sites	Common water quality indicators					nutrient enrichment indicators			
	BOD5	pH	TEMP	TON	TRAN	DIN	MRP	DOX	IEWQI
DB010	100	100	100	25.00	100.00	0.00	77.270	52.27	73
DB015	100	100	100	57.00	100.00	0.00	38.640	50.00	74
DB020	100	100	100	41.00	100.00	0.00	59.090	51.14	73
DB210	82.86	100	100	69.00	100.00	0.00	56.820	82.73	76
DB120	75	100	100	85.50	100.00	29.41	43.180	76.82	79
DB300	55.71	100	100	47.50	100.00	0.00	0.000	79.55	67
DB310	45.71	100	100	50.50	100.00	0.00	0.000	95.45	68
DB320	43.29	100	100	59.00	100.00	0.00	0.000	60.82	68
DB330	57.14	100	100	93.50	80.00	56.86	0.000	98.05	78
DB340	75	100	100	95.00	100.00	66.67	18.180	43.27	84
DB350	57.14	100	100	94.50	100.00	64.71	0.000	80.50	83
DB420	71.43	100	100	94.00	100.00	49.02	0.000	91.73	82
DB410	62.86	100	100	87.50	100.00	0.00	0.000	86.36	77
DB220	71.43	100	100	93.00	100.00	62.75	68.180	98.27	87
DB510	100	100	100	99	100	90.2	2.27	80.32	92
DB560	100	100	100	99.5	100	92.16	86.36	78.05	96
DB730	100	100	100	91.5	100	62.75	50	95.45	87
DB610	100	100	100	94	100	68.63	68.18	90.91	90
DB570	100	100	100	100	100	96.08	95.45	83.32	98
DB540	100	100	100	100	100	96.08	97.73	77.27	98
DB450	82.86	100	100	94	100	49.02	0	75.45	82
DB550	100	100	100	98	100	84.31	77.27	76.5	94
DB580	100	100	100	98	100	88.24	97.73	72.73	96
DB740	100	100	100	91.5	100	62.75	68.18	95.45	89

Table 7.S12 Calculated sub-index, IEWQI values and impact of ambiguity on final score for various water quality indicators at different monitoring sites in Dublin Bay through the winter season.

Monitoring sites	Common water quality indicators					nutrient enrichment indicators			
	BOD5	pH	TEMP	TON	TRAN	DIN	MRP	DOX	IEWQI
DB010	85.71	100	100	0.00	100.00	0.00	61.700	94.17	70
DB015	100	100	100	16.50	100.00	0.00	42.550	72.48	70
DB020	100	100	100	18.50	73.00	0.00	0.000	61.74	62
DB210	100	100	100	50.50	100.00	0.00	8.510	86.96	72
DB120	89.57	100	100	69.50	100.00	0.00	29.790	71.74	75
DB300	100	100	100	35.00	100.00	0.00	0.000	95.65	71
DB310	100	100	100	65.50	100.00	0.00	0.000	78.26	75
DB320	100	100	100	45.00	100.00	0.00	0.000	95.65	72
DB330	100	100	100	65.50	100.00	0.00	0.000	78.26	75
DB340	100	100	100	79.00	80.00	25.40	0.000	91.30	75
DB350	100	100	100	78.50	80.00	0.00	0.000	100.00	74
DB420	89.57	100	100	85.00	100.00	22.22	0.000	73.91	78
DB410	79.29	100	100	73.50	100.00	0.00	0.000	69.57	74
DB220	100	100	100	82.50	100.00	33.33	10.640	95.65	80
DB510	100	100	100	94	100	74.6	31.91	84.78	88
DB560	100	100	100	91.5	100	69.84	53.19	95.65	88
DB730	100	100	100	94	100	74.6	70.21	91.3	91
DB610	100	100	100	94.5	100	73.02	23.4	82.61	88
DB570	100	100	100	95	100	77.78	44.68	86.96	90
DB540	100	100	100	95	100	79.37	48.94	86.96	90
DB450	100	100	100	95.5	100	80.95	57.45	86.96	91
DB550	100	100	100	95	100	79.37	55.32	86.96	91
DB580	100	100	100	96	100	82.54	53.19	84.78	91
DB740	100	100	100	91.5	100	69.84	70.21	95.65	90

Table 7.S13 Calculated sub-index, IEWQI values and impact of ambiguity on final score for various water quality indicators at different monitoring sites in Cork Harbour during the summer season.

Monitoring sites	Common water quality indicators					nutrient enrichment indicators			
	BOD5	pH	TEMP	TON	TRAN	DIN	MRP	DOX	IEWQI
LE040	100.00	100.00	100.00	25.00	100.00	0.00	77.27	52.27	73
LE030	100.00	100.00	100.00	57.00	100.00	0.00	31.82	50.00	73
LE110	100.00	100.00	100.00	41.00	100.00	0.00	54.55	51.14	72
LE120	82.86	100.00	100.00	69.00	100.00	0.00	54.55	82.73	76
LE140	55.71	100.00	100.00	47.50	100.00	0.00	0.00	79.55	67
LE130	45.71	100.00	100.00	50.50	100.00	0.00	0.00	95.45	68
LE150	43.29	100.00	100.00	59.00	100.00	0.00	0.00	60.82	68
LE160	57.14	100.00	100.00	93.50	80.00	56.86	0.00	98.05	78
Tivoli	75.00	100.00	100.00	95.00	100.00	66.67	9.09	43.27	84
LE170	57.14	100.00	100.00	94.50	100.00	64.71	0.00	80.50	83
LE180	62.86	100.00	100.00	87.50	100.00	0.00	0.00	86.36	77
BLKC*	71.43	100.00	100.00	93.00	100.00	62.75	77.27	98.27	88
LE220	100.00	100.00	100.00	99.00	100.00	90.20	9.09	80.32	92
LE210	100.00	100.00	100.00	91.50	100.00	62.75	54.55	95.45	88
LE310	100.00	100.00	100.00	94.00	100.00	68.63	77.27	90.91	91
LE330	82.86	100.00	100.00	94.00	100.00	49.02	0.00	75.45	82
LE340	78.86	100.00	100.00	98.00	100.00	84.31	77.27	76.50	92
LE410	84.29	100.00	100.00	87.00	65.00	27.45	0.00	0.00	71
LE420	86.43	100.00	100.00	98.50	50.00	76.47	54.55	72.73	82
LE430	71.43	100.00	100.00	98.50	80.00	80.39	77.27	9.09	87
LE440	79.43	100.00	100.00	67.50	99.00	0.00	0.00	53.55	72
LE450	84.29	100.00	100.00	98.50	100.00	86.27	77.27	36.36	92
LE540	83.57	100.00	100.00	99.50	65.00	92.16	54.55	0.00	86
LE500	74.29	100.00	100.00	0.00	100.00	0.00	9.09	88.64	66
LE550	75.71	100.00	100.00	97.00	100.00	76.47	77.27	18.18	89
HBLIN*	71.71	100.00	100.00	94.50	100.00	66.67	77.27	4.27	87
LE380	84.29	100.00	100.00	95.00	100.00	68.63	77.27	76.14	89
LE620	100.00	100.00	100.00	98.50	100.00	86.27	77.27	94.32	95
LE610	84.29	100.00	100.00	95.00	100.00	68.63	77.27	94.32	90
RLD*	70.00	100.00	100.00	96.00	100.00	68.63	0.00	99.55	85
LE630	100.00	100.00	100.00	99.00	100.00	86.27	77.27	93.18	95
LE810	78.00	100.00	100.00	100.00	100.00	92.16	100.00	97.73	97
LE820	76.43	100.00	100.00	99.00	100.00	90.20	77.27	81.82	93
LE505	85.71	100.00	100.00	0.00	100.00	0.00	31.82	68.18	67
LE510	73.14	100.00	100.00	19.00	100.00	0.00	31.82	88.64	67
LE520	78.57	100.00	100.00	28.50	100.00	0.00	54.55	98.86	70
LE530	76.43	100.00	100.00	71.00	100.00	0.00	54.55	72.73	76

Table 7.S14 Calculated sub-index, IEWQI values and impact of ambiguity on final score for various water quality indicators at different monitoring sites in Cork Harbour during the winter season.

Monitoring sites	Common water quality indicators					nutrient enrichment indicators			
	BOD5	pH	TEMP	TON	TRAN	DIN	MRP	DOX	IEWQI
LE040	85.71	96.00	100.00	0.00	100.00	0.00	50.85	79.31	68
LE030	88.57	100.00	100.00	0.00	50.00	0.00	23.73	68.97	57
LE110	82.86	100.00	100.00	20.00	100.00	0.00	59.32	89.66	70
LE120	80.00	100.00	100.00	0.00	50.00	0.00	52.54	82.76	58
LE140	82.86	100.00	100.00	0.00	20.00	0.00	45.76	93.10	55
LE130	82.86	100.00	100.00	0.00	20.00	0.00	1.69	89.66	53
LE150	82.43	100.00	100.00	42.00	100.00	2.24	57.63	37.41	71
LE160	84.43	100.00	100.00	49.00	100.00	12.69	50.85	44.83	72
Tivoli	87.14	100.00	100.00	32.00	100.00	0.00	64.41	21.90	70
LE170	82.43	100.00	100.00	46.00	100.00	8.21	59.32	65.03	72
LE180	84.71	100.00	100.00	49.00	100.00	11.94	52.54	78.45	72
BLKC*	84.14	100.00	100.00	55.00	100.00	23.13	67.80	14.86	74
LE220	0.00	100.00	100.00	0.00	50.00	0.00	0.00	79.31	50
LE210	0.00	100.00	100.00	0.00	45.00	0.00	0.00	82.76	50
LE310	92.86	100.00	100.00	0.00	100.00	0.00	33.90	31.03	67
LE330	88.57	100.00	100.00	31.50	100.00	0.00	37.29	53.45	69
LE340	100.00	100.00	100.00	53.00	100.00	18.66	45.76	43.10	74
LE410	88.29	100.00	100.00	53.50	100.00	23.88	52.54	82.76	74
LE420	92.86	100.00	100.00	35.00	100.00	0.00	40.68	86.21	71
LE430	88.29	100.00	100.00	35.00	100.00	0.00	52.54	82.76	71
LE440	89.57	100.00	100.00	30.00	100.00	0.00	49.15	79.31	70
LE450	88.57	100.00	100.00	53.50	100.00	25.37	57.63	86.21	75
LE540	89.00	100.00	100.00	65.00	100.00	42.54	54.24	82.76	78
LE500	89.71	100.00	100.00	0.00	100.00	0.00	0.00	96.55	67
LE550	87.86	100.00	100.00	0.00	100.00	0.00	0.00	72.41	66
HBLIN*	82.86	100.00	100.00	75.50	100.00	55.22	57.63	60.34	81
LE380	81.43	100.00	100.00	70.50	100.00	49.25	54.24	51.72	78
LE620	86.43	100.00	100.00	69.50	100.00	48.51	62.71	46.55	79
LE610	86.43	100.00	100.00	74.00	100.00	56.72	13.56	82.76	79
RLD*	87.57	100.00	100.00	76.50	100.00	61.19	66.10	34.83	82
LE630	82.86	100.00	100.00	69.50	100.00	47.76	40.68	98.28	78
LE810	92.86	100.00	100.00	92.50	100.00	85.82	62.71	87.07	91
LE820	87.57	100.00	100.00	76.50	100.00	61.19	62.71	87.07	83
LE505	78.57	100.00	100.00	9.50	100.00	20.90	49.15	98.28	69
LE510	100.00	100.00	100.00	95.00	100.00	91.04	69.49	70.69	93
LE520	100.00	100.00	100.00	91.00	100.00	84.33	72.88	70.69	92
LE530	100.00	100.00	100.00	87.50	100.00	79.10	57.63	67.24	89

Table 7.S15 Calculated sub-index, IEWQI values and impact of ambiguity on final score for various water quality indicators at different monitoring sites in Galway Bay during the summer season.

Monitoring sites	Common water quality indicators					nutrient enrichment indicators			
	BOD5	pH	TEMP	TON	TRAN	DIN	MRP	DOX	IEWQI
GY250	77.43	100.00	100.00	94.00	100.00	76.19	68.09	71.74	89
GY210	77.14	100.00	100.00	94.00	100.00	76.19	68.09	93.91	89
GY200	79.57	100.00	100.00	94.00	100.00	79.37	82.98	86.96	91
GY220	86.14	100.00	100.00	95.00	100.00	80.95	70.21	84.78	91
GY260	89.29	100.00	100.00	94.00	100.00	77.78	65.96	65.22	90
GY150	87.57	100.00	100.00	94.00	100.00	77.78	68.09	70.65	90
GY180	81.86	100.00	100.00	94.00	100.00	79.37	65.96	95.65	90
GY160	87.57	100.00	100.00	97.00	100.00	87.30	68.09	87.83	92
GY170	77.86	100.00	100.00	94.00	100.00	79.37	68.09	96.39	90
GY130	78.29	100.00	100.00	92.50	100.00	73.02	68.09	92.39	88
GY140	78.71	100.00	100.00	94.00	100.00	77.78	70.21	98.22	90
GY120	80.71	100.00	100.00	99.00	100.00	95.24	70.21	83.04	94
GY110	79.57	100.00	100.00	99.50	100.00	93.65	74.47	86.96	94
KA050	82.00	100.00	100.00	92.50	100.00	69.84	72.34	83.70	88
KA060	78.71	100.00	100.00	94.00	100.00	74.60	68.09	97.83	89
KA070	79.00	100.00	100.00	97.50	100.00	85.71	63.83	81.30	91
KA040	79.57	100.00	100.00	94.00	100.00	74.60	72.34	82.61	89
KA080	81.57	100.00	100.00	95.50	100.00	80.95	70.21	88.22	91
KA030	83.57	100.00	100.00	92.00	100.00	68.25	65.96	83.35	88
KA025	63.29	100.00	100.00	92.50	100.00	71.43	8.51	89.13	84
KA020	70.57	100.00	100.00	92.50	100.00	73.02	61.70	91.70	87
GY190	70.57	100.00	100.00	95.00	100.00	80.95	68.09	92.04	90

Table 7.S16 Calculated sub-index, IEWQI values and impact of ambiguity on final score for various water quality indicators at different monitoring sites in Galway Bay during the winter season.

Monitoring sites	Common water quality indicators					nutrient enrichment indicators			
	BOD5	pH	TEMP	TON	TRAN	DIN	MRP	DOX	IEWQI
GY250	91.00	100.00	100.00	89.50	100.00	65.06	70.00	73.52	87
GY210	88.00	100.00	100.00	89.00	100.00	69.88	58.00	56.20	86
GY200	82.29	100.00	100.00	95.00	100.00	86.75	78.00	74.00	92
GY220	84.29	100.00	100.00	95.00	100.00	85.54	60.00	72.00	90
GY260	78.57	100.00	100.00	95.00	100.00	86.75	68.00	73.00	91
GY150	79.57	100.00	100.00	95.50	100.00	87.95	78.00	80.00	92
GY180	88.00	100.00	100.00	95.50	100.00	86.75	58.00	74.00	91
GY160	90.29	100.00	100.00	82.50	100.00	53.01	70.00	68.00	84
GY170	79.57	100.00	100.00	93.00	100.00	79.52	70.00	64.00	89
GY130	78.29	100.00	100.00	95.00	100.00	85.54	68.00	64.00	90
GY140	83.57	100.00	100.00	94.00	100.00	81.93	56.00	71.00	89
GY120	82.14	100.00	100.00	95.00	100.00	85.54	50.00	62.00	89
GY110	82.14	100.00	100.00	90.00	100.00	72.29	66.00	78.00	87
KA050	86.00	100.00	100.00	88.00	100.00	66.27	88.00	82.00	89
KA060	82.86	100.00	100.00	88.50	100.00	65.06	84.00	88.00	88
KA070	83.29	100.00	100.00	85.00	100.00	59.04	78.00	80.00	86
KA040	82.86	100.00	100.00	89.00	100.00	67.47	86.00	82.00	89
KA080	83.71	100.00	100.00	93.00	100.00	75.90	84.00	72.00	90
KA030	82.14	100.00	100.00	88.00	100.00	63.86	60.00	84.00	85
KA025	84.29	100.00	100.00	63.00	100.00	0.00	80.00	0.00	76
KA020	83.43	100.00	100.00	81.00	100.00	49.40	60.00	58.00	81
GY190	83.57	100.00	100.00	85.00	100.00	2.41	0.00	78.00	77

Table 7.S17 Calculated sub-index, IEWQI values and impact of ambiguity on final score for various water quality indicators at different monitoring sites in Mulroy Bay over the summer season.

Monitoring sites	Common water quality indicators					nutrient enrichment indicators			
	BOD5	pH	TEMP	TON	TRAN	DIN	MRP	DOX	IEWQI
MB140	72.29	100.00	100.00	98.50	100.00	78.95	56.52	97.83	96
MB130	71.29	100.00	100.00	100.00	100.00	75.44	0.00	97.83	97
MB120	72.86	100.00	100.00	100.00	100.00	35.09	0.00	91.30	96
MB110	70.71	100.00	100.00	100.00	100.00	75.44	0.00	93.48	97
MB100	72.29	100.00	100.00	100.00	100.00	78.95	52.17	91.30	97
MB090	72.00	100.00	100.00	100.00	100.00	75.44	47.83	86.96	97
MB080	67.86	100.00	100.00	100.00	100.00	77.19	34.78	89.13	97
MB070	71.29	100.00	100.00	100.00	100.00	75.44	30.43	86.96	97
MB060	71.71	100.00	100.00	100.00	100.00	75.44	43.48	86.96	97
MB050	72.29	100.00	100.00	100.00	100.00	73.68	30.43	86.96	97
MB040	70.00	100.00	100.00	100.00	100.00	71.93	0.00	84.78	97
MB030	71.71	100.00	100.00	100.00	100.00	71.93	0.00	80.43	96
MB020	73.57	100.00	100.00	100.00	100.00	66.67	19.57	63.04	92
MB010	72.86	100.00	100.00	100.00	100.00	66.67	30.43	56.52	95

Table 7.S18 Calculated sub-index, IEWQI values and impact of ambiguity on final score for various water quality indicators at different monitoring sites in Mulroy Bay over the winter season.

Monitoring sites	Common water quality indicators					nutrient enrichment indicators			
	BOD5	pH	TEMP	TON	TRAN	DIN	MRP	DOX	IEWQI
MB140	88.14	100.00	100.00	98.50	100.00	86.84	100.00	84.52	89
MB130	87.14	100.00	100.00	100.00	100.00	94.74	100.00	69.05	86
MB120	67.14	100.00	100.00	100.00	100.00	94.74	100.00	54.76	78
MB110	89.71	100.00	100.00	100.00	100.00	94.74	100.00	50.00	86
MB100	86.86	100.00	100.00	100.00	100.00	94.74	100.00	45.24	88
MB090	90.29	100.00	100.00	100.00	100.00	94.74	100.00	38.10	87
MB080	94.00	100.00	100.00	100.00	100.00	94.74	100.00	34.52	87
MB070	93.14	100.00	100.00	100.00	100.00	94.74	100.00	35.71	86
MB060	93.57	100.00	100.00	100.00	100.00	94.74	100.00	40.48	87
MB050	86.00	100.00	100.00	100.00	100.00	94.74	100.00	76.19	86
MB040	87.00	100.00	100.00	100.00	100.00	94.74	100.00	40.48	85
MB030	90.57	100.00	100.00	100.00	100.00	97.37	88.10	54.76	85
MB020	88.14	100.00	100.00	100.00	100.00	94.74	0.00	76.19	84
MB010	86.43	100.00	100.00	100.00	100.00	94.74	80.95	35.71	84

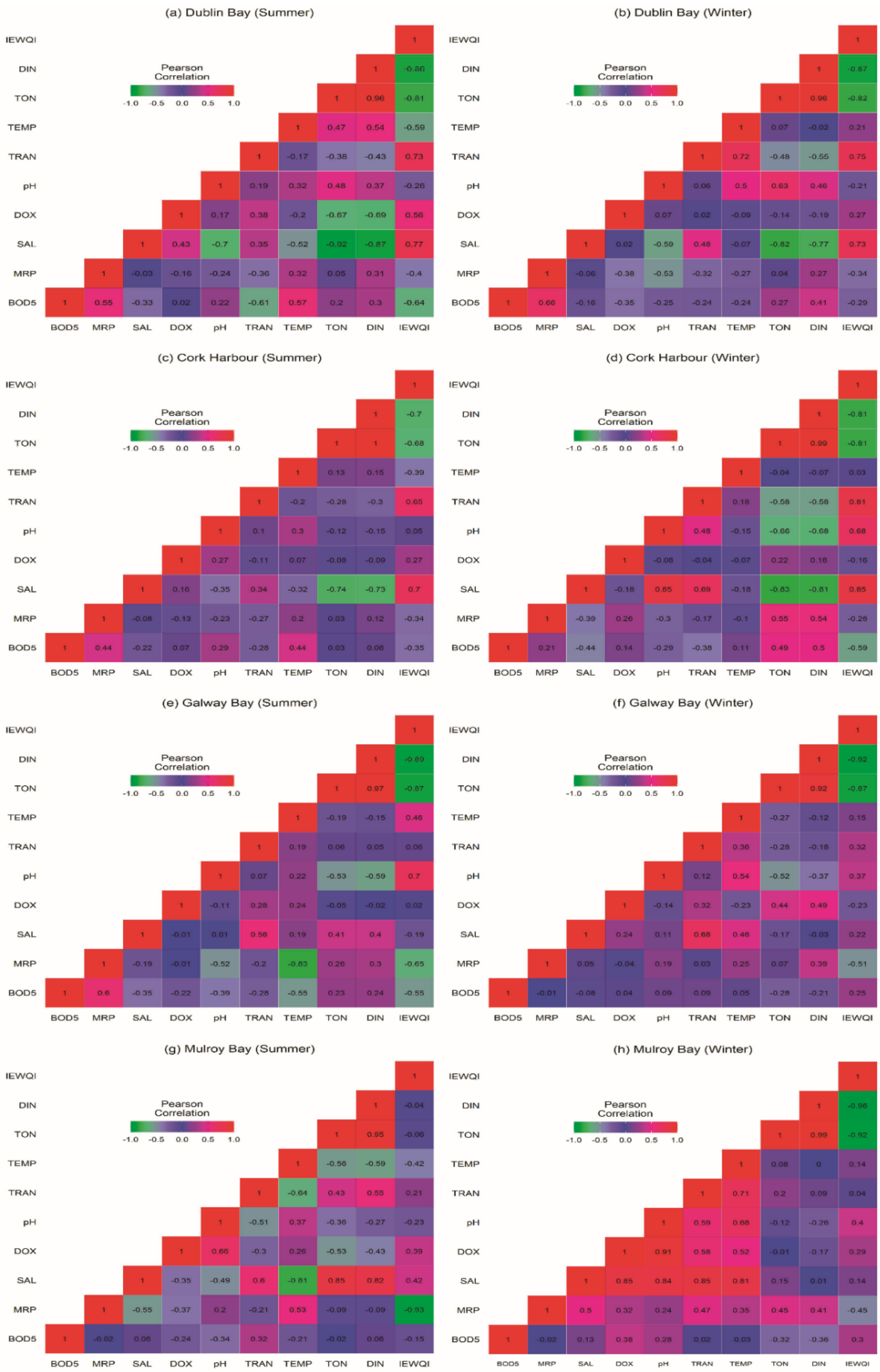


Figure 7.S1. Pearson correlation of selected indicators and IEWQI across different waterbodies in Ireland.

7.13.1. Assessment of water quality in Ireland (cont.)

Compared to the application domains, in Dublin Bay, the WQM model classified 58% (14) of monitoring sites as "good" and 42% (10) as "fair" water quality, whereas 46% (11) and 54% (13) were respectively, classified as "good" and "fair" water quality during the winter season (Figure 7.17). In terms of water body types, it can be seen from the assessment results in table 8 that the model classified all monitoring sites of coastal water quality as "good" status during both seasons, whereas it varied significantly for the transitional water over the winter season. The WQM technique classified transitional water quality at 29% (4) as "good" and 71% (10) as "fair" classes, while 7% (1) of sites were classified as "good" and 93% (13) of monitoring sites as "fair" classes (Table 7.S19).

In Cork Harbour, a considerable difference of water quality was found between summer and winter seasons for both coastal and transitional waterbodies (Table 7.S19). During summer, all coastal waterbodies monitoring sites classified as “good” class whereas 47% (14) and 53% (16) of transitional sites classified as “good” and “fair” classes, respectively. Unlike summer, both coastal and transitional monitoring sites water quality degraded during winter season. Only 19% (7) of monitoring sites classified as “good” status and 81% (30) of monitoring sites graded as “fair” class whereas relatively it varied during winter season, the model classified 43% (3) as “good” and 57% (4) as “fair” for coastal water quality whereas 13% (4) as “good” and 87% (26) as “fair” class for transitional water, respectively (Table 7.S19). In can seen form the figure 17 that comparatively most monitoring sites water quality downgraded during winter season. The results of water quality in Cork Harbour are consistence with earlier studies of Uddin et al., (2022a; 2022b). Those studies also have revealed the similar results for this domain.

The model classified 100% (22) of the monitoring sites for Galway Bay and Mulroy Bay as having "good" water quality throughout the summer, though the assessment outcomes were slightly different from those of the winter (Figure 7.17). During the winter, the WQM model rated the water quality at 91% (20) of the monitoring sites as "good," and at 9% (2) as "fair," while at 93% (13) of the sites in Mulroy Bay, the rating was "good," and at 7% (1), it was "fair" (Figure 7.17). It should be noted that the model assessed all ten coastal monitoring sites for Galway Bay as "good" and all fourteen monitoring sites, respectively, as "good" over the summer seasons (Table 7.S19).

Spatio-temporal variations of water quality and status at each monitoring site are presented in figures 7.S2 and 7.S3, respectively, for the summer and winter seasons across the application domains. There were a significant variation found of water quality between summer and winter seasons over the application domains.

Table 7. S19 Water quality status across the various domains in Ireland through the study period.

Application domains	Summer (2021)				Winter (2021)				Total monitoring sites	
	Coastal		Transitional		Coastal		Transitional			
	Good	Fair	Good	Fair	Good	Fair	Good	Fair	Coastal	Transitional
Dublin Bay	10 (100%)	0	4 (29%)	10 (71%)	10 (100%)	0	1 (7%)	13 (93%)	10	14
Cork harbour	7 (100%)	0	14 (47%)	16 (53%)	3 (43%)	4 (57 %)	4 (13 %)	26 (87%)	7	30
Galway Bay	10 (100 %)	0	12 (100%)	0	9 (90 %)	1 (10%)	11 (92%)	1 (8 %)	10	12
Mulroy Bay	14 (100 %)	0	0	0	13 (93 %)	1 (7 %)	0	0	14	0

Similar to Dublin Bay, most transitional sites in the upper and outer parts of the Cork Harbour had "fair" water quality during the summer [Figure 7.S2(b)], whereas the lower Harbour had "good" water quality. On the other hand, the upper harbour had comparable water quality during the winter. The finding shows that throughout the winter, the coastal water quality of the outer Harbour significantly improved. Figures 7.S2(b) and 7.S3(b) indicate that the transitional water quality has significantly declined over the winter period in comparison to the summer. The quality of the harbor's water decreases during the winter due to a variety of pressures, such as raw wastewater pressure, domestic waste pressure, agricultural pressure, nutrient loads, etc.(Barr and Mcelroy, 2019; Environmental Protection Agency, 2020; “News Releases 2022 | Environmental Protection Agency,” n.d.). The results of the spatio-temporal variability of water quality in Cork Harbour are consistent with the author’s earlier studies (Uddin et al., 2022a; 2022b). Moreover, the results of Cork Harbour water quality are in line with those earlier studies in the literature(Barr and Mcelroy, 2019; EPA, 2021, 2020).

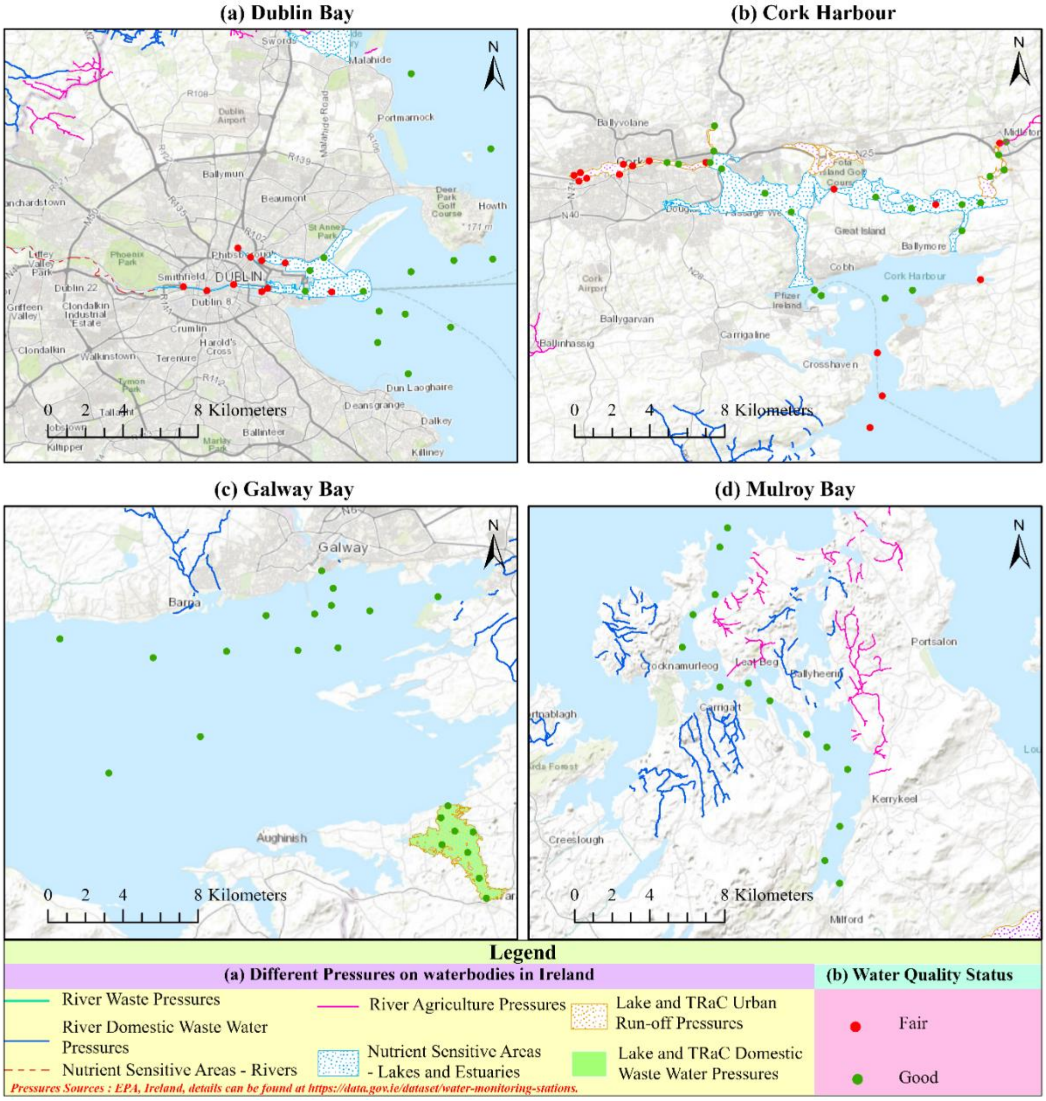


Figure 7.S2. States of water quality at different monitoring sites across the application domains in Ireland throughout the summer season.

As regards the Cork Harbour, like Dublin Bay, most transitional sites in the upper and outer parts of the Harbour's water quality were found to be "fair" during the summer season [Figure 7.S3(b)], whereas "good" water quality was found in the lower Harbour. On the other hand, during the winter season, similar water quality was found in the upper harbour. The results showed that the outer Harbour water quality (coastal) improved significantly through the winter period. Compared to summer, figures 7.S2(b) and 7.S3(b) show that transitional water quality has been degraded significantly over the winter period. Due to a number of pressures that may contribute to affecting harbour water quality, like raw wastewater, domestic waste pressure, agricultural pressure, nutrient loads, etc., the Harbour water quality declines during the winter period. The results of the spatio-temporal variability of water quality in Cork Harbour are consistent with the author’s earlier studies (Uddin et al., 2022a; 2022b).

Also, the results of Cork Harbour water quality are in line with those earlier studies in the literature (Trodd and Shane, 2018; Wall et al., 2020).

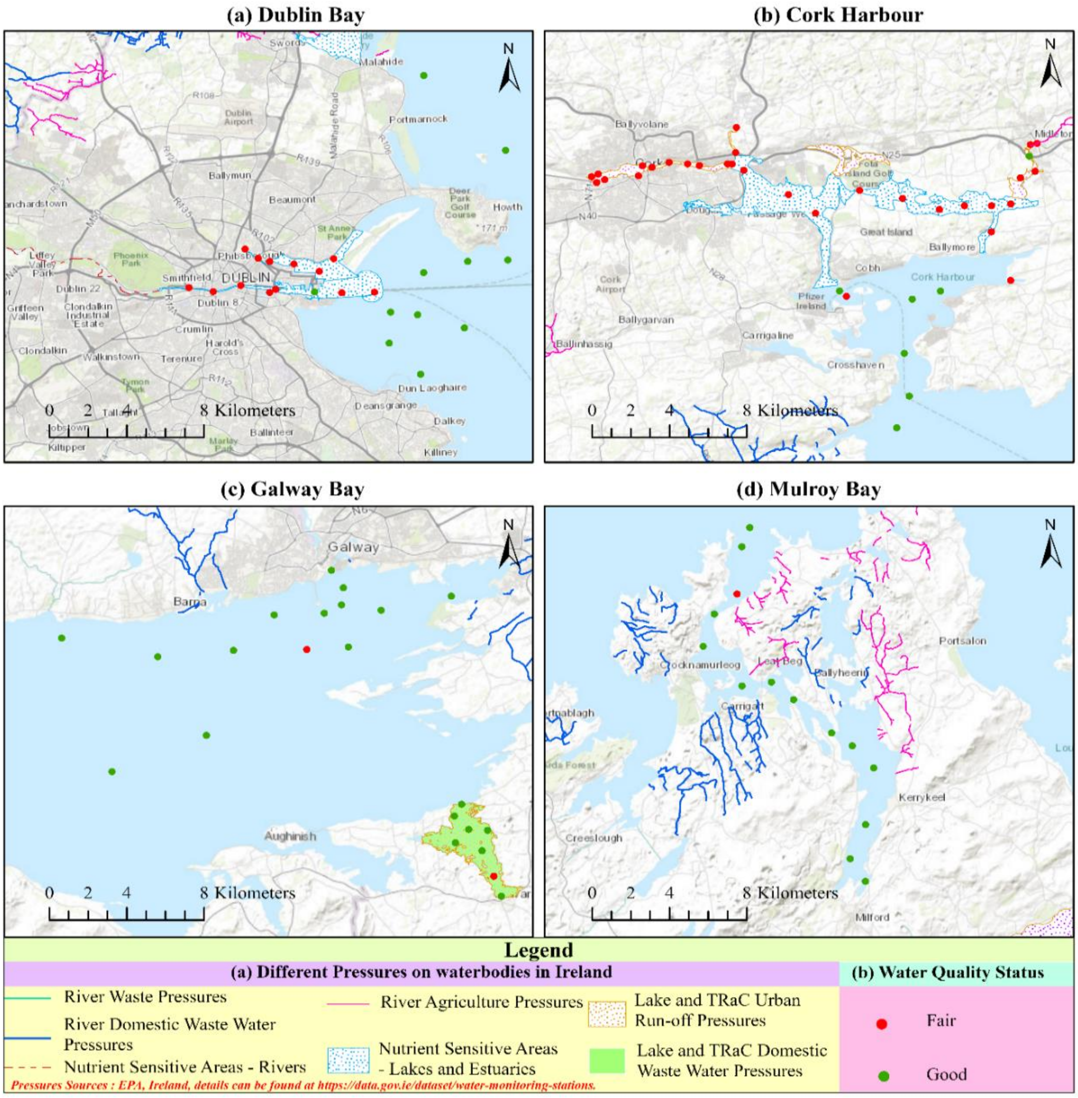


Figure 7.S3. States of water quality at different monitoring sites across the application domains in Ireland throughout the winter season.

In the case of Galway Bay and Mulroy Bay, interestingly, during the summer, all monitoring sites' water quality was found to be "good", whereas a significant difference was found in the winter season. Two sites in Galway Bay, one in the upper Bay (GY190), the other near the Kinvarra (KA025), saw a decline in water quality during the winter season; both sites' water quality was rated as "fair" [Figure 7.S2(c); 7.S3(c)]. Like other waterbodies, several factors has contributed to the decline in Galway Bay water quality through the winter period. As seen from the figures 7.18c and 7.19c, the Galway Bay has significant pressures of domestic wastewater. The Galway Bay experiences significant pressures of domestic wastewater, as shown in figures 7.S2(c) and 7.S3(c). The water quality of Gortnalughoge Bay (MB120) was determined to be "fair" during the winter. Due to this area's high sensitivity to nutrient components, according to the EPA, it may have a significant impact on nutrient elements in this area [Figure 7.S2(d); 7.S3(d)]. However, the results of the IEWQI model reflect the actual scenarios of water quality across the application domains under different pressures in the existing settings of domains. Moreover, the results of the present study are also in line with those of previous studies. The differences in water quality over the various domains between seasons may be due to the constituents of water quality indicators in terms of various factors like geospatial setting of the domains, different pressures on water bodies etc.

Appendix 8. Robust machine learning algorithms for predicting coastal water quality index

8.6.1 Description of various ML techniques

(i) Extreme Gradient Boosting (XGB)

Recently, boosting is the most widely used algorithm of ensemble supervise learning method in order to regression analysis. This algorithm composes many weak learners' models (Bourel and Segura, 2018). Thus far, a number of boosting techniquetechniques were developed including AdaBoost.MH, LogitBoost, GradientBoost, XGBoost, LightGBM, CatBoost etc. In this study, we utilized the XGBoost (XGB) for predicting WQIs because recently, several studies has revealed that the XGB is effective compare than other learning algorithm for regression analysis (Khan et al., 2021; Tanha et al., 2020). The detail of the algorithm can be found in Huan et al., (2020).

(ii) K-Nearest Neighbors (KNN)

KNN is one of the commonly used algorithm that technique predicts a new observation uses of the distance measures. A number ofSeveral distance measures used in KNN algorithm. They can be Euclidean, Manhattan, Minkowski distance. In this study, we used Minkowski distances function for the determination of k-nearest neighbours because this algorithm efficient for the small datasets (29 observations were used for this study). Detail algorithm can be found in (Modaresi and Araghinejad, (2014). The Minkowski distances is given as follows:

$$D = \left(\sum_{i=1}^{n} |p_i - q_i|^p\right)^{1/p} \qquad (8.2)$$

where n is the number of dimensions, p_i , q_i are the data points and p refers the order of the norm.

(iii) Decision Tree (DT) algorithm

DT is another supervised algorithm that is widely used for both classification and regression analysis in ML technique. It splits a large dataset into smaller homogenous datasets easily. In this study, the DT was performed using the approach described by Chen et al., (2020). The DT model building process can be expressed as follows:

$$DT_r = \sum_{n=1}^{n} \sum_{i \epsilon R_j} \left(y_i - \hat{y}_{R_j} \right)^2 \qquad (8.3)$$

Where DT_r refers to the decision tree model, *n* is the number of the observation, R_j is the observation region, y_i and $\hat{y}_{R_j}$ are the eacheach individual response and mean response respectively for the training observation with nth data variables.

(iv) Random Forest (RF)

RF is one of the decision tree-based algorithms that applies multiple base models using subsets of the given data, whereas model decisions are made based on the average of each individual tree decision. It is widely used algorithm for regression analysis. The details algorithm were presented by Liaw and Wiener, (2002). In this study, boosting algorithm was utilised to develop the prediction model.

(v) Extra Tree (ExT) algorithm

ExT is another common tree basedtree-based ensemble algorithm that is widely used for classification and regression analysis. Relatively, the ExT algorithm is much faster than the RF method. It allows all original observations to be predicted without any subsampling. In this study, this algorithm was performed following the approach described in (Hannan and Anmala, 2021).

(vi) Linear Regression (LR)

LR is one of the most common and extensively used algorithm for predicting water quality. Recently, several studied were utilized this technique to predict water quality (Grbčić et al., 2021; Kadam et al., 2019). LR algorithm can be found details in Grbčić et al., (2021). It is defined as follows:

$$y = b_0 + b_1x_1 + b_2x_2 + \cdots b_nx_n \qquad (8.4)$$

where *y* is the MLR-predicted index score, b_0 is constant, x_n is the MLR inputs for the n^{th} WQ parameters, and b_n is the regression coefficient for the n^{th} input.

(vii) Support Vector Machine (SVM) algorithm

SVM is the combination of various supervised learning techniques, which commonly used for the classification and regression purposes (Jalal and Ezzedine, 2019; Modaresi and Araghinejad, 2014). In 1992, this method was developed by Boser and Guyon, although the basic foundation was established by Vapnik in 1995 (Vapnik, 2000). Principally the SVM algorithm differ from the traditional neural networks (NN) algorithm; it uses the structural risk minimization technique for the regression model where the NN used empirical risk minimization functions (Modaresi and Araghinejad, 2014). In this study, the SVM was performed according to Li et al., (2013) approach. The SVM mathematical expression can be defined as follows:

$$Minimize: \qquad R_{sum}(\omega, \varepsilon^*) = \frac{1}{2}||\omega||^2 + C\sum_{i=1}^{n}(\varepsilon_i + \varepsilon_i^*) \qquad (8.5)$$

Subject:

$$d_i - \omega\varphi(x_i) + b_i \leq \epsilon + \varepsilon_i$$
$$\omega\varphi(x_i) + b_i - d_i \leq \epsilon + \varepsilon_i$$
$$\varepsilon_i, \varepsilon_i^* \geq 0, i = 1,2 \ldots, n,$$

where ω is the normal vector, $\frac{1}{2}||\omega||^2$ refers to the regularization factor, C is the error penalty factor, b is the bias, $\varphi(x_i)$is the features space, ϵ is the error function, x_i is the input vector, $d_i$refers to the response variable, n is the number of features in the training dataset, ε_i and ε_i^* are the upper and lower excess deviation respectively (Haghiabi et al., 2018). Where radial basis function (RBF) kernel is defined as follows:

$$K(x_i, x_j) = \exp(-\gamma||\, x_i - x_j||)^2, \gamma > 0 \qquad (8.6)$$

where $x_i and\ x_j$ are inputs variables, and γ is the regularization indicator.

(viii) Gaussian Naïve Bayes (GNB)

GNB is the extended form of the Naïve Bayes algorithm which allows the Gaussian normal distribution of continuous data (Hassan et al., 2021). It is powerful algorithm for predictive model. This algorithm uses prior and posterior probabilities in order to avoid the overfitting problems and biases in predictive model automatically. The GNB assumption in regression analysis is that the continuous values associated with each response follow a normal distribution (Malek et al., 2022). In this research, the GNB algorithms was performed according to the procedure of Varalakshmi et al., (2017).

The likelihood of the features is can becan be defined as follows:

$$P(x_i|y) = \frac{1}{\sqrt{2\pi\sigma_y^2}} exp\left(-\frac{\left(x_i - \mu_y\right)^2}{2\sigma_y^2}\right) \tag{8.7}$$

Where, $P(x_i|y)$ is the probability of x given y, σ is the standard deviation of input variables and μ_y is the mean value of given data variables.

These algorithms were chosen for this study because, recently, many researchers have utilised them to predict the water quality as well as WQI values. A number of researchof research has revealed that those algorithms could be effective and they found higher accuracy to predict water quality or WQI values (Bui et al., 2020; Hafeez et al., 2019; Khan et al., 2021; Modaresi and Araghinejad, 2014). The details of the procedure are presented in Figure 8.2 (above). In order toTo implement these algorithms, the present study was used the Python programming language on the Google Colab cloud computing platform. It is a very convenient environment, and it enables users to run a variety of advanced machine learning models using the Python language.

List of Tables:

Table 8.S1 A summary of the various ML techniques in predicting water quality.

Regions	Applied algorithms	Type of waterbody	Purposes	Suggested algorithm(s)	Reference
Asia					
Bangladesh	Multiple Linear Regression, Support Vector Regression, Gradient Boosting Regression, Random Forest Regression	Lake	To predict water quality index and water quality status	Support Vector Regression for predicting WQI score and Gradient Boosting Regression for predicting water quality status	Islam Khan et al. (2021)
China	Random forest	Lake	To develop a turbidity prediction model	The performance of Random forest was found outperforming other ML algorithms from literature	Zhang et al. (2021)
Hong Kong	Artificial neural networks and Support vector machine	Coastal water	To predict marine water quality	Artificial neural networks in terms of calculation time	Deng et al. (2021)
India	Traditional ML algorithms (Naive Bayes, Logistic regression, Support vector machine, Decision trees, Random Forest) and Auto ML algorithms (Baseline, Linear, Extra Trees, Nearest Neighbors, CatBoost, LightGBM, Xgboost, and Neural Networks)	Lake	To predict water quality index	Auto ML algorithms	Venkata Vara Prasad et al. (2021)
	AutoKeras, Conventional Neural Network and Long Short-Term Memory	Lake	To predict water quality	AutoKeras	Prasad et al. (2022)
	Random Forest, Neural Network, Multinomial Logistic Regression, Bagged Tree Model, Support Vector Machine	-	To predict water quality index	Multinomial Logistic Regression	Hassan et al. (2021)
Iran	Artificial neural networks, Group method of data handling, Support vector machine	River	To predict water quality components	Support vector machine	Haghiabi et al. (2018)
Malaysia	Linear regression, Interaction regression, Robust regression, Stepwise regression, Support vector regression, Boosted trees ensemble regression, Bagged trees ensemble regression, XGBoost, Tree regression and Gaussian process regression	River	To predict water level	Gaussian process regression	Ahmed et al. (2022)
	Support vector machine and Least square-support vector machine	River basin	To predict water quality index	Least square- support vector machine	Leong et al. (2021)
South Korea	Explainable artificial intelligence, XGBoost	River	To predict chlorophyll-a	XGBoost	Park et al. (2022)

Vietnam	Boosting-based algorithms (adaptive boosting, gradient boosting, histogram-based gradient boosting, light gradient boosting, and extreme gradient boosting), Decision tree-based algorithms (decision tree, extra trees, and random forest), and Artificial neural networks -based algorithms (multilayer perceptron, radial basis function, deep feed-forward neural network, and convolutional neural network)	River	To estimate and predict water quality index	XGBoost	Khoi et al. (2022)
Australia					
New Zealand	Naive model, Multiple linear regression, Dynamic regression, regression tree, Markov chain, Classification tree, Random forests, Multinomial logistic regression, Discriminant analysis and Bayesian network	River	to predict water quality via *E. coli*	Bayesian network	Avila et al. (2018)
Africa					
Algeria	Multilinear regression, Random forest, M5P tree, Random subspace, Additive regression, Artificial neural network, Support vector regression, Locally weighted linear regression	Groundwater	To generate and predict water quality index	Multilinear regression	Kouadri et al. (2021)
Nigeria	Artificial neural networks	River	To predict water quality index	ANN	Ubah et al. (2021)
Europe					
Croatia	Gradient Boosting algorithms (Catboost, Xgboost), Random Forests, Support Vector Regression and Artificial Neural Networks	Coastal water	To predict coastal water quality	Catboost	(Grbčić et al., 2021)
Italy	Random Forest and Deep feed-forward Neural Network	River	To predict water quality	Deep feed-forward Neural Network	Zanoni et al. (2022)
Turkey	Multilayer perceptron neural network, Multilayer perceptron neural network-Firefly Algorithm	Lake	To predict water level	Multilayer perceptron neural network-Firefly Algorithm	Ghorbani et al. (2018)
North America					
USA	Multiple linear regression, Partial least square, Sparse partial least square, Random forest, and Bayesian network	Lakes	To Improve the robustness of beach water quality modelling	Performance of the five studied ML models varied significantly at different sites as well as for different years	Wang et al. (2021)
South America					
Brazil	Artificial neural networks	Rivers, streams, lakes	To predict resilience of water resources	Artificial neural networks	Imani et al. (2021)

Table 8.S2 EPA's water quality monitoring sites descriptions in Cork harbor, Ireland.

EPA_ID	User ID	lat.	long.	Site description
LE030	1	51.892	-8.5062	Lee (Cork) Estuary Upper
LE040	2	51.8947	-8.5106	Lee (Cork) Estuary Upper
LE110	3	51.8965	-8.4997	Lee (Cork) Estuary Upper
LE120	4	51.8934	-8.4946	Lee (Cork) Estuary Upper
LE130	5	51.9002	-8.4663	Lee (Cork) Estuary Upper
LE140	6	51.8953	-8.4692	Lee (Cork) Estuary Upper
LE150	7	51.89946	-8.459071	Lee (Cork) Estuary Lower
LE160	8	51.90193	-8.446311	Lee (Cork) Estuary Lower
LE170	9	51.90049	-8.423487	Lee (Cork) Estuary Lower
LE180	10	51.90137	-8.402429	Lee (Cork) Estuary Lower
LE200	11	51.92602	-8.395003	Glashaboy Estuary
LE210	12	51.91892	-8.396046	Glashaboy Estuary
LE220	13	51.90678	-8.396375	Glashaboy Estuary
LE310	14	51.89827	-8.390053	Lough Mahon
LE330	15	51.8867	-8.3565	Lough Mahon
LE340	16	51.8778	-8.3361	Lough Mahon
LE380	17	51.8378	-8.3126	Cork Harbour
LE420	18	51.8851	-8.2708	North Channel Great Island
LE430	19	51.8798	-8.2432	North Channel Great Island
LE450	20	51.8817	-8.204	North Channel Great Island
LE500	21	51.9168	-8.1766	Owenacurra Estuary
LE505	22	51.9111	-8.17401	Owenacurra Estuary
LE510	23	51.906	-8.1773	Owenacurra Estuary
LE540	24	51.8826	-8.1895	North Channel Great Island
LE550	25	51.8691	-8.204	North Channel Great Island
LE620	26	51.8366	-8.2633	Cork Harbour
LE630	27	51.8105	-8.269	Outer Cork Harbour
LE810	28	51.7899	-8.2652	Outer Cork Harbour
LE820	29	51.7746	-8.2745	Outer Cork Harbour

Table 8.S3 Averaged concentration of water quality indicators in Cork Harbour for 2020 (January – December), and ML models predictors and response are presented respectively.

User ID	SAL*	Ml model Predictors										Response
	(psu)	CHL (mg/m^3)	DOX (mg/l)	MRP (mg/l)	DIN (mg/l)	AMN (mg/l)	BOD (mg/l)	pH -	TEMP (0c)	TON (mg/l)	TRAN (m/depth)	WQM-WQIs
1	0.83	1	69.33	0.011	3.423	0.26	1.37	7.6	15	3.17	0	41
2	0.83	1.9	103.3	0.011	2.258	0.06	3.55	7.9	15.43	2.2	0	44.3
3	1.78	2.033	98	0.015	1.992	0.025	1.3	7.7	16.8	1.97	0	45.7
4	0.85	1.45	93.33	0.018	2.64	0.039	1.33	7.7	16.13	2.6	0	44.3
5	5.55	2.5	89.33	0.028	2.394	0.06	1.25	7.8	15.83	2.3	1.5	35.3
6	2.70	2.067	93.33	0.025	2.357	0.057	1.2	7.7	15.53	2.3	0	45.2
7	19.8	4.283	90.17	0.025	1.001	0.11	1.86	7.8	15.83	0.89	2.18	51.2
8	18.5	3.25	88.83	0.027	1.105	0.16	0	7.8	15.75	0.95	2.26	49
9	21.4	7.518	102	0.019	0.731	0.12	2	7.9	15.84	0.65	1.77	56.1
10	20.4	7.8	109.2	0.014	0.709	0.1	0	8.1	15.68	0.61	1.9	57
11	0.88	2.6	101.3	0.064	6.021	0.021	1.9	7.7	14.83	6	0	44.8
12	0.85	2	103	0.046	4.587	0.02	0	7.8	14.77	4.57	0	44.8
13	13.6	5.967	101	0.023	1.351	0.068	2.17	7.9	16.6	1.28	0.75	44.6
14	22.7	7.6	112.5	0.015	0.584	0.09	2.48	8.3	15.7	0.14	1.53	63.5
15	29.0	9.442	123.7	0.011	0.246	0.11	2.38	8.3	15.82	0.14	1.65	68.3
16	27.0	10.233	121.3	0.011	0.234	0.09	2.48	8.3	15.7	0.14	1.53	68.7
17	28.6	10.433	119.5	0.008	0.12	0.056	2.55	8.2	15.57	0.064	1.83	71.5
18	28.1	8.85	136.2	0.022	0.092	0.035	2.7	8.3	16.6	0.057	1.53	72.5
19	27.4	9.6	130.8	0.012	0.077	0.028	2.25	8.3	16.17	0.048	1.8	72.6
20	28.9	7.65	120.7	0.034	0.076	0.036	1.1	8.23	15.4	0.04	2.3	72.7
21	0.90	3.15	106.7	0.024	4.861	0.027	2	7.8	16.27	4.83	0	45.3
22	0.93	1.8	104.3	0.021	5.186	0.19	1.3	7.8	15.07	5.17	0	42.5
23	16.9	9.82	133.2	0.02	2.382	0.064	3.2	8.2	16.9	2.318	1.05	33.1
24	29.4	9.8	124	0.008	0.066	0.03	1.1	8.3	15.65	0.036	2.03	72.9
25	28.9	6.467	121.8	0.013	0.075	0.038	2.48	8.2	15.73	0.037	2.23	72.6
26	29.9	5.06	110.3	0.007	0.052	0.04	1.68	8.2	14.5	0.017	3.87	62.8
27	30.1	4.175	105.3	0.014	0.064	0.036	2	8.2	14.17	0.28	3.4	70.8
28	26.2	3.167	113.7	0.018	0.056	0.031	1.65	8.2	14.8	0.026	5.6	73.3
29	26.2	2.7	103	0.017	0.038	0.038	1.1	8.1	13.9	0	4.83	63.2

**SAL concentration only used for the determination of water quality indicators standard threshold.*

Table 8.S4 The detailed applicable values of each of the criteria for the entire range of salinities (SAL).

Salinity Median psu	DIN Median mg/l N	MRP Median µg/l P	Chlorophyll Median µg/l	Chlorophyll 95 %ile µg/l	Dissolved Oxygen % Saturation 5 %ile	Dissolved Oxygen % Saturation 95 %ile
0	2.600	60	15.0	30.0	70	130
1	2.529	60	15.0	30.0	70	130
2	2.459	60	15.0	30.0	70	130
3	2.388	60	15.0	30.0	70	130
4	2.318	60	15.0	30.0	70	130
5	2.247	60	15.0	30.0	70	130
6	2.176	60	15.0	30.0	70	130
7	2.106	60	15.0	30.0	70	130
8	2.035	60	15.0	30.0	70	130
9	1.965	60	15.0	30.0	70	130
10	1.894	60	15.0	30.0	70	130
11	1.824	60	15.0	30.0	70	130
12	1.753	60	15.0	30.0	70	130
13	1.682	60	15.0	30.0	70	130
14	1.612	60	15.0	30.0	70	130
15	1.541	60	15.0	30.0	70	130
16	1.471	60	15.0	30.0	70	130
17	1.400	60	15.0	30.0	70	130
18	1.336	59	14.7	29.4	71	129
19	1.272	58	14.4	28.9	71	129
20*	1.208	57	14.2	28.3	72	128
21	1.144	56	13.9	27.8	72	128
22	1.081	54	13.6	27.2	73	127
23	1.017	53	13.3	26.7	73	127
24	0.953	52	13.1	26.1	74	126
25	0.889	51	12.8	25.6	74	126
26	0.825	50	12.5	25.0	75	125
27	0.761	49	12.2	24.4	76	124
28	0.697	48	11.9	23.9	76	124
29	0.633	47	11.7	23.3	77	123
30	0.569	46	11.4	22.8	77	123
31	0.506	44	11.1	22.2	78	122
32	0.442	43	10.8	21.7	78	122
33	0.378	42	10.6	21.1	79	121
34	0.314	41	10.3	20.6	79	121
35	0.250	40	10.0	20.0	80	120

** in this study, the SAL median value was 20.47. The color red indicates the threshold of regarding parameters.*

Table 8.S5 Predicted WQM-WQIs of various ML models at each monitoring site in Cork Harbour for 2020.

User ID	XGB	KNN	DT	RF	ExT	LR	SVM	GNB
1	41.00	44.16	41.00	41.33	41.00	36.32	54.52	35.31
2	44.31	44.30	44.30	44.49	44.30	51.88	56.08	49.35
3	45.67	44.82	45.70	45.06	45.70	42.77	55.80	45.93
4	44.31	44.34	44.30	43.61	44.30	42.04	55.55	43.73
5	35.36	45.00	35.30	39.18	35.30	43.05	55.38	45.47
6	45.17	44.34	45.20	44.76	45.20	48.50	55.56	46.65
7	51.21	45.00	51.20	50.58	51.20	48.30	55.46	50.99
8	48.92	45.00	49.00	48.62	49.00	50.47	55.39	51.85
9	56.07	55.80	56.10	56.06	56.10	55.16	56.10	56.21
10	57.04	62.04	57.00	57.21	57.00	61.35	56.48	61.22
11	44.81	44.34	44.80	44.48	44.80	39.47	55.92	38.21
12	44.79	44.34	44.80	44.55	44.80	49.54	56.02	45.53
13	44.63	52.30	44.60	45.96	44.60	48.34	56.01	50.30
14	63.52	65.62	63.50	63.98	63.50	62.50	56.65	61.28
15	68.29	71.04	68.30	68.52	68.30	66.88	57.23	66.13
16	68.68	70.82	68.70	68.80	68.70	67.16	57.12	65.49
17	71.46	70.76	71.50	71.21	71.50	66.68	57.04	65.70
18	72.48	63.88	72.50	71.91	72.50	68.39	57.76	68.73
19	72.60	63.88	72.60	72.40	72.60	68.21	57.55	68.59
20	72.70	70.76	72.70	72.33	72.70	71.99	57.07	68.10
21	45.27	44.34	45.30	44.78	45.30	35.20	56.22	40.20
22	42.51	44.34	42.50	43.11	42.50	41.85	56.08	42.04
23	33.11	63.88	33.10	41.50	33.10	51.65	57.62	57.90
24	72.86	71.04	72.90	72.41	72.90	69.86	57.25	68.60
25	72.59	71.04	72.60	72.08	72.60	66.98	57.11	66.38
26	62.83	65.48	62.80	65.41	62.80	68.85	56.53	67.51
27	70.78	59.44	70.80	69.28	70.80	70.80	56.25	65.35
28	73.21	65.48	73.30	70.72	73.30	65.42	56.69	69.26
29	63.20	55.80	63.20	65.03	63.20	69.98	56.13	67.58

References

Ahmed, A.N., Yafouz, A., Birima, A.H., Kisi, O., Huang, Y.F., Sherif, M., Sefelnasr, A., El-Shafie, A., 2022. Water level prediction using various machine learning algorithms: a case study of Durian Tunggal river, Malaysia. Eng. Appl. Comput. Fluid Mech. 16, 422–440. https://doi.org/10.1080/19942060.2021.2019128

Avila, R., Horn, B., Moriarty, E., Hodson, R., Moltchanova, E., 2018. Evaluating statistical model performance in water quality prediction. J. Environ. Manage. 206, 910–919. https://doi.org/10.1016/j.jenvman.2017.11.049

Bourel, M., Segura, A.M., 2018. Multiclass classification methods in ecology. Ecol. Indic. 85, 1012–1021. https://doi.org/10.1016/j.ecolind.2017.11.031

Chen, K., Chen, H., Zhou, C., Huang, Y., Qi, X., Shen, R., Liu, F., Zuo, M., Zou, X., Wang, J., Zhang, Y., Chen, D., Chen, X., Deng, Y., Ren, H., 2020. Comparative analysis of surface water quality

prediction performance and identification of key water parameters using different machine learning models based on big data. Water Res. 171, 115454. https://doi.org/10.1016/j.watres.2019.115454
Deng, T., Chau, K.W., Duan, H.F., 2021. Machine learning based marine water quality prediction for coastal hydro-environment management. J. Environ. Manage. 284, 112051. https://doi.org/10.1016/j.jenvman.2021.112051
Ghorbani, M.A., Deo, R.C., Karimi, V., Yaseen, Z.M., Terzi, O., 2018. Implementation of a hybrid MLP-FFA model for water level prediction of Lake Egirdir, Turkey. Stoch. Environ. Res. Risk Assess. 32, 1683–1697. https://doi.org/10.1007/s00477-017-1474-0
Grbčić, L., Družeta, S., Mauša, G., Lipić, T., Lušić, D.V., Alvir, M., Lučin, I., Sikirica, A., Davidović, D., Travaš, V., Kalafatović, D., Pikelj, K., Fajković, H., Holjević, T., Kranjčević, L., 2021. Coastal water quality prediction based on machine learning with feature interpretation and spatio-temporal analysis.
Haghiabi, A.H., Nasrolahi, A.H., Parsaie, A., 2018. Water quality prediction using machine learning methods. Water Qual. Res. J. 53, 3–13. https://doi.org/10.2166/wqrj.2018.025
Hannan, A., Anmala, J., 2021. Classification and Prediction of Fecal Coliform in Stream Waters Using Decision Trees (DTs) for Upper Green River Watershed, Kentucky, USA. Water 2021, Vol. 13, Page 2790 13, 2790. https://doi.org/10.3390/W13192790
Hassan, Md. Mehedi, Hassan, Md. Mahedi, Akter, L., Rahman, M.M., Zaman, S., Hasib, K.M., Jahan, N., Smrity, R.N., Farhana, J., Raihan, M., Mollick, S., 2021. Efficient Prediction of Water Quality Index (WQI) Using Machine Learning Algorithms. Human-Centric Intell. Syst. 1, 86. https://doi.org/10.2991/hcis.k.211203.001
Huan, J., Li, H., Li, M., Chen, B., 2020. Prediction of dissolved oxygen in aquaculture based on gradient boosting decision tree and long short-term memory network: A study of Chang Zhou fishery demonstration base, China. Comput. Electron. Agric. 175, 105530. https://doi.org/10.1016/j.compag.2020.105530
Imani, M., Hasan, M.M., Bittencourt, L.F., McClymont, K., Kapelan, Z., 2021. A novel machine learning application: Water quality resilience prediction Model. Sci. Total Environ. 768, 144459. https://doi.org/10.1016/j.scitotenv.2020.144459
Islam Khan, M.S., Islam, N., Uddin, J., Islam, S., Nasir, M.K., 2021. Water quality prediction and classification based on principal component regression and gradient boosting classifier approach. J. King Saud Univ. - Comput. Inf. Sci. https://doi.org/10.1016/j.jksuci.2021.06.003
Jalal, D., Ezzedine, T., 2019. Performance analysis of machine learning algorithms for water quality monitoring system. 2019 Int. Conf. Internet Things, Embed. Syst. Commun. IINTEC 2019 - Proc. 86–89. https://doi.org/10.1109/IINTEC48298.2019.9112096
Kadam, A.K., Wagh, V.M., Muley, A.A., Umrikar, B.N., Sankhua, R.N., 2019. Prediction of water quality index using artificial neural network and multiple linear regression modelling approach in Shivganga River basin, India. Model. Earth Syst. Environ. 5, 951–962. https://doi.org/10.1007/s40808-019-00581-3
Khoi, D.N., Quan, N.T., Linh, D.Q., Nhi, P.T.T., Thuy, N.T.D., 2022. Using Machine Learning Models for Predicting the Water Quality Index in the La Buong River, Vietnam. Water 14, 1552. https://doi.org/10.3390/w14101552
Kouadri, S., Elbeltagi, A., Islam, A.R.M.T., Kateb, S., 2021. Performance of machine learning methods in predicting water quality index based on irregular data set: application on Illizi region (Algerian southeast). Appl. Water Sci. 11, 1–20. https://doi.org/10.1007/s13201-021-01528-9
Leong, W.C., Bahadori, A., Zhang, J., Ahmad, Z., 2021. Prediction of water quality index (WQI) using support vector machine (SVM) and least square-support vector machine (LS-SVM). Int. J. River Basin Manag. 19, 149–156. https://doi.org/10.1080/15715124.2019.1628030
Li, W., Yang, M., Liang, Z., Zhu, Y., Mao, W., Shi, J., Chen, Y., 2013. Assessment for surface water quality in Lake Taihu Tiaoxi River Basin China based on support vector machine. Stoch. Environ. Res. Risk Assess. 27, 1861–1870. https://doi.org/10.1007/s00477-013-0720-3
Liaw, A., Wiener, M., 2002. Classification and Regression by randomForest 2.
Malek, N.H.A., Wan Yaacob, W.F., Md Nasir, S.A., Shaadan, N., 2022. Prediction of Water Quality Classification of the Kelantan River Basin, Malaysia, Using Machine Learning Techniques. Water. https://doi.org/10.3390/w14071067
Modaresi, F., Araghinejad, S., 2014. A comparative assessment of support vector machines, probabilistic neural networks, and K-nearest neighbor algorithms for water quality classification. Water Resour. Manag. 28, 4095–4111. https://doi.org/10.1007/s11269-014-0730-z
Park, J., Lee, W.H., Kim, K.T., Park, C.Y., Lee, S., Heo, T.Y., 2022. Interpretation of ensemble learning to predict water quality using explainable artificial intelligence. Sci. Total Environ. 832, 155070.

https://doi.org/10.1016/j.scitotenv.2022.155070
Prasad, D.V.V., Venkataramana, L.Y., Kumar, P.S., Prasannamedha, G., Harshana, S., Srividya, S.J., Harrinei, K., Indraganti, S., 2022. Analysis and prediction of water quality using deep learning and auto deep learning techniques. Sci. Total Environ. 821, 153311. https://doi.org/10.1016/j.scitotenv.2022.153311
Tanha, J., Abdi, Y., Samadi, N., Razzaghi, N., Asadpour, M., 2020. Boosting methods for multi-class imbalanced data classification: an experimental review. J. Big Data 7. https://doi.org/10.1186/s40537-020-00349-y
Ubah, J.I., Orakwe, L.C., Ogbu, K.N., Awu, J.I., Ahaneku, I.E., Chukwuma, E.C., 2021. Forecasting water quality parameters using artificial neural network for irrigation purposes. Sci. Rep. 11, 1–13. https://doi.org/10.1038/s41598-021-04062-5
Vapnik, V.N., 2000. The Nature of Statistical Learning Theory. Nat. Stat. Learn. Theory. https://doi.org/10.1007/978-1-4757-3264-1
Varalakshmi, P., Vandhana, S., Vishali, S., 2017. Prediction of water quality using Naive Bayesian algorithm. 2016 8th Int. Conf. Adv. Comput. ICoAC 2016 224–229. https://doi.org/10.1109/ICoAC.2017.7951774
Venkata Vara Prasad, D., Senthil Kumar, P., Venkataramana, L.Y., Prasannamedha, G., Harshana, S., Jahnavi Srividya, S., Harrinei, K., Indraganti, S., 2021. Automating water quality analysis using ML and auto ML techniques. Environ. Res. 202, 111720. https://doi.org/10.1016/j.envres.2021.111720
Wang, L., Zhu, Z., Sassoubre, L., Yu, G., Liao, C., Hu, Q., Wang, Y., 2021. Improving the robustness of beach water quality modeling using an ensemble machine learning approach. Sci. Total Environ. 765, 142760. https://doi.org/10.1016/j.scitotenv.2020.142760
Zanoni, M.G., Majone, B., Bellin, A., 2022. A catchment-scale model of river water quality by Machine Learning. Sci. Total Environ. 838, 156377. https://doi.org/10.1016/j.scitotenv.2022.156377
Zhang, Y., Yao, X., Wu, Q., Huang, Y., Zhou, Z., Yang, J., Liu, X., 2021. Turbidity prediction of lake-type raw water using random forest model based on meteorological data: A case study of Tai lake, China. J. Environ. Manage. 290, 112657. https://doi.org/10.1016/j.jenvman.2021.112657

Appendix 9. An improved methodology for the assessment of trophic status for coastal and transitional waters using machine learning and artificial intelligence approaches

Table 9.S1 Averaged concentrations of water quality indicators in **Cork Harbour, 2021**. The guideline values (thresholds) adopted for the Cork Harbour are included at the bottom and values in bold indicate compliance failures.

Monitoring sites	SAL (psu)	Common water quality indicators					nutrient enrichment indicators				
		BOD5 (mg/l)	pH -	TEMP (^{0}C)	TON (mg/l as N)	TRAN (m/depth)	CHL (µg/l)	DIN (mg/l)	MRP (mg/l as P)	DOX (% sat)	CHL (µg/l)
LE040	5.10	0.00	8.2	17.8	1.50	1.50	4	**1.54**	0.010	89.50	4.0
LE030	17.08	0.00	8.0	16.8	0.86	1.10	1.7	**0.92**	0.030	89.00	1.7
LE110	11.09	0.00	8.1	17.3	1.18	1.30	2.85	**1.23**	0.020	89.25	2.85
LE120	27.63	1.20	8.1	16.6	0.62	1.50	5.3	**0.68**	0.020	96.20	5.3
LE140	0.30	3.10	8.4	17.1	1.05	1.00	4.1	**1.09**	**0.050**	104.50	4.1
LE130	2.30	3.80	8.4	17.4	0.99	1.00	3.3	**1.06**	**0.060**	101.00	3.3
LE150	20.11	3.97	8.2	18.3	0.82	1.00	19.17	**1.01**	**0.130**	91.38	19.17
LE160	30.03	3.00	8.0	16.9	0.13	**0.80**	18	0.22	**0.050**	99.57	18
Tivoli	30.80	1.75	8.1	16.4	0.10	1.10	3.36	0.17	0.040	112.48	3.36
LE170	30.18	3.00	8.1	16.8	0.11	1.00	7.97	0.18	**0.050**	104.29	7.97
LE180	31.14	2.60	7.9	17.2	0.25	1.13	2.98	**0.88**	**0.300**	97.00	2.98
BLKC*	32.55	2.00	8.1	16.3	0.14	1.40	5.34	0.19	0.010	100.38	5.34
LE220	31.50	0.00	8.1	13.8	0.02	2.00	1.24	0.05	0.040	104.33	1.24
LE210	33.90	0.00	8.0	7.2	0.17	1.00	0.74	0.19	0.020	99.00	0.74
LE310	33.60	0.00	8.0	7.3	0.12	1.20	0.62	0.16	0.010	98.00	0.62
LE330	31.38	1.20	8.1	13.9	0.12	1.84	1.88	0.26	**0.050**	105.40	1.88
LE340	32.00	1.48	8.1	14.0	0.04	1.96	0.8	0.08	0.010	105.17	0.8
LE410	31.73	1.10	8.0	17.4	0.26	**0.65**	7.18	0.37	**0.050**	77.80	7.18
LE420	30.70	0.95	8.1	18.2	0.03	**0.50**	7.2	0.12	0.020	106.00	7.2
LE430	31.20	2.00	8.2	17.9	0.03	**0.80**	6.9	0.1	0.010	120.00	6.9
LE440	31.60	1.44	8.1	17.3	0.65	**0.99**	7.15	**0.71**	**0.070**	110.22	7.15
LE450	32.05	1.10	8.1	16.9	0.03	1.50	8.7	0.07	0.010	114.00	8.7
LE540	32.20	1.15	8.2	17.6	0.01	**0.65**	3.8	0.04	0.020	125.50	3.8
LE500	0.10	1.80	8.1	16.2	**4.10**	1.00	1.55	4.12	0.040	102.50	1.55
LE550	31.85	1.70	8.2	17.2	0.06	1.80	9.15	0.12	0.010	118.00	9.15
HBLIN*	31.96	1.98	8.2	15.8	0.11	2.00	2.36	0.17	0.010	78.94	2.36
LE380	32.20	1.10	8.2	16.2	0.10	2.00	2.95	0.16	0.010	105.25	2.95
LE620	33.83	0.00	8.1	15.4	0.03	3.00	1.76	0.07	0.010	101.25	1.76
LE610	32.20	1.10	8.15	15.82	0.10	2.00	2.36	0.16	0.01	101.25	2.36
RLD*	4.30	2.10	8.2	18.2	0.08	1.13	3.36	0.16	**0.05**	100.10	3.36
LE630	34.03	0.00	8.1	15.38	0.02	3.40	3.05	0.07	0.01	101.50	3.05
LE810	34.05	1.54	8.1	15.4	0.00	3.50	4.42	0.04	0	99.50	4.42
LE820	34.20	1.65	8.1	15.1	0.02	3.75	2.65	0.05	0.01	96.00	2.65

LE505	0.30	1.00	8	16.2	**4.60**	1.00	0.53	**4.63**	0.03	107.00	0.53
LE510	22.80	1.88	7.98	16.25	1.62	1.00	8.98	**1.69**	0.03	97.50	8.98
LE520	23.75	1.50	7.98	16.45	1.43	1.00	4.35	**1.49**	0.02	100.25	4.35
LE530	27.80	1.65	8.1	16.65	0.58	1.10	3.15	**0.64**	0.02	106.00	3.15
Criteria	**Media n = 31**	**0 - 7**	**5.0 - 9.0**	**25**	**0 - 2**	**>1**	**11.1 - 22.2**	**0 - 0.51**	**0 - 0.044**	**78 - 122**	***11.1 - 22.2***
	Breached		ML predictors		ML response						

Table 9.S2 Determining the moving thresholds (guideline) values for the nutrient indicators based on the entire range of salinities using the ATSEBI system.

Salinity Median (psu)	DIN Median (mg/l N)	MRP Median (µg/l P)	Chlorophyll Median (µg/l)	Chlorophyll 95 %ile (µg/l)	Dissolved Oxygen 5 %ile (% Saturation)	Dissolved Oxygen 95 %ile (% Saturation)
0	2.600	60	15.0	30.0	70	130
1	2.529	60	15.0	30.0	70	130
2	2.459	60	15.0	30.0	70	130
3	2.388	60	15.0	30.0	70	130
4	2.318	60	15.0	30.0	70	130
5	2.247	60	15.0	30.0	70	130
6	2.176	60	15.0	30.0	70	130
7	2.106	60	15.0	30.0	70	130
8	2.035	60	15.0	30.0	70	130
9	1.965	60	15.0	30.0	70	130
10	1.894	60	15.0	30.0	70	130
11	1.824	60	15.0	30.0	70	130
12	1.753	60	15.0	30.0	70	130
13	1.682	60	15.0	30.0	70	130
14	1.612	60	15.0	30.0	70	130
15	1.541	60	15.0	30.0	70	130
16	1.471	60	15.0	30.0	70	130
17	1.400	60	15.0	30.0	70	130
18	1.336	59	14.7	29.4	71	129
19	1.272	58	14.4	28.9	71	129
20	1.208	57	14.2	28.3	72	128
21	1.144	56	13.9	27.8	72	128
22	1.081	54	13.6	27.2	73	127
23	1.017	53	13.3	26.7	73	127
24	0.953	52	13.1	26.1	74	126
25	0.889	51	12.8	25.6	74	126
26	0.825	50	12.5	25.0	75	125
27	0.761	49	12.2	24.4	76	124
28	0.697	48	11.9	23.9	76	124
29	**0.633**	**47**	**11.7**	**23.3**	**77**	**123**
30	**0.569**	**46**	**11.4**	**22.8**	**77**	**123**
31	**0.506**	**44**	**11.1**	**22.2**	**78**	**122**
32	0.442	43	10.8	21.7	78	122
33	**0.378**	**42**	**10.6**	**21.1**	**79**	**121**
34	0.314	41	10.3	20.6	79	121
35	0.250	40	10.0	20.0	80	120

**Red and bold indicated that the median SAL values were used for the determination the threshold values of nutrients indicators in the present study across the four application domains through the study year.*

Table 9.S3 Optimized hyper-parameters of various ML models during testing period for predicting CHL.

Model parameters	XGBoost	CatBoost	RF	DT	ExT	MLR	KNN	SVM	GNB	DNN
n_estimators	100	100	10	100	100	100	-	30	200	1500
learning_rate	0.1	0.1	-	-	-	-	-	-	-	0.2
dropout_rate	-	-	-	-	-	-	-	-	-	0.6
weight_constrint	-	-	-	-	-	-	-	-	-	1
Momentum	-	-	-	-	-	-	-	-	-	0.9
max.depth	10	8	20	10	20				-	-
gamma	0	-	-	-	-	-	-	auto	-	-
booster	gbtree		-	-	-	-	-		-	-
l2_leaf_reg	-	3	-	-	-	-	-	-	-	-
Kernel		-	-	-	-	-	-	RBF	-	-
subsample	1	-	-	-	-	-	-	-	-	-
colsample_bytree	1	-	-	-	-	-	-	-	-	-
base_score	0.5	-	-	-	-	-	-	-	-	-
reg_lamda	1	-	-	-	-	-	-	-	-	-
bootstrap	True	-	True	-	True	-	-	-	-	-
cv.folds	10	-		-	-	-	-	-	-	-
random_state	1	-	1	-	1	-	-	-	-	-
Objective	reg.linear	-	-	-	-	-	-	-	-	-
criterion	-	-	*Squared_error*	-	*Squared_error*	-	-	-	-	-
max_leaf_nodes			20	10	5	-	10	-	-	-
min_samples_leaf			5	3	1	-	-	-	-	-
epsilon	-	-	-	-	-	-	-	0.1	-	-
Degree	-	-	-	-	-	-	-	5	-	-
shrinking	-	-	-	-	-	-	-	True	-	-
fit_intercept	-	-	-	-	-	TRUE	-	-	-	-
n_neighbors	-	-	-	-	-	-	20	-	-	-
weight	-	-	-	-	-	-	uniform	-	-	-
metrics	-	-	-	-	-	-	minkowski	-	-	-
power_parameters	-	-	-	-	-	-	2	-	-	

Table 9.S4 Comparison between actual and predicted CHL in Cork Harbour of various ML techniques.

Monitoring sites	XGBoost		RF		ExT		MLR		SVM		GNB		DNN		CatBoost		KNN		DT	
	A	P	A	P	A	P	A	P	A	P	A	P	A	P	A	P	A	P	A	P
LE040	4.0	4.0	4.0	4.4	4.0	4.0	4.0	3.9	4.0	3.0	4.0	3.7	4.0	6.3	4.0	3.9	4.0	3.8	4.0	4.0
LE030	1.7	1.7	1.7	4.4	1.7	1.7	1.7	3.6	1.7	2.9	1.7	3.6	1.7	1.9	1.7	1.9	1.7	3.8	1.7	1.7
LE110	2.9	2.9	2.9	4.4	2.9	2.9	2.9	3.8	2.9	3.0	2.9	3.7	2.9	3.0	2.9	2.9	2.9	3.8	2.9	2.9
LE120	5.3	5.3	5.3	4.5	5.3	5.3	5.3	4.0	5.3	3.2	5.3	4.0	5.3	3.6	5.3	3.8	5.3	3.9	5.3	5.3
LE140	4.1	4.1	4.1	6.1	4.1	4.1	4.1	5.2	4.1	4.0	4.1	5.1	4.1	10.0	4.1	4.1	4.1	4.9	4.1	4.1
LE130	3.3	3.3	3.3	5.4	3.3	3.3	3.3	5.5	3.3	3.4	3.3	5.3	3.3	13.7	3.3	3.4	3.3	4.5	3.3	3.3
LE150	3.4	3.4	3.4	5.2	3.4	3.4	3.4	4.8	3.4	4.2	3.4	4.6	3.4	3.3	3.4	3.3	3.4	4.7	3.4	3.4
LE160	8.0	7.9	8.0	6.3	8.0	8.0	8.0	5.1	8.0	4.0	8.0	4.9	8.0	8.3	8.0	7.5	8.0	4.9	8.0	8.0
Tivoli	3.0	3.0	3.0	4.3	3.0	3.0	3.0	4.8	3.0	3.6	3.0	4.7	3.0	10.3	3.0	3.1	3.0	4.0	3.0	3.0
LE170	5.3	5.3	5.3	4.7	5.3	5.3	5.3	4.3	5.3	3.6	5.3	4.3	5.3	4.9	5.3	5.2	5.3	4.6	5.3	5.3
LE180	1.2	1.2	1.2	2.0	1.2	1.2	1.2	2.5	1.2	1.3	1.2	2.8	1.2	0.9	1.2	1.3	1.2	3.3	1.2	1.2
BLKC*	0.7	0.7	0.7	1.7	0.7	0.7	0.7	0.2	0.7	0.8	0.7	1.0	0.7	0.8	0.7	0.8	0.7	3.1	0.7	0.7
LE220	0.6	0.6	0.6	1.7	0.6	0.6	0.6	0.2	0.6	0.8	0.6	0.9	0.6	0.8	0.6	0.8	0.6	3.1	0.6	0.6
LE210	1.9	1.9	1.9	1.7	1.9	1.9	1.9	3.0	1.9	1.9	1.9	3.3	1.9	0.9	1.9	2.0	1.9	4.0	1.9	1.9
LE310	0.8	0.8	0.8	1.7	0.8	0.8	0.8	3.1	0.8	2.1	0.8	3.3	0.8	0.9	0.8	2.1	0.8	4.0	0.8	0.8
LE330	7.2	7.2	7.2	4.9	7.2	7.2	7.2	4.0	7.2	3.6	7.2	3.9	7.2	7.0	7.2	7.0	7.2	4.3	7.2	7.2
LE340	7.2	7.2	7.2	6.1	7.2	7.2	7.2	5.4	7.2	4.1	7.2	4.9	7.2	9.0	7.2	7.0	7.2	4.6	7.2	7.2
LE410	6.9	6.9	6.9	6.1	6.9	6.9	6.9	6.0	6.9	4.5	6.9	5.5	6.9	10.3	6.9	3.7	6.9	4.7	6.9	6.9
LE420	7.2	7.2	7.2	6.1	7.2	7.2	7.2	5.1	7.2	4.3	7.2	4.8	7.2	7.1	7.2	7.0	7.2	5.0	7.2	7.2
LE430	8.7	8.7	8.7	5.5	8.7	8.7	8.7	4.7	8.7	3.9	8.7	4.5	8.7	4.2	8.7	3.2	8.7	4.4	8.7	8.7
LE440	3.8	3.8	3.8	6.1	3.8	3.8	3.8	5.8	3.8	3.9	3.8	5.3	3.8	6.0	3.8	3.9	3.8	4.7	3.8	3.8
LE450	1.6	1.6	1.6	2.3	1.6	1.6	1.6	4.4	1.6	3.8	1.6	4.4	1.6	2.5	1.6	1.7	1.6	4.6	1.6	1.6
LE540	9.2	9.1	9.2	5.7	9.2	9.2	9.2	5.1	9.2	4.3	9.2	4.8	9.2	9.1	9.2	3.6	9.2	4.5	9.2	9.2
LE500	2.4	2.4	2.4	2.2	2.4	2.4	2.4	3.0	2.4	2.5	2.4	3.3	2.4	2.7	2.4	2.4	2.4	3.8	2.4	2.4
LE550	3.0	3.0	3.0	3.9	3.0	3.0	3.0	3.9	3.0	2.9	3.0	3.9	3.0	2.6	3.0	2.9	3.0	4.2	3.0	3.0
HBLIN*	1.8	1.8	1.8	2.2	1.8	1.8	1.8	2.7	1.8	2.2	1.8	2.9	1.8	3.3	1.8	1.7	1.8	3.4	1.8	1.8
LE380	2.4	2.4	2.4	2.2	2.4	2.4	2.4	3.6	2.4	2.5	2.4	3.7	2.4	2.2	2.4	2.1	2.4	4.0	2.4	2.4
LE620	3.4	3.4	3.4	4.5	3.4	3.4	3.4	5.2	3.4	4.0	3.4	4.9	3.4	14.0	3.4	3.6	3.4	4.9	3.4	3.4
LE610	3.1	3.1	3.1	2.2	3.1	3.1	3.1	2.5	3.1	2.5	3.1	2.7	3.1	3.9	3.1	1.8	3.1	3.4	3.1	3.1
RLD*	4.4	4.4	4.4	2.2	4.4	4.4	4.4	2.9	4.4	2.8	4.4	3.1	4.4	4.3	4.4	2.4	4.4	3.8	4.4	4.4
LE630	2.7	2.7	2.7	2.0	2.7	2.7	2.7	2.5	2.7	2.8	2.7	2.9	2.7	4.5	2.7	2.6	2.7	3.9	2.7	2.7
LE810	0.5	0.5	0.5	2.3	0.5	0.5	0.5	4.4	0.5	3.5	0.5	4.2	0.5	0.9	0.5	0.7	0.5	4.4	0.5	0.5
LE820	9.0	8.9	9.0	4.8	9.0	9.0	9.0	4.3	9.0	3.7	9.0	4.3	9.0	3.1	9.0	3.6	9.0	4.3	9.0	9.0

LE505	4.4	4.4	4.4	5.4	4.4	4.4	4.4	4.4	4.4	3.7	4.4	4.3	4.4	3.1	4.4	4.2	4.4	4.2	4.4	4.4
LE510	3.2	3.2	3.2	5.6	3.2	3.2	3.2	4.7	3.2	4.0	3.2	4.5	3.2	4.6	3.2	3.2	3.2	4.6	3.2	3.2

**A = Actual, and P = Predicted ASTI scores.*

Table 9.S5 Models (ATSEBI and newly proposed ASTI) input (water quality indicators) for assessing trophic status in Cork Harbour, 2021 and model outputs.

Monitoring sites	Input (ATSEBI system, whereas only CHL used for ASTI)				Models output			
	MRP (µg/l)	DOX (% sat.)	DIN (mg/l)	CHL (µg/l)	ATSEBI system (Existing)	ASTI (Proposed method)		
					Trophic status	ASTI (Actual)	ASTI (Predicted)	Trophic status
LE040	0.01	89.5	1.54	4	Intermediate	63.96	63.96	Moderate
LE030	0.03	89	0.92	1.7	Intermediate	84.68	84.68	Unpolluted
LE110	0.02	89.25	1.23	2.85	Intermediate	74.32	74.32	Moderate
LE120	0.02	96.2	0.68	5.3	Intermediate	52.25	52.25	Moderate
LE140	0.05	104.5	1.09	4.1	Intermediate	63.06	63.06	Moderate
LE130	0.06	101	1.06	3.3	Intermediate	70.27	70.27	Moderate
LE150	0.13	91.38	1.01	19.17	Intermediate	0.00	0.00	Hypereutrophic
LE160	0.05	99.57	0.22	18	Unpolluted	0.00	0.00	Hypereutrophic
Tivoli	0.04	112.48	0.17	3.36	Unpolluted	69.73	69.73	Moderate
LE170	0.05	104.29	0.18	7.97	Unpolluted	28.20	28.20	Hypereutrophic
LE180	0.3	97	0.88	2.98	Intermediate	73.15	73.15	Moderate
BLKC*	0.01	100.38	0.19	5.34	Unpolluted	51.89	51.89	Moderate
LE220	0.04	104.33	0.05	1.24	Unpolluted	88.83	88.83	Unpolluted
LE210	0.02	99	0.19	0.74	Unpolluted	93.33	93.33	Unpolluted
LE310	0.01	98	0.16	0.62	Unpolluted	94.41	94.41	Unpolluted
LE330	0.05	105.4	0.26	1.88	Unpolluted	83.06	83.06	Unpolluted
LE340	0.01	105.17	0.08	0.8	Unpolluted	92.79	92.79	Unpolluted
LE410	0.05	77.8	0.37	7.18	Intermediate	35.32	35.31	Eutrophic
LE420	0.02	106	0.12	7.2	Unpolluted	35.14	35.13	Eutrophic
LE430	0.01	120	0.1	6.9	Unpolluted	37.84	37.84	Eutrophic
LE440	0.07	110.22	0.71	7.15	Intermediate	35.59	35.59	Eutrophic
LE450	0.01	114	0.07	8.7	Unpolluted	21.62	21.62	Hypereutrophic
LE540	0.02	125.5	0.04	3.8	Unpolluted	65.77	65.77	Moderate
LE500	0.04	102.5	4.12	1.55	Intermediate	86.04	86.04	Unpolluted
LE550	0.01	118	0.12	9.15	Unpolluted	17.57	17.57	Hypereutrophic
HBLIN*	0.01	78.94	0.17	2.36	Unpolluted	78.74	78.74	Moderate
LE380	0.01	105.25	0.16	2.95	Unpolluted	73.42	73.42	Moderate
LE620	0.01	101.25	0.07	1.76	Unpolluted	84.14	84.14	Unpolluted
LE610	0.01	101.25	0.16	2.36	Unpolluted	78.74	78.74	Moderate
RLD*	0.05	100.1	0.16	3.36	Unpolluted	69.73	69.73	Moderate
LE630	0.01	101.5	0.07	3.05	Unpolluted	72.52	72.52	Moderate
LE810	0	99.5	0.04	4.42	Unpolluted	60.18	60.18	Moderate
LE820	0.01	96	0.05	2.65	Unpolluted	76.13	76.13	Moderate
LE505	0.03	107	4.63	0.53	Intermediate	95.23	95.23	Unpolluted
LE510	0.03	97.5	1.69	8.98	Intermediate	19.10	19.10	Hypereutrophic
LE520	0.02	100.25	1.49	4.35	Intermediate	60.81	60.81	Moderate
LE530	0.02	106	0.64	3.15	Intermediate	71.62	71.62	Moderate
N = 37	***0.44***	***78-122***	***0.506***	***11.1 -22.2***		-		

**red indicates the indicator(s) of water quality have breached the guideline values.*

Table 9.S6 Models (ATSEBI and newly proposed ASTI) input (water quality indicators) for assessing trophic status in Dublin Bay, 2021 and model outputs.

Monitoring sites	Input (ATSEBI system, whereas only CHL used for ASTI)				Models output			
	MRP (µg/l)	DOX (% sat.)	DIN (mg/l)	CHL (µg/l)	ATSEBI system (Existing)	ASTI (Proposed method)		
					Trophic status	ASTI (Actual)	ASTI (Predicted)	Trophic status
DB010	0.01	89.50	1.54	4.00	Intermediate	63.96	63.96	Moderate
DB015	0.03	89.00	0.92	1.70	Intermediate	84.68	84.68	Unpolluted
DB020	0.02	89.25	1.23	2.85	Intermediate	74.32	74.32	Moderate
DB210	0.02	96.20	0.68	5.30	Intermediate	52.25	52.25	Moderate
DB120	0.02	94.90	0.36	10.92	Unpolluted	1.62	8.40	Hypereutrophic
DB300	0.05	104.50	1.09	4.10	Intermediate	63.06	63.06	Moderate
DB310	0.06	101.00	1.06	3.30	Intermediate	70.27	70.27	Moderate
DB320	0.13	91.38	1.01	19.17	Intermediate	0.00	0.00	Hypereutrophic
DB330	0.05	99.57	0.22	18.00	Unpolluted	0.00	0.00	Hypereutrophic
DB340	0.04	112.48	0.17	3.36	Unpolluted	69.74	69.74	Moderate
DB350	0.05	104.29	0.18	7.97	Unpolluted	28.20	28.20	Hypereutrophic
DB420	0.08	101.82	0.26	3.90	Unpolluted	64.86	64.86	Moderate
DB410	0.30	97.00	0.88	2.98	Intermediate	73.12	73.12	Moderate
DB220	0.01	100.38	0.19	5.34	Unpolluted	51.89	51.89	Moderate
DB510	0.04	104.33	0.05	1.24	Unpolluted	88.83	88.83	Unpolluted
DB560	0.01	104.83	0.04	1.73	Unpolluted	84.38	84.38	Unpolluted
DB730	0.02	99.00	0.19	0.74	Unpolluted	93.33	93.33	Unpolluted
DB610	0.01	98.00	0.16	0.62	Unpolluted	94.41	94.41	Unpolluted
DB570	0.00	103.67	0.02	0.80	Unpolluted	92.76	92.76	Unpolluted
DB540	0.00	105.00	0.02	1.80	Unpolluted	83.78	83.78	Unpolluted
DB450	0.04	105.40	0.26	1.88	Unpolluted	83.05	83.04	Unpolluted
DB550	0.01	105.17	0.08	0.80	Unpolluted	92.76	92.76	Unpolluted
DB580	0.00	106.00	0.06	1.36	Unpolluted	87.73	87.73	Unpolluted
DB740	0.01	99.00	0.19	0.92	Unpolluted	91.71	91.71	Unpolluted
N = 24	***0.46***	***77 - 123***	***0.569***	***11.1 – 22.2***		-		

**red indicates the indicator(s) of water quality have breached the guideline values.*

Table 9.S7 Models (ATSEBI and newly proposed ASTI) input (water quality indicators) for assessing trophic status in Galway Bay, 2021 and model outputs.

Monitoring sites	Input (ATSEBI system, whereas only CHL used for ASTI)				Models output			
	MRP (µg/l)	DOX (% sat.)	DIN (mg/l)	CHL (µg/l)	ATSEBI system (Existing)	ASTI (Proposed method)		
					Trophic status	ASTI (Actual)	ASTI (Predicted)	Trophic status
GY250	0.01	106.50	0.15	0.97	Unpolluted	91.64	91.26	Unpolluted
GY210	0.02	101.40	0.15	1.08	Unpolluted	90.69	90.27	Unpolluted
GY200	0.01	103.00	0.13	1.61	Unpolluted	86.12	85.50	Unpolluted
GY220	0.01	96.50	0.12	1.03	Unpolluted	91.12	90.72	Unpolluted
GY260	0.02	108.00	0.14	0.15	Unpolluted	98.71	96.61	Unpolluted
GY150	0.01	106.75	0.14	1.95	Unpolluted	83.19	82.43	Unpolluted
GY180	0.02	101.00	0.13	1.95	Unpolluted	83.19	82.43	Unpolluted
GY160	0.01	102.80	0.08	2.28	Unpolluted	80.31	79.42	Unpolluted
GY170	0.01	100.83	0.13	3.06	Unpolluted	73.62	72.43	Moderate
GY130	0.01	101.75	0.17	1.20	Unpolluted	89.66	89.19	Unpolluted
GY140	0.01	100.41	0.14	2.52	Unpolluted	78.28	77.30	Moderate
GY120	0.01	103.90	0.03	1.42	Unpolluted	87.76	87.21	Unpolluted
GY110	0.01	103.00	0.04	1.00	Unpolluted	91.38	90.99	Unpolluted
KA050	0.01	103.75	0.19	1.07	Unpolluted	90.78	90.36	Unpolluted
KA060	0.02	99.50	0.16	0.84	Unpolluted	92.76	92.43	Unpolluted
KA070	0.02	104.30	0.09	0.78	Unpolluted	93.28	92.97	Unpolluted
KA040	0.01	104.00	0.16	0.91	Unpolluted	92.16	91.80	Unpolluted
KA080	0.01	102.71	0.12	1.50	Unpolluted	87.07	86.49	Unpolluted
KA030	0.02	103.83	0.20	1.61	Unpolluted	86.12	85.50	Unpolluted
KA025	0.04	102.50	0.18	5.05	Unpolluted	56.47	54.50	Moderate
KA020	0.02	101.91	0.17	8.39	Unpolluted	27.67	24.41	Hypereutrophic
GY190	0.01	101.83	0.12	1.32	Unpolluted	88.62	88.11	Unpolluted
N = 22	***0.47***	***77-123***	***0.633***	***11.7-23.3***		-		

**red indicates the indicator(s) of water quality have breached the guideline values.*

Table 9.S8 Models (ATSEBI and newly proposed ASTI) input (water quality indicators) for assessing trophic status in Mulroy Bay, 2021 and model outputs.

Monitoring sites	Input (ATSEBI system, whereas only CHL used for ASTI)				Models output			
					ASTEB_IE	ASTI (Proposed method)		
	MRP (µg/l)	DOX (% sat.)	DIN (mg/l)	CHL (µg/l)	Trophic status	ASTI (Actual)	ASTI (Predicted)	Trophic status
MB140	0.00	103.25	0.05	0.46	Unpolluted	95.62	95.76	Unpolluted
MB130	0.00	106.50	0.02	0.64	Unpolluted	93.90	94.23	Unpolluted
MB120	0.00	109.50	0.02	0.71	Unpolluted	93.24	93.60	Unpolluted
MB110	0.00	110.50	0.02	0.61	Unpolluted	94.22	94.53	Unpolluted
MB100	0.00	111.50	0.02	0.68	Unpolluted	93.52	93.87	Unpolluted
MB090	0.00	113.00	0.02	0.82	Unpolluted	92.24	92.66	Unpolluted
MB080	0.00	113.75	0.02	0.63	Unpolluted	94.00	94.32	Unpolluted
MB070	0.00	113.50	0.02	0.40	Unpolluted	96.19	95.92	Unpolluted
MB060	0.00	112.50	0.02	1.10	Unpolluted	89.57	90.14	Unpolluted
MB050	0.00	105.00	0.02	0.98	Unpolluted	90.71	91.22	Unpolluted
MB040	0.00	112.50	0.02	0.53	Unpolluted	94.95	95.23	Unpolluted
MB030	0.01	109.50	0.01	0.92	Unpolluted	91.24	91.71	Unpolluted
MB020	0.08	105.00	0.02	0.65	Unpolluted	93.81	94.14	Unpolluted
MB010	0.01	113.50	0.02	0.72	Unpolluted	93.14	93.51	Unpolluted
N = 14	***0.42***	***79-121***	***0.378***	***10.6-21.1***		-		

**red indicates the indicator(s) of water quality have breached the guideline values.*

Appendix 10. FORTRAN programming codes for computing IEWQI scores

```
!===========================================================
! IRISH WATER QUALITY INDEX MODEL
! SHORT FORM IS "IEWQI" MODEL FOR MARINE WATERS
!=============================================================
! WRITTEN BY MD GALAL UDDIN,
! PhD. CANDIDATE, CIVIL ENGINEERING
! UNIVERSITY OF GALWAY, IRELAND
!====================================================
! SUPERVISED BY DR. AGNIESZKA I. OLBERT,
! DR. STEPHEN NASH AND DR. AZIZUR
!====================================================
! VERSION HISTORY
! FIRST VESRSION: 18 MAY 2020.
! SENCOND VERSION: 06 APRIL 2021
! THIRD VERSION: 07 SEPTEMBER 2022
! FOURTH VERSION: 10 DECEMBER 2022
!====================================================
! LIST OF ALL MAJOR VARIABLES IN IEWQI MODEL
!====================================================
! WATER QUALITY INDICATORS
!====================================================
!SAL    = SALINITY
!TEMP   = TEMEPERATURE
!PH     = WATER PH
!DOX    = DISSOLVED OXYGEN
!TON    = TOTAL ORGANIC NITROGEN
!DIN    = DISSOLVED INORGANIC NITROGEN
!MRP    = MOLYBDATE REACTIVE PHOSPHORUS
!BOD     = BIOLOGICAL OXYGEN DEMAND
!TRAN   = WATER TRANSPARENCY
!===================================================
!MODEL SUBINDEX PARAMETERS
!===================================================
!SISAL  = SUBINDEX OF SALINITY
!SITEMP = SUBINDEX OF TEMP
!SIPH   = SUBINDEX OF PH
!SIDIN  = SUBINDEX OF DIN
!SIDOX  = SUBINDEX OF DOX
!SITON  = SUBINDEX OF TON
!SIMRP  = SUBINDEX OF MRP
!SIBOD  = SUBINDEX OF BOD
!SITRAN = SUBINDEX OF TRAN
!=================================================
!MODEL WEIGHTING PARAMETERS
!=================================================
!WSAL   = WEIGHT OF SALINITY
!WTEMP= WEIGHT OF TEMPERATURE
!WPH    = WEIGHT OF WATERR PH
!WDOX   = WEIGHR OF DISSOLVED OXYGEN
!WTON   = WEIGHT OF TON
!WDIN   = WEIGHT OF DIN
!WMRP   = WEIGHT OF MRP
!WTON   = WEIGHT OF TON
!WBOD   = WEIGHT OF BOD
!============================================================
!OTHER ESSENTIAL ABBREVIATIONS
!DINUB = DISSOLVED OXYGEN UPPER BOUND
!MRPUB = MOLYBODATE REACTIVE PHOSPHATE UPPER BOUND
!DOXLB = DISSOLVED OXYGEN LOWER BOUND
!DOXUB = DISSOLVED OXYGEN UPPER BOUND
!================================================================
!WATER QUALITY PARAMETERS UNITS                                       !
!================================================================
!SALINITY               = PSU
!TEMPERATURE            = 0 CELCIUS
!PH                     = ---
!DISSOLVED OXYGEN       = % SATURATION
!TOTAL ORGANIC NITROGEN = MG/L
!AMMONICAL NITROGEN     = MG/L
!PHOSPHATE              = µG/L
!CHLOROPHILL            = µG/L
!NITRATE                = MG/L
!===================================================================
```

```
!MODULE FOR THE CALCULATION OF SALINITY MEDIAN VALUE                !
!===================================================================
MODULE DATAMED
IMPLICIT NONE
INTEGER, PRIVATE :: I,N,J,K,L
INTEGER, PARAMETER:: TN = 37  !TOTAL NUMBER OF CASES
REAL, DIMENSION(100) :: SAL   !SALINITY CONCENTRATION
REAL :: TEMPS,MEDIAN   !FOR SALINITY MEDIAN
!MAIN PROGRAM FOR ESTIMATING WQI SCORES
REAL:: BOD, SIBOD, BODUB,BODLB               !VARIABLES FOR BOD
REAL:: DIN, SIDIN, DINUB, DINLB              !VARIABLES FOR DIN
REAL:: MRP, SIMRP, MRPUB, MRPLB              !VARIABLES FOR MRP
REAL:: TEMP, SITEMP                  !VARIABLES FOR TEMP
REAL :: PH, SIPH, PHUB,PHLB, PHMU,PHML       !VARIABLES FOR PH
REAL:: DOX, SIDOX, DOXLB,DOXUB,DOXMB !VARIABLES FOR DOX
REAL :: TON,SITON,TONUB,TONLB         !VARIABLES FOR TON
REAL:: TRAN, SITRAN, TRANUB,TRANLB    !VARIABLES FOR TRAN
!MULTIPLICATION OF SUBINDEX AND WEIGHT VARIABLES
REAL:: MBOD, MDIN,MMRP,MTEMP,MPH,MDOX,MTON,MTRAN,WQM
!VARIABLES FOR INDICATORS WEIGHT
REAL:: WBOD, WDIN,WMRP,WTEMP,WPH,WDOX,WTON,WTRAN
CONTAINS
!======================================================!
!SUBROUTINE FOR CALCULATING SALINITY MEDIAN VALUE       !
!======================================================!
SUBROUTINE MEDIANVALUE
REAL :: TEMP,MEDIAN,EVEN
REAL, DIMENSION(:), ALLOCATABLE:: SAL
OPEN (21, FILE = 'SALMEDIAN.DAT', STATUS='UNKNOWN')
  READ(*,*)
  N     = TN !NUMBER OF SALINITY DATA OR MONITORING SITES
  ALLOCATE(SAL(N))
  OPEN (1, FILE = 'SALDATA.DAT', STATUS='OLD')
  READ(1,*)(SAL(I),I=1,N)
  CLOSE(1)
  WRITE(*,*) SAL
!DO LOOP FOR SORTING SALINITY DATA
  DO I=1,N-1
    DO J=1,N-1
      IF(SAL(J) > SAL(J+1)) THEN
      TEMP=SAL(J)
      SAL(J)=SAL(J+1)
      SAL(J+1)=TEMP
      END IF
    END DO
  END DO
  WRITE(*,*) SAL
 !FUNCTION FOR CLACULATING MEDIAN VALUE
IF ((N/2*2) /= N) THEN
      MEDIAN=SAL((N+1)/2)
    ELSE IF ((N/2*2) == N) THEN
      EVEN= (SAL(N/2)+SAL((N+2)/2))
      MEDIAN=EVEN/2
  END IF
  WRITE(21,10) NINT(MEDIAN)
  PRINT*, "MEDIAN SALINITY IS =", NINT(MEDIAN)
       10 FORMAT (10I6.2)
       CLOSE(1)
       CLOSE(21)
       RETURN
 END SUBROUTINE
!======================================================!
!SUBROUTINE FOR DETERMINING THE INDICATORS THRESHOLDS   !
!BASED ON THE SALINTY MEDIAN VALUE ACCORDING TO WFD AND !
!EPA,IRELAND GUIDELINES FOR TrC WATERBODIES            !
!======================================================!
SUBROUTINE THRESHOLDS
IMPLICIT NONE
REAL :: MEDIAN,DINLB,DINUB,MRPLB,MRPUB,DOXLB,DOXUB
OPEN (501, FILE = 'SALMEDIAN.DAT', STATUS='UNKNOWN')
OPEN(502, FILE ='DINUB.DAT', STATUS = 'UNKNOWN')
OPEN(503, FILE ='MRPUB.DAT', STATUS = 'UNKNOWN')
OPEN(504, FILE ='DOXULB.DAT', STATUS = 'UNKNOWN')
READ (501,*) MEDIAN
IF (MEDIAN .EQ. 0) THEN
          DINUB = 2.60
```

```
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
 WRITE(502,46) DINUB
 WRITE(503,46) MRPUB
 WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 1) THEN
        DINUB = 2.53
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
     ELSE IF (MEDIAN .EQ. 2) THEN
        DINUB = 2.46
        MRPUB = 0.060
        DOXLB = 70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
 ELSE IF (MEDIAN .EQ. 3) THEN
        DINUB = 2.39
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
 ELSE IF (MEDIAN .EQ. 4) THEN
        DINUB = 2.32
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
 ELSE IF (MEDIAN .EQ. 5) THEN
        DINUB = 2.25
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
 ELSE IF (MEDIAN .EQ. 6) THEN
        DINUB = 2.18
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
 ELSE IF (MEDIAN .EQ. 7) THEN
        DINUB = 2.11
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
 ELSE IF (MEDIAN .EQ. 8) THEN
        DINUB = 2.04
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
 ELSE IF (MEDIAN .EQ. 9) THEN
```

```
        DINUB = 1.97
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 10) THEN
        DINUB = 1.89
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB= 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 11) THEN
        DINUB = 1.82
        MRPUB = 0.060
        DOXLB = 70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 12) THEN
        DINUB = 1.75
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 13) THEN
        DINUB = 1.68
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 14) THEN
        DINUB = 1.61
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 15) THEN
        DINUB = 1.54
        MRPUB = 0.060
        DOXLB =70.00
        DOXUB = 130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 16) THEN
        DINUB = 1.47
        MRPUB = 0.060
        DOXLB= 70.00
        DOXUB =130.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 17) THEN
        DINUB = 1.40
        MRPUB = 0.060
        DOXLB = 70.00
        DOXUB = 130.00
```

```
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 18) THEN
        DINUB = 1.34
        MRPUB = 0.059
        DOXLB =71.00
        DOXUB = 129.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 19) THEN
        DINUB = 1.27
        MRPUB = 0.058
        DOXLB =71.00
        DOXUB = 129.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 20) THEN
        DINUB = 1.21
        MRPUB = 0.057
        DOXLB =72.00
        DOXUB = 128.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 21) THEN
        DINUB = 1.14
        MRPUB = 0.056
        DOXLB =72.00
        DOXUB = 128.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 22) THEN
        DINUB = 1.08
        MRPUB = 0.054
        DOXLB =73.00
        DOXUB = 127.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 23) THEN
        DINUB = 1.02
        MRPUB = 0.053
        DOXLB =73.00
        DOXUB = 127.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 24) THEN
        DINUB = 0.95
        MRPUB = 0.052
        DOXLB =74.00
        DOXUB = 126.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 25) THEN
        DINUB = 0.89
        MRPUB = 0.051
        DOXLB = 74.00
        DOXUB = 126.0
        WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
        WRITE(502,46) DINUB
        WRITE(503,46) MRPUB
        WRITE(504,46) DOXLB, DOXUB
```

```
ELSE IF (MEDIAN .EQ. 26) THEN
       DINUB = 0.83
       MRPUB = 0.050
       DOXLB = 75.00
       DOXUB = 125.0
       WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
       WRITE(502,46) DINUB
       WRITE(503,46) MRPUB
       WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 27) THEN
       DINUB = 0.76
       MRPUB = 0.049
       DOXLB =76.00
       DOXUB = 124.0
       WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
       WRITE(502,46) DINUB
       WRITE(503,46) MRPUB
       WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 28) THEN
       DINUB = 0.70
       MRPUB = 0.048
       DOXLB =76.00
       DOXUB = 124.0
       WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
       WRITE(502,46) DINUB
       WRITE(503,46) MRPUB
       WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 29) THEN
       DINUB = 0.63
       MRPUB = 0.047
       DOXLB =77.00
       DOXUB = 123.0
       WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
       WRITE(502,46) DINUB
       WRITE(503,46) MRPUB
       WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 30) THEN
       DINUB = 0.57
       MRPUB = 0.046
       DOXLB =77.00
       DOXUB = 123.0
       WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
       WRITE(502,46) DINUB
       WRITE(503,46) MRPUB
       WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 31) THEN
       DINUB = 0.51
       MRPUB = 0.044
       DOXLB =78.00
       DOXUB = 122.0
       WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
       WRITE(502,46) DINUB
       WRITE(503,46) MRPUB
       WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 32) THEN
       DINUB = 0.44
       MRPUB = 0.043
       DOXLB =78.00
       DOXUB = 122.0
       WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
       WRITE(502,46) DINUB
       WRITE(503,46) MRPUB
       WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 33) THEN
       DINUB = 0.38
       MRPUB = 0.042
       DOXLB =79.00
       DOXUB = 121.0
       WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
       WRITE(502,46) DINUB
       WRITE(503,46) MRPUB
       WRITE(504,46) DOXLB, DOXUB
ELSE IF (MEDIAN .EQ. 34) THEN
       DINUB = 0.31
       MRPUB = 0.041
       DOXLB =79.00
```

```
           DOXUB = 121.0
           WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
           WRITE(502,46) DINUB
           WRITE(503,46) MRPUB
           WRITE(504,46) DOXLB, DOXUB
   ELSE IF (MEDIAN .EQ. 35) THEN
           DINUB = 0.25
           MRPUB = 0.040
           DOXLB = 80.00
           DOXUB = 120.0
           WRITE (*,46) DINUB, MRPUB, DOXLB, DOXUB
           WRITE(502,46) DINUB
           WRITE(503,46) MRPUB
           WRITE(504,46) DOXLB, DOXUB
   ELSE
           DINUB = 0.0
           MRPUB = 0.0
           DOXLB = 0.0
           DOXUB = 0.0
  WRITE(502,46) DINUB
  WRITE(503,46) MRPUB
  WRITE(504,46) DOXLB, DOXUB
   46 FORMAT (F10.3)
  END IF
  CLOSE(501)
  CLOSE(502)
  CLOSE(503)
  CLOSE(504)
  RETURN
 END SUBROUTINE THRESHOLDS
!SUBROUTIN FOR CALCULATION SUBINDEX VALUES WRITTEN ACCORDING
!TO IEWQI MODEL. EQUTIONS ARE AVIABLE AT
!https://doi.org/10.1016/j.watres.2022.118532
!====================================================================
!SUBROUTINE FOR CALCULATING DISSOLVED OXYGEN SUB-INDEX
!====================================================================
SUBROUTINE DOXSI(SIDOX, DOXLB)
IMPLICIT NONE
REAL :: DOX, SIDOX, DOXLB, DOXUB,DOXMB
OPEN(125,FILE="DOXULB.DAT", STATUS ="OLD")
READ(125,33) DOXLB, DOXUB
PRINT*, "DOXLB IS=", DOXLB
PRINT*, "DOXUB IS=", DOXUB
         33 FORMAT (F10.2)
!READ STANDARD THRESHOLDS FOR DOX
               DOXLB = DOXLB
               DOXMB = 100.0
               DOXUB = DOXUB
OPEN(1, FILE="DOX.DAT", STATUS ="OLD")
OPEN(2, FILE="SIDOX.DAT", STATUS ="UNKNOWN")
   READ(*,*)
     DINUB = DINUB      !DIN UPPER BOUND
         MRPUB = MRPUB  !MRP UPPER BOUND
         DOXLB = DOXLB  !DOX LOWER BOUND
         DOXUB = DOXUB  !DOX UPPER BOUND
DO I = 1, TN
READ(1,10) DOX
10 FORMAT (F6.2)
IF ((DOX .GE. DOXLB) .AND. (DOX .LE. DOXMB))THEN
       SIDOX = ((DOX - DOXLB)/(DOXMB -DOXLB)*100)  !EQ(5)
       ELSE IF((DOX .GE. DOXMB) .AND. (DOX .LE. DOXUB))THEN
       SIDOX = (100-((DOX - DOXMB)/(DOXUB -DOXMB)*100)) !EQ(6)
       ELSE
       SIDOX = 0.0
       END IF
       WRITE(2,11) SIDOX
       11 FORMAT (F6.2)
       END DO
CLOSE(1)
CLOSE(2)
     RETURN
     END SUBROUTINE
!====================================================================
!SUBROUTINE FOR CALCULATING MRP SUB INDEX
!====================================================================
SUBROUTINE MRPSI(SIMRP, MRPUB)
```

```
IMPLICIT NONE
REAL :: MRP, SIMRP, MRPUB, MRPLB
OPEN(126,FILE="MRPUB.DAT", STATUS ="OLD")
READ(126,33) MRPUB
PRINT*, "MRPUB IS=", MRPUB
         33 FORMAT (F10.2)
!READ STANDARD THRESHOLDS FOR MRP
               MRPLB = 00.00  !MRP LOWER BOUND
               MRPUB = MRPUB  !MRP UPPER BOUND
OPEN(3, FILE="MRP.DAT", STATUS ="OLD")
OPEN(4, FILE="SIMRP.DAT", STATUS ="UNKNOWN")
DO I = 1,TN
READ(3,12) MRP
12 FORMAT (F6.2)
IF ((MRP .GE. MRPLB) .AND. (MRP .LE. MRPUB))THEN
       SIMRP = (100-(100*MRP)/(MRPUB -MRPLB))!EQ.(4)
       ELSE
       SIMRP = 0.0
       END IF
       WRITE(4,13) SIMRP
       13 FORMAT (F6.2)
       END DO
CLOSE(3)
CLOSE(4)
     RETURN
     END SUBROUTINE
!====================================================================
!SUBROUTINE FOR CALCULATING DIN SUB INDEX
!====================================================================
SUBROUTINE DINSI(SIDIN, DINUB)
IMPLICIT NONE
REAL :: DIN, SIDIN, DINUB, DINLB
OPEN(127,FILE="DINUB.DAT", STATUS ="OLD")
READ(127,33) DINUB
PRINT*, "DINUB IS=", DINUB
         33 FORMAT (F10.2)
!READ STANDARD THREHOLDS FOR DIN
               DINLB = 00.00  !DIN LOWER BOUND (THRESHOLD)
               DINUB = DINUB  !DIN UPPER BOUND (THRESHOLD)
OPEN(7, FILE="DIN.DAT", STATUS ="OLD")
OPEN(8, FILE="SIDIN.DAT", STATUS ="UNKNOWN")
DO I = 1,TN
READ(7,12) DIN
12 FORMAT (F6.2)
IF ((DIN .GE. DINLB) .AND. (DIN .LE. DINUB))THEN
       SIDIN = (100-(100*DIN)/(DINUB - DINLB)) !EQ.(4)
       ELSE
       SIDIN = 0.0
       END IF
       WRITE(8,13) SIDIN
       13 FORMAT (F6.2)
       END DO
CLOSE(7)
CLOSE(8)
     RETURN
     END SUBROUTINE
!====================================================================
! SUBROUTINE FOR CALCULATING TRAN SUB INDEX
!====================================================================
SUBROUTINE TRANSI(SITRAN, TRAN)
IMPLICIT NONE
REAL :: TRAN, SITRAN, TRANUB, TRANLB
               TRANUB = 1.00
               TRANLB = 0.00

OPEN(9, FILE="TRAN.DAT", STATUS ="OLD")
OPEN(10, FILE="SITRAN.DAT", STATUS ="UNKNOWN")
DO I = 1,TN
READ(9,12) TRAN
12 FORMAT (F6.2)
IF (TRAN .LT. TRANUB)THEN
       SITRAN = (TRAN - TRANLB)/(TRANUB - TRANLB)*100 ! !EQ.(4)
       ELSE IF (TRAN .GE. TRANUB) THEN
       SITRAN = 100.0
       END IF
       WRITE(10,13) SITRAN
```

```
        13 FORMAT (F6.2)
        END DO
CLOSE(9)
CLOSE(10)
     RETURN
     END SUBROUTINE
!===================================================================
!SUBROUTINE FOR CALCULATING BOD5 SUB INDEX
!=================================================================== SUBROUTINE
BODSI(SIBOD, BOD)
IMPLICIT NONE
REAL :: BOD, SIBOD,BODUB, BODLB
               BODUB = 7.00 !BOD UPPER BOUND(THRESHOLD)
               BODLB = 0.00 !BOD LOWER BOUND(THRESHOLD)
OPEN(11, FILE="BOD.DAT", STATUS ="OLD")
OPEN(12, FILE="SIBOD.DAT", STATUS ="UNKNOWN")
DO I = 1,TN
READ(11,12) BOD
12 FORMAT (F6.2)
        IF ((BOD.GE. BODLB) .AND. (BOD .LE. BODUB))THEN
        SIBOD = (100-(100*BOD)/(BODUB - BODLB))        !EQ (4)
        ELSE
        SIBOD = 0.0
        END IF
        WRITE(12,13) SIBOD
        13 FORMAT (F6.2)
        END DO
CLOSE(11)
CLOSE(12)
     RETURN
     END SUBROUTINE
!===================================================================
! SUBROUTINE FOR CALCULATING TON SUB-INDEX
!===================================================================
SUBROUTINE TONSI(SITON, TON)
IMPLICIT NONE
REAL :: TON,SITON,TONUB,TONLB
               TONUB = 2.00
               TONLB = 0.00
OPEN(15, FILE="TON.DAT", STATUS ="OLD")
OPEN(16, FILE="SITON.DAT", STATUS ="UNKNOWN")
DO I = 1,TN
READ(15,12) TON
12 FORMAT (F6.2)
        IF ((TON .GE. TONLB) .AND. (TON .LE. TONUB))THEN
        SITON = (100-(100*TON)/(TONUB - TONLB))       !EQ(4)
        ELSE
        SITON = 0.0
        END IF
        WRITE(16,13) SITON
        13 FORMAT (F6.2)
        END DO
CLOSE(15)
CLOSE(16)
     RETURN
     END SUBROUTINE
!===================================================================
! SUBROUTINE FOR CALCULATING PH SUB-INDEX                            !
!===================================================================
SUBROUTINE PHSI(SIPH, PH)
IMPLICIT NONE
REAL :: PH, SIPH, PHUB,PHLB, PHMU,PHML
               PHUB = 9.00
               PHML = 7.50    !PH MID LOWER
               PHMU = 8.50 !PH MID UPPER
               PHLB = 5.00
OPEN(17, FILE="PH.DAT", STATUS ="OLD")
OPEN(18, FILE="SIPH.DAT", STATUS ="UNKNOWN")
DO I = 1,TN
READ(17,12) PH
12 FORMAT (F6.2)
        IF ((PH .GE. PHML) .AND. (PH .LE. PHMU))THEN
        SIPH = 100.00
        ELSE IF ((PH .GE. PHLB).AND.(PH .LE.PHML))THEN
        SIPH = ((PH - PHLB)/(PHML -PHLB)*100)  !EQ (5)
        ELSE IF((PH .GE. PHMU) .AND. (PH .LE. PHUB))THEN
```

```
        SIPH = (100-((PH - PHMU)/(PHUB -PHMU)*100))  !EQ(6)
        ELSE
        SIPH = 0.00
        END IF
        WRITE(18,13) SIPH
        13 FORMAT (F6.2)
        END DO
CLOSE(17)
CLOSE(18)
     RETURN
     END SUBROUTINE
!=======================================================================
! SUBROUTINE FOR CALCULATING TEMP SUB-INDEX                            !
!==========================================================================
SUBROUTINE TEMPSI(SITEMP, TEMP)
IMPLICIT NONE
REAL :: TEMP, SITEMP
OPEN(19, FILE="TEMP.DAT", STATUS ="OLD")
OPEN(20, FILE="SITEMP.DAT", STATUS ="UNKNOWN")
DO I = 1,TN
READ(19,12) TEMP
12 FORMAT (F6.2)
        IF (TEMP .LE. 25) THEN
        SITEMP = 100.00
        ELSE
        SITEMP = 0.00
        END IF
        WRITE(20,13) SITEMP
        13 FORMAT (F6.2)
        END DO
CLOSE(19)
CLOSE(20)
     RETURN
     END SUBROUTINE
!===============================================================
!SUBROUTINE FOR MULTIPLICATING INDICATORS SUBINDEX AND WEIGHT   !
!===============================================================
SUBROUTINE MSIW(SIBOD,WBOD)
IMPLICIT NONE
!MULTIPLICATION OF SUBINDEX AND WEIGHT VARIABLES
REAL:: MBOD, MDIN,MMRP,MTEMP,MPH,MDOX,MTON,MTRAN
! PARAMETERS SUBINDEX VARIABLES
REAL:: SIBOD,SIDIN,SIMRP,SITEMP,SIPH,SIDOX,SITON,SITRAN
!PARAMETERS WEIGHT VARIABLES
REAL:: WBOD, WDIN,WMRP,WTEMP,WPH,WDOX,WTON,WTRAN

!READ PARAMETERS WEIGHT VALUES
READ (*,770)
                      WBOD   = 0.083
                      WDIN   = 0.194
                      WMRP   = 0.111
                      WTEMP  = 0.056
                      WPH    = 0.139
                      WDOX   = 0.028
                      WTON   = 0.222
                      WTRAN  = 0.167
770 FORMAT (F6.3)
!READ INDICATORS SUBINDEX VALUES
OPEN(91,FILE ='SIBOD.DAT',   STATUS = 'OLD')
OPEN(92, FILE='SIDIN.DAT', STATUS = 'OLD')
OPEN(93, FILE='SIMRP.DAT',   STATUS = 'OLD')
OPEN(94, FILE='SITEMP.DAT',  STATUS = 'OLD')
OPEN(95, FILE='SIPH.DAT',  STATUS = 'OLD')
OPEN(96, FILE='SIDOX.DAT',  STATUS = 'OLD')
OPEN(120, FILE='SITON.DAT',  STATUS = 'OLD')
OPEN(131,FILE ='SITRAN.DAT',  STATUS = 'OLD')
OPEN(122, FILE ='MBOD.DAT',   STATUS = 'UNKNOWN')
OPEN(123, FILE ='MDIN.DAT',  STATUS = 'UNKNOWN')
OPEN(124, FILE ='MMRP.DAT',    STATUS = 'UNKNOWN')
OPEN(125, FILE ='MTEMP.DAT',   STATUS = 'UNKNOWN')
OPEN(126, FILE ='MPH.DAT',    STATUS = 'UNKNOWN')
OPEN(127, FILE ='MDOX.DAT',   STATUS = 'UNKNOWN')
OPEN(128, FILE ='MTON.DAT',   STATUS = 'UNKNOWN')
OPEN(129, FILE ='MTRAN.DAT',    STATUS = 'UNKNOWN')
!DO LOOP FOR THE MULTIPLICATION OF SI-INDEX AND WEIGHT
DO  I = 1, TN
```

```
  READ(91,10) SIBOD
  READ(92,10) SIDIN
  READ(93,10) SIMRP
  READ(94,10) SITEMP
  READ(95,10) SIPH
  READ(96,10) SIDOX
  READ(120,10) SITON
  READ(131,10) SITRAN
  10 FORMAT (F6.2)
          MBOD  = (SIBOD**2)*WBOD
       MDIN = (SIDIN**2)*WDIN
       MMRP = (SIMRP**2)*WMRP
       MTEMP = (SITEMP**2)*WTEMP
       MPH = (SIPH**2)*WPH
       MDOX = (SIDOX**2)*WDOX
       MTON = (SITON**2)*WTON
          MTRAN = (SITRAN**2)*WTRAN
 WRITE (122,100) MBOD
 WRITE (123,100) MDIN
 WRITE (124,100) MMRP
 WRITE (125,100) MTEMP
 WRITE (126,100) MPH
 WRITE (127,100) MDOX
 WRITE (128,100) MTON
 WRITE (129,100) MTRAN
100 FORMAT (F12.2)
END DO
CLOSE(91)
CLOSE(92)
CLOSE(93)
CLOSE(94)
CLOSE(95)
CLOSE(96)
CLOSE(120)
CLOSE(121)
CLOSE(131)
CLOSE(132)
CLOSE(122)
CLOSE(123)
CLOSE(124)
CLOSE(125)
CLOSE(126)
CLOSE(127)
CLOSE(128)
CLOSE(129)
     RETURN
     END SUBROUTINE
!==========================================================
!SUBROUTINE FOR CALCULATING THE SUMSIWT SCORES                !
!==========================================================
SUBROUTINE WQMWQI(MBOD,MTRAN)
IMPLICIT NONE
REAL :: MBOD,MDIN,MMRP,MTEMP,MPH,MDOX,MTON,MTRAN,WQM
!READ MULTIPLY VALUES OF PARAMETERS SUBINDEX AND WEIGHT
OPEN (71, FILE = 'MBOD.DAT',   STATUS = 'OLD')
OPEN (72, FILE = 'MDIN.DAT',   STATUS = 'OLD')
OPEN (73, FILE = 'MMRP.DAT',   STATUS = 'OLD')
OPEN (74, FILE = 'MTEMP.DAT',  STATUS = 'OLD')
OPEN (75, FILE = 'MPH.DAT',    STATUS = 'OLD')
OPEN (76, FILE = 'MDOX.DAT',   STATUS = 'OLD')
OPEN (77, FILE = 'MTON.DAT',   STATUS = 'OLD')
OPEN (79, FILE = 'MTRAN.DAT',  STATUS = 'OLD')
OPEN(51,  FILE = 'WQM.DAT',    STATUS = 'UNKNOWN')
DO  I = 1, TN
        READ (71,35) MBOD
        READ (72,35) MDIN
        READ (73,35) MMRP
        READ (74,35) MTEMP
        READ (75,35) MPH
        READ (76,35) MDOX
        READ (77,35) MTON
        READ (79,35) MTRAN
        35 FORMAT (F12.2)
!CALCULATE SUM OF MULTIPL RESULTS OF SUBINDEX AND WEIGHT
!WEIGHTED QUARDATIC MEAN(WQM) AGGRIGATION FUNTION
   IEWQM = NINT(SQRT(MBOD+MDIN+MMRP+MTEMP+MPH+MDOX+MTON+MTRAN))
```

```
    WRITE (51,610) (IEWQM)
    610 FORMAT (F6.2)
   END DO
CLOSE(71)
CLOSE(72)
CLOSE(73)
CLOSE(74)
CLOSE(75)
CLOSE(76)
CLOSE(77)
CLOSE(78)
CLOSE(79)
CLOSE(51)
RETURN
END SUBROUTINE
END MODULE
!==================================================================!
!MAIN PROGRAM FOR COMPUTING IEWQI SCORES                           !
!==================================================================!
PROGRAM WQMWQIMODEL
!CALL MODULE PROGRAM
!USED MODULE DATAMED
USE DATAMED
!CALL SUBROUTINES
CALL MEDIANVALUE      !SUBROUTINE FOR COMPUTING SALINITY MEDIAN VALUE
CALL THRESHOLDS       !SUBROUTINE FOR IDENTIFYING THRESHOLDS VALUES
CALL BODSI(SIBOD, BOD) !CALL SUBROUTINE FOR CALCULATING BOD SUBINDEX
CALL DINSI(SIDIN, DINUB)!CALL SUBROUTINE DIN SUBINDEX CALCULATOR
CALL MRPSI(SIMRP, MRPUB)!CALL SUBROUTINE FOR CALCULATING MRP SUBINDEX
CALL TEMPSI(SITEMP, TEMP)!CALL SUBROUTINE FOR CALCULATING TEMP SUBINDEX
CALL PHSI(SIPH, PH)!CALL SUBROUTINE FOR CALCULATING PH SUBINDEX
CALL DOXSI(SIDOX, DOXLB) CALL SUBROUTINE FOR CALCULATING DOX SUBINDEX
CALL TONSI(SITON, TON) !CALL SUBROUTINE FOR CALCULATING TON SUBINDEX
CALL TRANSI(SITRAN,TRAN)!CALL SUBROUTINE FOR CALCULATING TRAN SUBINDEX
CALL MSIW(SIBOD,WBOD)  !CALL SUBROUTINE FOR THE SI AND WIGHT MULTIPLIER
CALL WQMWQI(MBOD,MTRAN)!CALL SUBROUTINE FOR COMPUTING IEWQI SCORE
END PROGRAM
!===========================END PROGRAM ============================!
```