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A novel machine learning application: Water quality resilience prediction model

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Abstract

Resilience-informed water quality management embraces the growing environmental challenges and provides greater accuracy by unpacking the systems' characteristics in response to failure conditions in order to identify more effective opportunities for intervention. Assessing the resilience of water quality requires complex analysis of influential parameters which can be challenging, time consuming and costly to compute. It may also require building detailed conceptual and/or physically process-based models that are difficult to build, calibrate and validate. This study utilises Artificial Neural Network (ANN) to develop a novel application to predict water quality resilience to simplify resilience evaluation. The Fuzzy Analytic Hierarchy Process method is used to rank water basins based on their level of resilience and to identify the ones that demand prompt restoration strategies. The commonly used 'magnitude * duration of being in failure state' quantification method has been used to formulate and evaluate resilience. A 17-years long water quality dataset from the 22 water basins in the State of São Paulo, Brazil, was used to train and test the ANN model. The overall agreement between the measured and simulated WQI resilience values is satisfactory and hence, can be used by planners and decision makers for improved water management. Moreover, comparative analyses show similarities and differences between the 'level of criticalities' reported in each zone by Environment Agency of the state of São Paulo (CETESB) and by the resilience model in this study.

Keywords: Artificial neural network, Analytic hierarchy process, Fuzzy logic, Triangular fuzzy number, Machine learning, Resilience, Water quality

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1 Introduction

Historically, environmental status of water resources in an area is assessed against pre-defined water quality (WQ) standards. For this purpose, spatial and temporal changes (e.g. monthly or annually) of WQ parameters (or WQ indexes) are collected and used to identify and assess WQ characteristics due to natural and man-made influences (Chounlamany et al., 2017) or for life cycle assessment of geomorphological dynamics (Tooth, 2018). In line with this, risk-based approaches are also commonly used to tackle the sparsity of WQ data and the limitations of statistical methods to reconstruct the time-series for WQ analysis (Maier et al., 2001; Hart et al., 2003; Mondal and Wasimi, 2007; Sarang et al., 2008; Asefa et al., 2014; Hoque et al., 2013, 2016). However, in practice, there are limitations to traditional WQ assessment methods and approaches used due to first, a high degree of uncertainty in emerging threats; second, time blindness of risk measures used; third, complexity of their consequences (Park et al., 2012; Sweetapple et al., 2018). Some latest studies have proposed resilience as a complementary measure to risk for a more robust decision-making in WQ management (Sweetapple et al., 2018). These studies focus on the promotion of key drivers, attributes and role players' adaptive capacities to cope with changing conditions rather than the use of control-based risk management (van Den Hoek et al., 2011; Hoque et al., 2012; Mallya et al., 2018). Conventional WQ management relies on the ability to project future change in order to design restoration strategies to well-known and defined problems (Pahl-Wostl et al. 2011). Therefore, the assessment methods used, tend to overlook the collective interaction of magnitude, frequency, and duration of failing periods as long as the overall performance (e.g., annual average) can fairly satisfy the desired standards. This approach can potentially become more difficult to maintain under highly variable future with numerous interconnected stressors leading to failure incidents (Zimmerman et al. 2008; Butler et al., 2016). Resilience-informed water quality management embraces the growing environmental challenges and provides greater accuracy by unpacking the systems' characteristics in response to failure conditions in order to identify more effective opportunities for intervention.

Drawing on the above discussion, resilience-informed WQ assessment requires WQ data and information that are generally expensive and time-consuming to collect, particularly for large-scale and complex catchments (Cumming, 2011; Rowny and Stewart, 2012; Zeng et al., 2013; Li et al., 2014). Building

surrogate models and/or methods proved to be effective methods in water quality (WQ) management to evaluate and demonstrate the relationship between different components in a system - particularly the effect of different interventions. Historically, Machine Learning (ML) techniques such as Artificial Neural Network (ANN) have been widely used for prediction and forecasting in water quality studies (Mitrović et al., 2019; Ahmed et al., 2019; Zhu and Heddam, 2020; Antanasijević et al., 2020), especially in WQ predictions (Palani et al., 2008; Singh et al., 2009; Khalil et al., 2011; Khan and See, 2016; Seo et al., 2016) and also in WQ indexes predictions (Gazzaz et al., 2015; Elshemy and Meon, 2017). In addition, there are many advantages of using ANNs for prediction purposes such as: eliminating the need for *a priori* knowledge of the underlying process and the existing complex relationships of the system elements (Kalin et al., 2010; Sarkar and Pandey, 2015). ANNs are often combined with other AI-based and/or evolutionary techniques to improve quality and accuracy of predictions in various applications for analysis and decision-making (Chau, 2006; Kuo et al., 2006; Zhang and Lai, 2011; Chen and Liu, 2015; Chen et al., 2015; Mahmoudi et al., 2016; Noori et al., 2020). Moreover, there are several studies based on multiple linear regression methods combined with AI methods to develop WQ models (Ji et al., 2017; Slaughter et al., 2017; Tomas et al., 2017; Wu et al., 2018; Antanasijević et al., 2020; Rajaei et al., 2020).

In recent years, advancement and innovations have been made in relation to resilience-informed disasters management (such as flood resilience) but very limited studies are available in the context of WQ management, partly due to non-acute and less visible impacts and consequences. To the date of this paper, WQ resilience has been quantified and analysed in a few studies using adaptive cycle algorithm (Li et al., 2016), functionality loss metrics and evolutionary algorithm-based optimisation (Zhang et al., 2020) and remained functionality metrics (Hoque et al., 2012; Sweetapple et al., 2018). These studies rely on case studies' data sets/archives and physical models to evaluate resilience and validate the results which are quite challenging. Having a resilience predictive model, in conjunction with the existing evaluation methods, can support WQ resilience management by reducing the reliance on physical data/model for evaluation and validation purposes and additionally, it can support future planning for resilience by making predictions. To date of this paper such model is yet to be studied and this is the gap that this study aims to tap in. Hence, the key novelty of this research embeds in development of a new model to predict WQI

resilience. It should be noted that this paper will not introduce any new machine learning method or algorithms, rather, it utilises the commonly used algorithms and methods in a new application (i.e., resilience-informed WQ assessment).

In general, three stages can be defined for resilience-informed WQ management at a catchment level: 1. modelling, assessing, evaluating resilience of the catchment; 2. prioritising the areas (e.g. (sub)-catchments) needing restorative intervention on the basis of their resilience level; and 3. determining the appropriate intervention to those most at risk. This paper focuses on the first stage and how it can inform prioritisation process in the second stage.

In this study, the resilience prediction model is set up for the case study of São Paulo city in Brazil to identify vulnerable contaminated areas (so-called critical zones or sub-catchments). Prediction of resilience (spatially/temporally) provides a tool for resilience planning by capturing the trend of resilience fluctuations (e.g., on an annual basis) in order to characterize, design and evaluate adaptation strategies. This predictive model can potentially assist key stakeholders and decision-makers in CETESB in their annual planning for environmental improvement.

In this paper, the study methodology is explained in Section 3 with the discussion of measuring water quality resilience and ANN structure. In this section, the Fuzzy Analytic Hierarchy Process (FAHP) conceptual model with the mathematical representation of that is also explained. In Section 4, we have discussed the procedure of identifying the critical zones based on the developed model. The results and associated discussions based on the outcomes have been described in Section 5. The study limitations have been also critically evaluated in this section. The conclusions with the future direction have been drawn in the last section.

2 Material and methods

The methodology section is twofold: the first part describes the development of WQ resilience evaluation framework (i.e. *stage 1* mentioned above); and the second part focuses on the integration of the ANN model as a surrogate for calculating WQ values (i.e. *stage 2* mentioned above).

The first stage (Section 2.4) explores the feasibility of integrating historical data and conventional machine learning techniques (ANNs) to develop a novel resilience predictive model for WQ without the need of costly physical models. In the second stage (Section 2.5), the widely studied Analytical Hierarchy Process (AHP) (Saaty, 1982; Saaty, 1977) is adopted for the prioritisation process adopting a fuzzy approach due to its simplicity and effectiveness in this kind of problem (Kahraman et al., 2004; Moktadir et al., 2017).

This predictive model can assist key stakeholders and decision-makers in two possible ways; first, in creating effective long-term actions to promote regional water resources resilience; second, in developing strategies that focus on desirable priorities such as environmental compliance, social equity or economic prosperity. The predictive model is particularly useful to overcome the challenges of costly and time-consuming manual data collection. In addition to being costly, manual data collection has its own challenges such as significant accessibility and safety issues particularly in the case study used. Also, data quality is critical in improving model accuracy and reducing uncertainty; and it can significantly be affected by the lack of automated monitoring systems. It should be noted that this is a feasibility study and not a comprehensive evaluation of the approach.

2.1 Case study

Surface water resources in the state of São Paulo (SP) in Brazil have been used as a case study in this research. SP is located southeast of Brazil with a state area of 248,000 km² and is the most populous state in Brazil (IBGE, 2014). It is divided into 22 Hydrographic Units of Water Resources Management (UGRHI) (Instituto Socioambiental, 2009) with three river basin districts and seven distinct climates. Surface water and groundwater resources together account for about 80% and 20% of water supply in SP, respectively. It has benefited from rapid economic and urban growth over recent decades which has come at the cost of compromising the quality of local water resources. This reduction in WQ has occurred for various reasons, mainly water management conflicts and the absence of clear long-term sustainable development plans for both urban areas and wastewater infrastructure. Environment Agency of the state of São Paulo (CETESB) operates 425 manual and 44 automatic freshwater quality monitoring stations (in total: 469 stations) and the number of collected WQ samples could vary from one season to

another in each station depending on climatic conditions. These data are used by CETESB for WQ management in the state of SP.

2.2 Water quality data

Decision makers in CETESB and the imposed environmental and social concerns of unsustainable developments in the state of SP have created the need for a great deal of information to be collected in response to public policies and the monitoring of their effects. To aid this data collection and analysis, CETESB has developed water quality indexes (WQI) that process increasing quantities of information, in a systematic and accessible way for decision makers. The main advantages of the indexes are the ease of communication with the lay public, the status greater than the isolated variables and the fact that it represents an average of several variables in a single number by combining different units of measure into a single unit (CETESB-Appendix C, 2017).

This study will focus on the impairment of surface WQ due to organic substances (mainly arisen from the lack of sufficient and efficient sewage collection and treatment systems) and in relation to aquatic life. Therefore, Table 1 in Supplementary Information (SI) outlines CETESB's three relevant WQIs (IQA, IET, and IVA) for decision-making on WQ policies and in line with the focus of this paper.

This study uses the average monthly values of CETESB's WQI (shown in Table 2 in SI) from 2000-2017 (in total 17 years of data) (CETESB, 2000-2017) to develop the predictive WQ resilience model, which provides a consistent and long-term data set ideal for ANN calibration and validation. As the data published by CETESB from 2010 onwards were more comprehensive, it was necessary to use data sets from latter years i.e. the first 16 years in this study, to develop a more accurate predictive model. The 2017 data set was then used for prediction validation purpose. The data used are publicly available in CETESB's annual reports and published after rigorous evaluations in terms of quality and accuracy. The data sets are of high quality, resolution, coverage and are used for policy and decision-making, on environmental matters in the region; therefore, no significant data pre-processing was needed (further details can be found in section 2 in SI). The water quality data used in this study are collected by CETESB from 469 automatic and manual monitoring stations across the State of São Paulo and WQIs are evaluated. These stations are spatially wide-spread, well-representing the whole study area. The quality of the monitoring stations is continuously

monitored and improved by CETESB. The data collected represent temporal changes in wet and dry seasons. The collection sites cover the surface water resources such as rivers, streams, lakes, branches, and places of transposition to reservoirs. WQI time series are used to calculate the annual resilience values that are used for ranking of the zones using a fuzzy algorithm which will be discussed in section 2.5 in the paper.

In addition to that, to evaluate resilience in terms of locally-defined acceptable levels of WQ, CETESB has introduced service thresholds and descriptive classification ranges for WQIs as shown in Table 2 in SI (CETESB, 2017). The greater IQA value indicates a better quality of surface water resources while this is opposite for IET and IVA (the lower, the better). These thresholds are used throughout the study for resilience evaluation. It should be noted that in this study the lower limits of the ‘average quality class’ in Table 2 in SI (i.e., 36 for IQA, 3.4 for IVA and 52 for IET), are used as the standard threshold (i.e. P_0 in Eq.(2) in SI) for each WQI. This is in line with CETESB’s approach to ‘average quality’ as an acceptable threshold.

2.3 Water quality resilience formulation

In this study, WQ resilience is defined as the capacity of a surface water resource system to cope with, and recover from contamination in order to maintain the required level of service and comply with predefined WQ standards to protect people and the environment.

It is important to make a distinction between the emerging concept of resilience and the commonly used assimilative capacity in WQ assessment. Traditionally, assimilative capacity utilises process-based modelling to build a relationship between WQ and quantity to assess whether a waterbody can meet pre-determined criteria for its ecological function and designated use. In other words, assimilative capacity tends to be reliability-driven (i.e. ‘Fail-Safe’ approach) aiming to avoid/prevent failures. On the other hand, resilience embraces assimilative capacity to improve its resistance capacity (one of the characteristics of resilience), but it also takes a ‘Safe-Fail’ approach in order to maximise its adaptation capacity to tackle emerging challenges (and their uncertainties) and to minimise adverse impacts (Butler et al., 2016). Further information about some potential differences between traditional environmental assessment method and resilience-based assessment methods have been provided in section 1 in the enclosed SI.

Several metrics/measures have been developed and introduced in literature to quantify resilience for different contexts in different water systems (Hashimoto et al., 1982; Fowler et al., 2003; Matrosov et al., 2012; Jung, 2013; Paton et al., 2014; Butler et al., 2016). This study inspired by the ‘volume-based resilience metrics’ method, introduced in the study by Roach et al. (2018), and formulated by Hasan et al. (2019) and McClymont et al. (2020), to encapsulate a suitable resilience-based performance metric for WQ evaluation. Details about formulation of WQR can be found in section 3 in SI. Additionally, details have been provided on data preparation and pre-processing in section 2 in SI.

2.4 Stage 1 - predictive water quality resilience model

As mentioned above, *Stage 1* focuses on development of the predictive WQ resilience model and its output can be the resilience value predicted in a zone (or a station in a zone) in the study area. The predictive WQ resilience model integrates the WQ resilience evaluation method (section 2.3) and the ANN. This model can be used to assess water resource adaptive capacity in order to identify the most vulnerable/critical contaminated UGRHIs (so-called zones in this paper) without the need for a great deal of costly data collection and time-consuming system modelling. Additionally, it can enable water and environment sectors to map the spatial and temporal dynamics of resilience fluctuations across the study area and time (Hasan et al., 2019), without direct characterisation of the influential factors (e.g., land use pattern, hydrological parameters, etc.). The proposed predictive model can be utilised to make predictions of future WQ resilience and therefore, enables proactive resilience planning. The key advantage of the predictive model is that it can be integrated into complex process-based models, for example as a surrogate to assess WQ resilience in ungauged catchments or for a fast resilience evaluation to enhance resilience-informed land-water system planning. It should be noted that resilience thresholds (how much resilience is needed, feasible, good enough, acceptable, low, high, etc.) have been recognised as playing a key role in resilience planning strategies and to the best of the authors’ knowledge, these thresholds are yet to be developed due to the complexity and challenges involved. The predictive model can assist and facilitate in the development of these resilience thresholds.

2.4.1 ANN structure

ANN and its algorithms have played a crucial role in predicting, modelling and classifying WQ parameters. The predictive model developed in this study is a multilayer perceptron neural network (MLPNN). This ANN model is formed in three layers: input layer that contains WQI values in a zone (IQA or IET or IVA), hidden layers and output layer having the dependent variable (i.e. the predicted resilience value associated with each WQI in a zone). It should be noted that, in this study, separated networks for each WQI have been produced (i.e. three separated networks). This reflects CETESB' approach to distinct remedial planning for surface water protection as defined in Table 1 in SI.

A log-sigmoid function widely used as a transform function to update weights and biases in the hidden layer and a linear transfer function for the output layer. All these layers contain a number of interconnected neurons (i.e., processing units). The optimal number of neurons in the hidden layer is proceeded by trial and error using the backpropagation (BP) algorithm and the mean square error (MSE). In this study, the best network training results were achieved with 11, 10 and 13 neurons in the hidden layer for IQA, IET and IVA datasets, respectively.

Fig.1a demonstrates the overall architecture of the predictive model in this study with WQI as the input neuron (IQA or IET or IVA) and its associated resilience value predicted, in output layer. Fig.1b demonstrates the network architecture in 'training phase'. In training phase, the input layer has 22 input neurons representing annual WQI (i.e., IQA or IET or IVA) in each of 22 UGRHIs (or zones) and their associated resilience values (using Eq. (3) in section 3 in SI). Hence, the total number of input neurons adds up to 44 for each WQI in this phase. Table 1 summarises the details of the network in training phase and also illustrates the number of epochs, gradient and Mu values for each input dataset in training phase and also illustrates the number of epochs, gradient and Mu values for each input dataset.

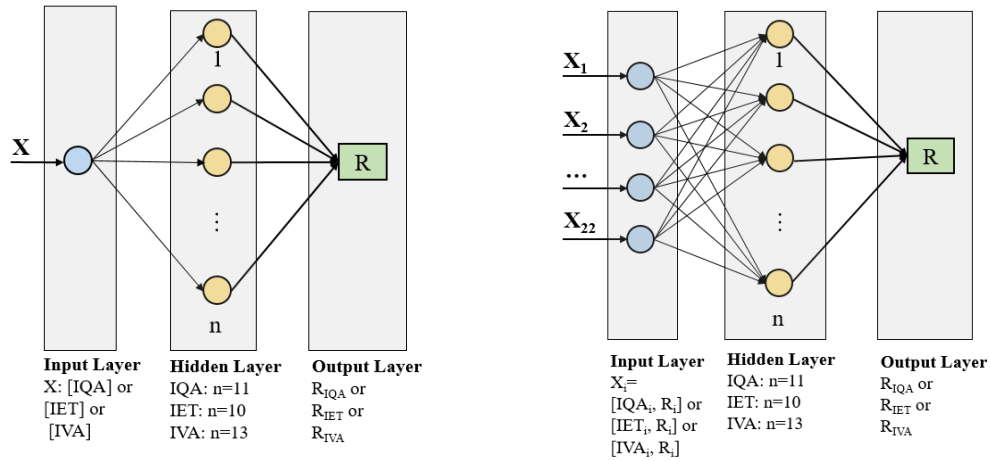


Fig. 1- ANN predictive model; a) Architecture of the predictive network and b) Predictive network architecture in the 'training phase'.

Table 1 - Structure of the predictive model in 'training phase' for each WQL.

Input datasets	Total number of input neurons	Hidden neurons	Transfer functions for Hidden layers	Output dataset	Total number of output neurons	Transfer function for output layer	Epochs	Gradient	Mu
[IQA, R _{IQA}]	44	11	Log-Sigmoid	R _{IQA}	1	Linear	60	9.6178	0.1
[IET, R _{IET}]	44	10		R _{IET}	1		22	0.1977	0.01
[IVA, R _{IVA}]	44	13		R _{IVA}	1		30	0.0025	0.0001

In this study, a feed-forward back propagation ANN (i.e., ANN trained using the Levenberg-Marquardt (LM) method), which has been widely used in developing predictive models for water systems (Sarkar and Pandey, 2015), is set to approximate WQ resilience. For this purpose, LM algorithm is used in the curve fitting process, Bayesian Regularization (BR) algorithm is used for nonlinear regression conversions during training process, and Scaled Conjugate Gradient (SCG) algorithm is used for batch learning method while computing the errors. These are commonly well-performed ANN algorithms in a wide range of applications (including WQ evaluations) (Xiang et al., 2006; Palani et al., 2008; Singh et al., 2009; Najah et al., 2013; Sarkar and Pandey, 2015; Seo et al., 2016).

The BR back propagation method is used for its accurate predictions in training (Alvisi and Franchini, 2011; Ha and Stenstrom, 2003; Malekmohammadi, et al., 2009). A batch mode of training is applied to enter the inputs to the network before the weights to be updated utilising SCG algorithm. The network training is finished when the specified number of epochs or training accuracy is achieved. The number of epochs represents the time needed for training of the network. If the training time is shorter, the network

architecture is more efficient. Similarly, the fewer number of weights indicate that the net will better generalize to validation, test, and new data with the same statistical attributes.

Given the ANN structure, each input dataset (Table 1) was randomly distributed into a 70% set for training, 15% set for validation and 15% set for testing, using the 469 WQ monitoring stations collected data across the 22 zones in São Paulo state.

It should be noted that authors are aware of further studies that could be conducted to identify the most suitable ANN algorithms and functions in a more systematic way. However, this is a feasibility study aiming to explore the possibility of developing a reliable model for resilience prediction in a water system application.

2.5 Stage 2 - predictive model application: to identify the critical zones

Stage 2 embraces CETESB's approach in prioritisation of zones most in need for interventions. This could be easily implemented by evaluating the resilience of each zone. However, due to the existing conflicting interactions among the three WQIs, identification and prioritisation of critical zones can be quite challenging. Hence, this study has developed a multi-criteria ranking method by integrating predicted resilience in each zone (i.e. the outcomes of the Stage 1) and Fuzzy Logic to overcome the abovementioned challenge. In line with this, FAHP method has been utilised in this study for its proven robustness and flexibility in resolving multi-criteria decision-making problems. It should be noted that, there are several approaches available in AHP methods such as weighted linear optimisation approach, ABC clustering approaches (Lolli et al., 2014) and triangular fuzzy number (TFN). In the context of this application and using TFN, there are several approaches that have been explored such as distance-based trapezoidal fuzzy number, graded mean integration representation and pairwise comparison matrix (Zhang and Ma, 2014). The step-by-step process is illustrated in Fig.6 in SI.

2.5.1 Step 1: set the geometric fuzzy

In this step, a fuzzy algorithm is used to measure the importance of each WQI for each monitoring station based on its overall resilience value (from Stage 1) over the time period of study. Fuzzy analysis has been used in this study because of its inherent ability and flexibility in solving multi-criteria decision-making

problems with embedded vagueness and uncertainties. Fuzzy linguistic labels are particularly great assets in the methodology to represent significant intensity in the context of resilience levels/thresholds.

TFN has been utilised in this study because of its proven simplicity and suitability to scale the ‘significance intensity’ (i.e. importance) of each WQI (in each station) based on its evaluated resilience value; and the multi-criteria system required (IET, IQA, IVA) to create the perception of different alternatives according to the criterion (wang et al., 2016). It should be noted that TFN is used in this study based on the pairwise comparison matrix. The TFN scales shown for each WQI in Table 2, have been widely used for group assessment and approximation (Dagdeviren and Yüksel, 2008; Wang et al., 2008). A set of membership functions have been defined and used by the triplet (l, m, n), as shown in section 4, Eq. (6) and Fig. 3 in SI, in relation to the required fuzzy algorithm.

In this study, l , m and n are the representatives for the upper, middle and lower values in a fuzzy AHP, adopted from TFN by Kahraman et al. (2004). A knowledge contrivance is created by utilising AHP (Saaty, 1977), which is a technique to solve multi-criteria-based complex systems. To facilitate the decision-making process in this study, linguistic variables (e.g. high quality, poor quality, etc.) (Zadeh, 1975) are created and scaled to categorise resilience as presented in Table 2 (high resilience, low resilience, etc).

Table 2 – ‘Significance intensity’ of WQI by AHP and TFN (Kahraman et al., 2004).

IQA Resilience			IVA/IET Resilience		
Significance intensity	FAHP Scale (λ)	TFN Scale (l, m, n)	Significance intensity	FAHP Scale (σ)	TFN Scale (l, m, n)
Very low resilience (very poor WQ)	1	(0.1,0.2,0.3)	Very high resilience (very high WQ)	6	(0.9, 1.0,1.0)
Low resilience (poor WQ)	2	(0.3,0.4,0.5)	High resilience (high WQ)	5	(0.8,0.9,1.0)
Average resilience (average WQ)	3	(0.5,0.6,0.7)	Good resilience (good WQ)	4	(0.7,0.8,0.9)
Good resilience (good WQ)	4	(0.7,0.8,0.9)	Average resilience (average WQ)	3	(0.4,0.5,0.6)
High resilience (high WQ)	5	(0.9,1.0,1.0)	Low resilience (poor WQ)	2	(0.0,0.1,0.2)
			Very low resilience (very poor WQ)	1	(0.0,0.1,0.2)

In this study, the ‘criticality’ (of the zones) is set using TFN and scaled between 0 (resilient) and 1 (critical).

2.5.2 Step 2: set the global index of monitoring stations

In this step, a fuzzy-based global index is developed to measure the overall importance of each zone. The global index will be used to identify the critical zones based on their overall resilience value. Eq.(1) calculates the aforementioned global index using FAHP and TFN scales shown in Table 3.

$$\delta_k^z = \lambda_j \times \sigma_j \quad (1)$$

where, δ_k^z denotes the fuzzy global index associated to a zone ($z=1,...,22$); λ and σ are the significance intensity of each monitoring station in a zone (Table 3); and k denotes the number of monitoring stations in a zone.

2.5.3 Step 3: set the fuzzy weight of each WQI

In this step, the weight of each WQI is determined by fuzzy mean using TFN scale (in Table 3), indicating the ‘significance intensity (importance)’ of that WQI, in its zone (as shown in Eq. (2)):

$$\underline{w}_z = \left[\frac{l_i}{\sum_{i=1}^k l_i}, \frac{m_i}{\sum_{i=1}^k m_i}, \frac{n_i}{\sum_{i=1}^k n_i} \right] \quad (2)$$

where, $\underline{w}$ denotes the fuzzy mean; l , m and n are the membership functions (as shown in Table 2); k represents the number of stations in a zone; and z represents the zone number. $\underline{w}_z$ is then used to evaluate the total weight of each WQI, across the 22 zones, by combining the entire upper and lower values and dividing them by the sum of the α -cut values as shown in Eq. (3).

$$W_{idx} = \left(\frac{\alpha(W_{z_{lower}})}{\sum_{i=1}^z \alpha_i}, \frac{\alpha(W_{z_{upper}})}{\sum_{i=1}^z \alpha_i} \right) \quad z = 1, \dots, 22 \quad (3)$$

where, W_{idx} denotes the fuzzy weight of each WQI; α denotes the cut values in the crisp values; z presents the number of zones; $\underline{w}_{z_{lower}}$ and $\underline{w}_{z_{upper}}$ are the upper and lower bounds of the α -cut values, respectively, using the weighting average method (Kim and Park, 1990; Klir and Yuan, 1995). It should be noted that the factors belonging to the IQA have five α -cut values and IET have IVA, six cut values.

2.5.4 Step 4: defuzzify the total weight of each WQI

In this step, W_{idx} is defuzzified using Eq.(4). This process interprets membership degrees into a specific decision.

$$W_{idx_T} = \left[\gamma \left(W_{idx(w_{z_{lower}})} \right) \times (1 - \gamma) \left(W_{idx(w_{z_{upper}})} \right) \right]; \gamma \in [0,1] \quad W_{id} = \left[\gamma \left(\frac{\alpha(w_{in})}{\sum_{i=1}^z \alpha_i} \right) \times (1 - \gamma) \left(\frac{\alpha(w_{il})}{\sum_{i=1}^z \alpha_i} \right) \right]; \gamma \in [0,1] \quad (4)$$

where, W_{idx_T} denotes the total weight of each WQI in a zone; γ represents optimism index (i.e. reflects risk-taking attitude of decision makers); z presents the number of zones.

2.5.5 Step 5: fine-tune the parameters

In this step, the ANN parameters are fine-tuned until the minimum errors are obtained. The root mean square error (RMSE) method is used to calculate the errors.

2.5.6 Step 6: identify and rank the critical zones

Generally, the critical zones are determined using δ_k and W_{idx_T} as shown in Eq. (3). To identify the most critical zones, initially all zones are ranked based on their W_{idx_T} (for each WQI). The higher W_{idx_T} values represent more criticality (lower resilience) and the lower ones represent less criticality (higher resilience).

The ranking process follows the ‘stack principle’ in a standard data structure for a given list. In other words, the ‘stack’ contains the most critical zones. For example, if the stack contains a lower W_{idx_T} for IQA (i.e. less critical) in one zone and a higher W_{idx_T} for IQA in the next one (i.e. more critical), then the stack pops that zone and pushes the new one. In this study, it includes the highest values for IET and IVA and the lowest values for IQA in a monitoring station (see Eq. (5)). Eq. (5) illustrates the critical monitoring stations based on the combined WQI importance. This study only considers a zone with more than two critical stations for each WQI. Drawing on these, each monitoring station can be expressed by Eq. (3):

$$CS_i^k = \text{Maximise: } \sum_{i=1}^n [(W_{idx_T}|IVA_z|, \sum_{i=1}^z \delta_i^k) \& (W_{idx_T}|IET_z|, \sum_{i=1}^z \delta_i^k)] + \text{Minimise: } (W_{idx_T}|IQA_z|, \sum_{i=1}^z \delta_i^k) \quad (5)$$

where, CS_i^k denotes the identified critical monitoring stations in each zone (based on combined WQI); n denotes the number of monitoring stations (it varies for each WQI); z and k present the number of zones and monitoring stations in that zone, respectively; δ denotes the global index value.

Drawing on Eq. (5), Eq. (6) is finally used to identify the most critical zones in the case study area using W_{idx_T} and CS_i^k .

$$Z = [CS_z]; \forall_{stations} W_{id} = \left[\gamma \left(\frac{\alpha(w_{in})}{\sum_{i=1}^z \alpha_i} \right) \times (1 - \gamma) \left(\frac{\alpha(w_{il})}{\sum_{i=1}^z \alpha_i} \right) \right]; \gamma \in [0,1] \quad (6)$$

where, Z denotes the critical zones across the case study area (i.e. 22 zones); CS_z is the number of critical stations in each zone.

3 Results and discussion

In this study, the network training stops as soon as any of the following conditions occur: (i) model performance in validation dataset decreases abruptly in successive iterations; (ii) the maximum number of epochs of 100 is reached.

Fig.2 depicts the overall performance of the neural network based on the training, validation and testing dataset for IQA and IET and IVA. In this figure, the best validation performance occurred at epoch 54, 16

and 24 for IQA, IET and IVA, respectively, showing Mean Squared Error (MSE) trend during the learning procedure. The decreasing trend of the validation set confirms that there is no over-fitting in the model.

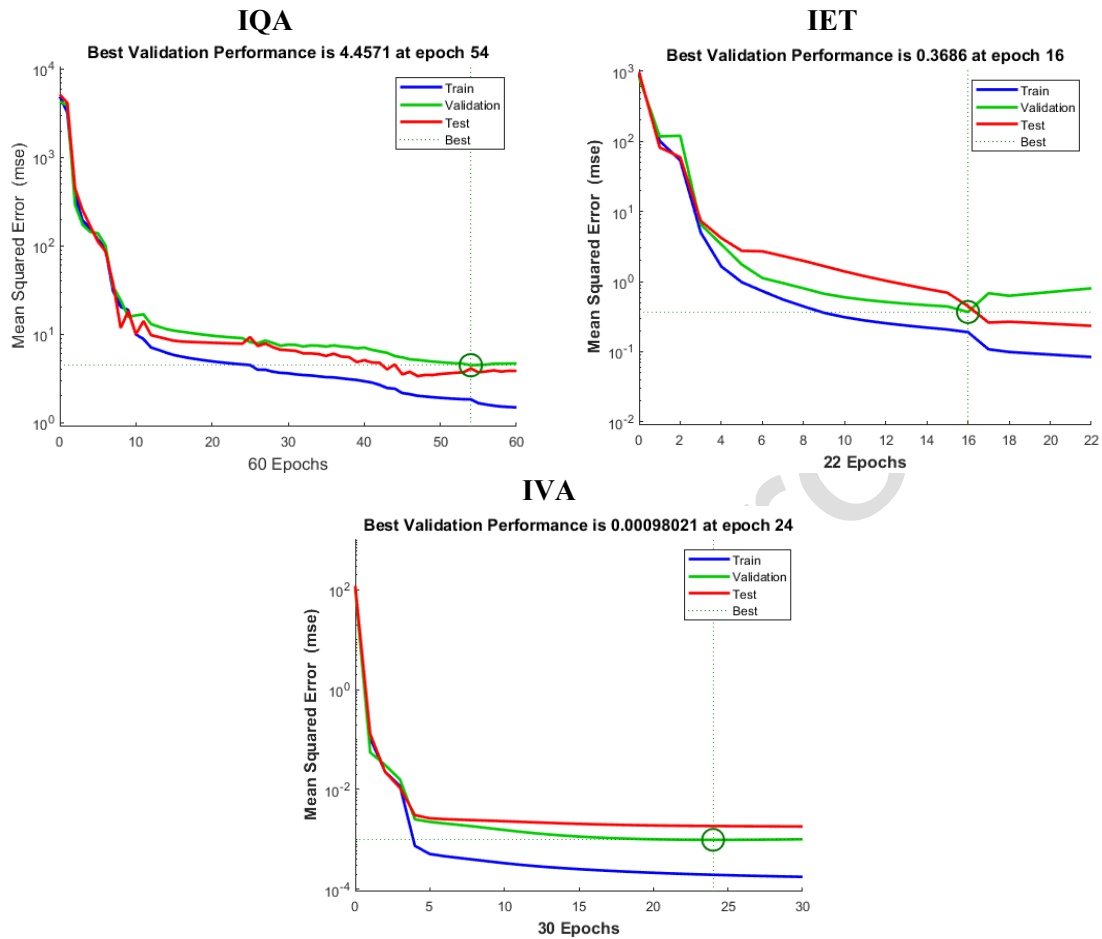


Fig. 2 - ANN performance.

Fig.3 demonstrates the scatter plots of the calculated WQI resilience values using Eq.(2) in SI and their corresponding ANN-based resilience prediction model. The observations demonstrate that there is a reasonable approximation by the ANN model across the spectrum of the evaluated WQI resilience values. Therefore, the overall agreement between the measured and simulated WQI resilience values (R values for IQA: 0.98814; IET: 0.99228; and IVA: 0.9999) are satisfactory. Similarly, a set of error histograms using student's T-test have been presented in Fig.4 in SI. Further details about the test can be found in the study by Hasan (2020).

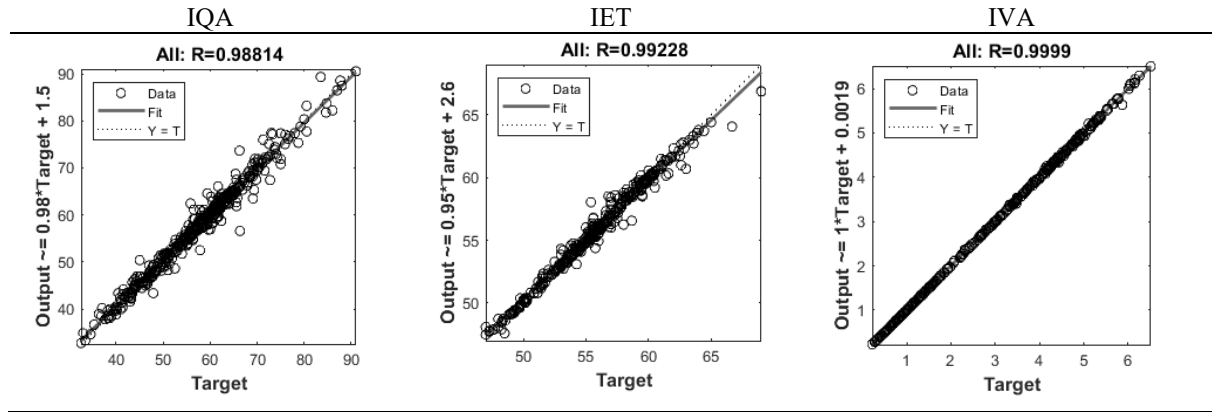


Fig. 3 - ANN model validation results.

Fig. 4 illustrates the *MSE* and *R* values of different algorithms for IQA, IET and IVA resilience predictions. It is noticeable in Fig. 4 that LM has performed better than BR and SCG for IQA and IET training. However, BR has performed significantly better with the testing dataset in the ANN model. Moreover, in all cases, SCG has shown the weakest performance. A possible reason is the poor convergence due to the adjustments of the weights and eigenvalues.

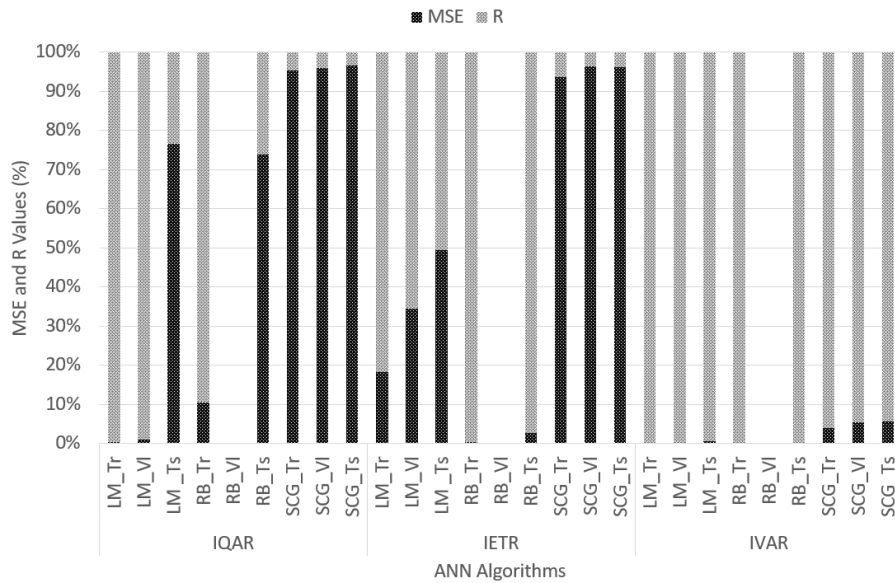


Fig. 4 - Performance evaluation of the utilised algorithms.

Table 3 shows the RMSE for the IQA, IET and IVA resilience, where it measures the differences between the resilience values predicted by the developed ANN-based resilience prediction model and the calculated WQI resilience values using Eq.(2) in SI. In other words, it shows the goodness-of-fit of generalization of the model. For the IET and IVA resilience, the BR performs significantly better compared to the LM and SCG in training, validation and testing purposes. Similarly, SCG performs poorest in all three WQIs. As a result, the SCG is not a suitable choice for predicting WQ resilience due to its poor accuracy in training,

validation and testing phases. In terms of accuracy, the BR is preferable than LM for IET and IVA resilience. However, the average RMSE is slightly better for LM in the dataset of IQA.

Table 3 - Average RMSE values of the applied algorithms.

Algorithm	RMSE for IQA	RMSE for IET	RMSE for IVA
LM	0.651	0.722	0.031
BR	0.670	0.076	0.011
SCG	4.635	3.479	0.227

Fig. 5 maps the identified critical (so-called vulnerable) zones utilising the predictive ANN-based resilience model and the FAHP method results for the case study area over the collective study period. The zones have been characterised descriptively by colour codes, varying from dark to light colours (most critical to least critical OR low resilience to high resilience). The observations illustrate that the Zones 5, 6, 7 and 9 have the lowest level of water resources resilience and therefore, in critical condition in São Paulo state. These zones are the most populated zones with rapid urban creeps and unsustainable developments leading to deteriorated WQ in the absence of sufficient and efficient wastewater collection and treatment infrastructures. However, prioritisation for intervention in critical Zones 5, 6, 7 and 9, where resources are limited, is required and according to the resilience-driven predictive model, Zone 5 has the most priority and Zone 7, the least.

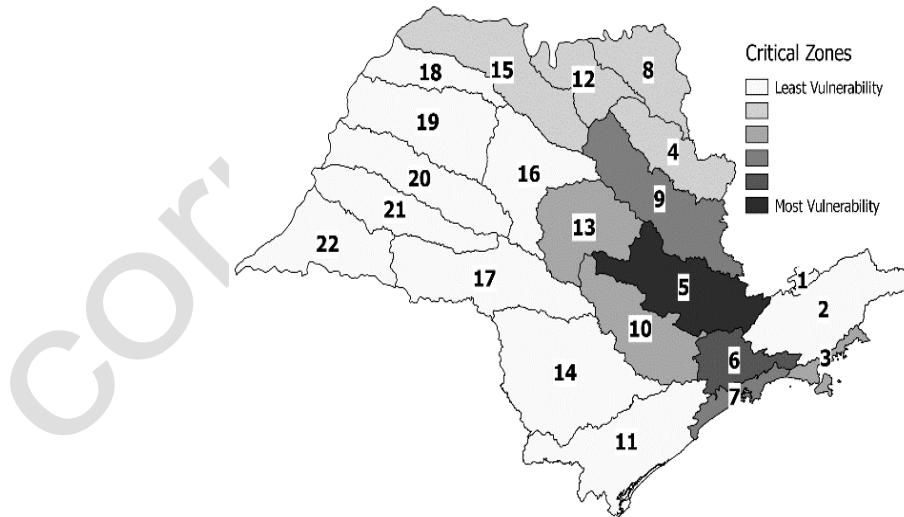


Fig. 5 –Mapped critical zones.

It is important to investigate the ranking of critical zones using the resilience-driven ranking method proposed in this study with CETESB's traditional approach in order to gain a better understanding of paradigm shift in WQ assessment. Details of these investigation can be found in section 6 and Fig. 5 in SI.

3.1 Limitations

This is a feasibility study to investigate the potential and suitability of using machine learning methods for resilience predictions in water engineering applications. Machine learning methods, and particularly artificial neural networks, have been commonly and successfully used in water systems management. On the other hand, resilience is a fast-growing concept proved to be an effective approach in preparing engineering systems to tackle and cope with emerging challenges. Authors believe that the integration of machine learning techniques to predict water quality resilience can provide an opportunity for more effective adoption of resilience to tackle the emerging challenges. This study is currently at its early stages and will be furthered in future studies. One potential improvement in horizon will be using more effective machine learning methods such as deep learning or deep reinforcement learning.

4 Conclusions

Planning water resources and related systems that are resilient in terms of delivering water of sufficient quality despite potential contamination that may occur in the catchment requires complex and integrated physical models that are challenging to build, characterize, and calibrate/validate. Moreover, these models rely on datasets that are costly and time consuming to collect. This study has focused on the application of a machine learning method (i.e. Artificial Neural Network), to develop a predictive model to evaluate resilience using readily available local data. This predictive model can support the key stakeholders and decision makers for targeted investments to improve resilience. The key advantage of the predictive model is that it can be integrated into complex process-based models to enhance resilience-informed land-water system planning. The predictive model can assist and facilitate in the development of the resilience thresholds.

This study has inspired by a ‘volume-based resilience metrics’ method for water quality resilience evaluation. It has also utilised a fuzzy-based algorithm to measure the criticality of water quality parameters with conflicting interactions. Additionally, the Fuzzy Analytical Hierarchy Process was used to develop a multi-criteria rating method to identify and rank the critical areas based on predicted resilience values.

The model was applied to and tested, using real data, for a case study in São Paulo state in Brazil. The results are satisfactory and demonstrate that the predictive model can make accurate predictions of

resilience. In this model, Bayesian Regularization algorithm offered better performance as compared to the Levenberg-Marquardt and Scaled Conjugate Gradient in making water quality resilience predictions and Scaled Conjugate Gradient showed the poorest performance. Additionally, the results indicated the low resilience identified in 45% of the 22 zones mainly located on the east and south east of the São Paulo state. These zones are the most populated zones with rapid unsustainable developments and climate change-induced risks leading to the deterioration of water resources quality in the absence of sufficient and efficient wastewater collection and treatment infrastructures.

The São Paulo state's environment agency (CETESB) publishes an annual report on the conditions of water resources quality across the whole region. There is a desire to incorporate 'resilience mapping' into this annual report for more effective resilience-informed planning. This can create an opportunity for adoption of the developed predictive model to assist decision makers' in CETESB in the future. Additionally, the integration of different machine learning techniques (e.g. deep reinforcement learning, recurrent neural network, convolutional neural network, etc.) with resilience-based methods could be further explored in order to create new techniques/methods for more effective adoption of 'resilience' in complex systems (e.g. integration of the resilience predictive model with physical models). Moreover, this study can potentially support reactive and planned maintenance for water supply. It also shows a direction for the researchers to implement the proposed model in various water reservoirs to measure water quality resilience, which may help to reduce the efforts of manual data collection. Therefore, the successful implementation of various machine learning algorithms in predicting water quality resilience is a new paradigm and can enrich the implementation of Artificial Intelligence and machine learning technologies to study the hydroinformatics and hydrodynamics arena. Furthermore, this model can be promoted and expanded by integration of real-time data monitoring systems for a more dynamic resilience prediction system.

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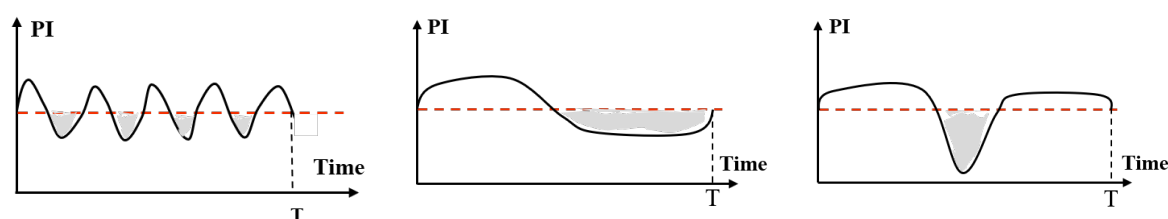
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Supplementary Information³

1. Traditional water assessment VS resilience-informed water assessment

In traditional assessment of WQ, commonly, annual (or monthly or even daily) average values are used to assess environmental status of the area against pre-defined environmental/ecological standards. This is the approach that CETESB takes in its reports to assess the WQ status of its UGRHs on an annual basis. This approach is simple, commonly used and can give reasonable assessment of the catchment environmental status. However, considering the growing challenges and their uncertainties, leading to water contamination incidents (e.g., more severe/frequent/prolonged), it is important to adopt an approach that can provide greater accuracy in terms of the system behaviour, the failure characteristics, and eventually the effective interventions needed. The traditional WQ assessment approaches tend to not be making a clear distinction between the characteristics of failing periods as long as the annual average can fairly satisfy the standards.

To further clarify this, Fig.1 in SI demonstrates three conceptual Figures (i.e., Fig.1a, Fig.1b and Fig.1c) that illustrate three different performance indicator (PI) time series of a given system with the same average values of PI in T (e.g., PI is the WQI in this study). From the conventional point of view, overall performance is acceptable as long as the annual average can meet the standard. However, having the resilience lens on, we need to unpack each time series and analyse its characteristics. The first time series (Fig.1a) represents small but quite frequent failures in the system indicating a system that fails easily but has good recoverability and resistance capacities in place, while the second one (Fig.1b) shows a system that does not fail frequently but clearly has low recoverability capacity in place although the failure is small; and the third one (Fig.1c) presents a system that fails rarely (e.g., once in T) and recovers quickly but the failure magnitude is considerable showing a low resistance capacity in the system. If these observations are put into the context of seven characteristics of resilience identified in 100ResilientCities (100RC, 2016), it is clear that the resilience-driven approach characterises the performance of a system much more precisely and hence, can lead to more appropriate and effective intervention strategies.



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(a)

(b)

(c)

Fig. 1 – Conceptual system performance curve, (a) small and frequent failures; (b) less frequent with prolonged and small failures; (c) less frequent with large, short failures

2. Data collection and pre-processing

This study uses the data collected by CETESB's from the WQ monitoring network across the region and are publicly available in CETESB's annual reports. These data sets are published after rigorous review and pre-processing works. Therefore, data sets are of high quality, resolution, coverage and accuracy, and no significant data pre-processing (as traditionally needed in raw data pre-processing) was needed in this study. However, some of the primary steps taken to prepare the data sets for the ANN model in this study, as follows:

- Gathering data from CETESB (e.g. raw data in pdf and then converted into csv and json formats by using Python and pandas library (Python Data Analysis Library, 2018);
- Cleaning data (e.g. to check the completeness and accuracy by using python and pandas library);
- Identifying missing data (e.g., using *dropna* and *fillna* functions in *pandas* library);
- Measuring data quality (e.g., validity, consistency, uniformity by manually random check as well as using *pydqc* (Chakki, 2018)).

3. Additional formulations on water quality resilience

In light of the discussion in section 2.3 in the manuscript, the resulting loss of system functionality (i.e., water contamination) is estimated using the concept of 'concentration severity' as Eq.(1) (see also Fig. 2):

$$Sev_i = \frac{WQ_{TF_i}}{WQ_{TC_i}} \quad (1)$$

where, i : index denoting WQ parameter analysed (1: IQA, 2: IVA, 3: IET); Sev_i : water contamination severity based on the 'magnitude $\times$ duration' concept for WQI i ; WQ_{TF_i} : cumulative breach of WQI i 's standard threshold (in Table 1 in the manuscript) as detailed in Eq.(2); WQ_{TC_i} : total WQI i 's standard threshold compliance over the study time period T ;

$$WQ_{TF_i} = \sum_{j=1}^n (WQ_{f_j} \times t_{f_j}) \quad (2)$$

where, i : index denoting WQ parameter analysed (1: IQA, 2: IVA, 3: IET); P_0 : WQ standard threshold (so-called performance threshold) as defined for each WQI in Table 1 in the manuscript and shown in Fig.2 here; j : index denoting each P_0 breach number in the study time period T for WQI i ; n : total number of P_0 breaches in the study time period T for WQI i ; WQ_{f_j} : magnitude of the WQI i in the j^{th} breach of P_0 in the study time period, i.e. magnitude of the water contamination; t_{f_j} : duration of the j^{th} breach of P_0 in the study time period T for WQI i , i.e. duration of time where WQI i has a value below or above the performance threshold P_0 (see Table 1 here).

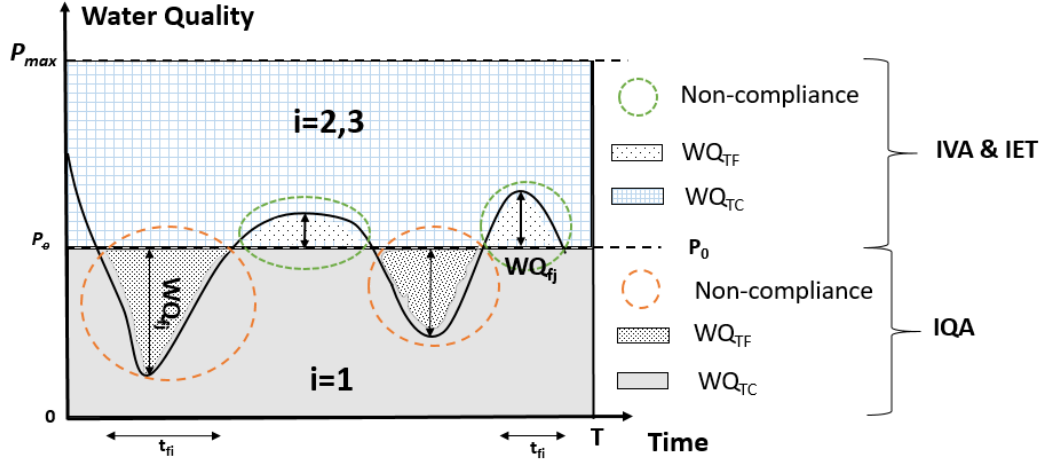


Fig. 2 - Schematic of the resilience evaluation curve

In this study, the ‘*remaining system functionality*’ (positive connotation of resilience) is used to quantify resilience (Fig. 2) and is calculated as Eq.(3):

$$R_i = 1 - Sev_i \quad (3)$$

where, R_i : resilience of a water resource system to water contamination; Sev_i : water contamination severity for WQI i ; i : index denoting water quality parameter analysed.

$$WQ_{fj} = P_0 - WQ_{jt} \quad (4)$$

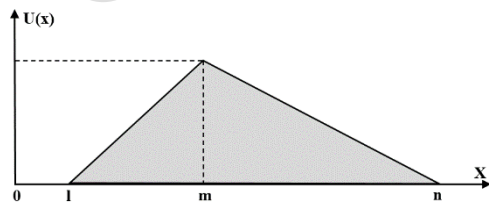
where, WQ_{fj} : magnitude of the WQI i in the j^{th} breach of P_0 in the study time period T ; P_0 : WQ standard threshold (so-called performance threshold) as defined for each WQI in Table 1 and shown in Fig.1 in the manuscript; WQ_{jt} : value of WQI, in time t in j^{th} breach of P_0 in the study time period T .

In this study, resilience is scaled between 0 and 1 using the most used scaling method of Min-Max (Eq.(5) -Hasan et al., 2019) for each WQI. It should be noted that the resilience normalisation is relative to the given time frame and also the maximum and minimum values of WQIs within that time frame.

$$R_i^n = (R_i - R_{min}) / (R_{max} - R_{min}) \quad (5)$$

where, R_i^n : the normalised resilience value; R_i is the actual resilience value; R_{min} and R_{max} : the minimum and maximum values for each WQI within the given time frame, respectively; i : index denoting water quality parameter analysed.

4. Triangular Fuzzy Number



$$U(x) = \begin{cases} (x - l) / (m - l), & l \leq x \leq m \\ (n - x) / (n - m), & m \leq x \leq n \\ 0, & \text{otherwise} \end{cases} \quad (6)$$

Fig. 3 - Distribution of triangular fuzzy number (Qiaoxiu, 2014)

where, l denotes the smallest likely value; m denotes the most probable value; and n denotes the largest possible value of any fuzzy event. In other words, m is the most probable value of the fuzzy number $U(x)$, l and n are the lower and upper bounds, respectively.

5. Error Histograms

Fig.4 shows target values and predicted values after training a feedforward neural network. The following diagrams indicate how predicted values are differing from the target values. Hence, the illustration reflects that the dataset fits well in the trained model. Further details about the test can be found in a study by Hasan (2020).

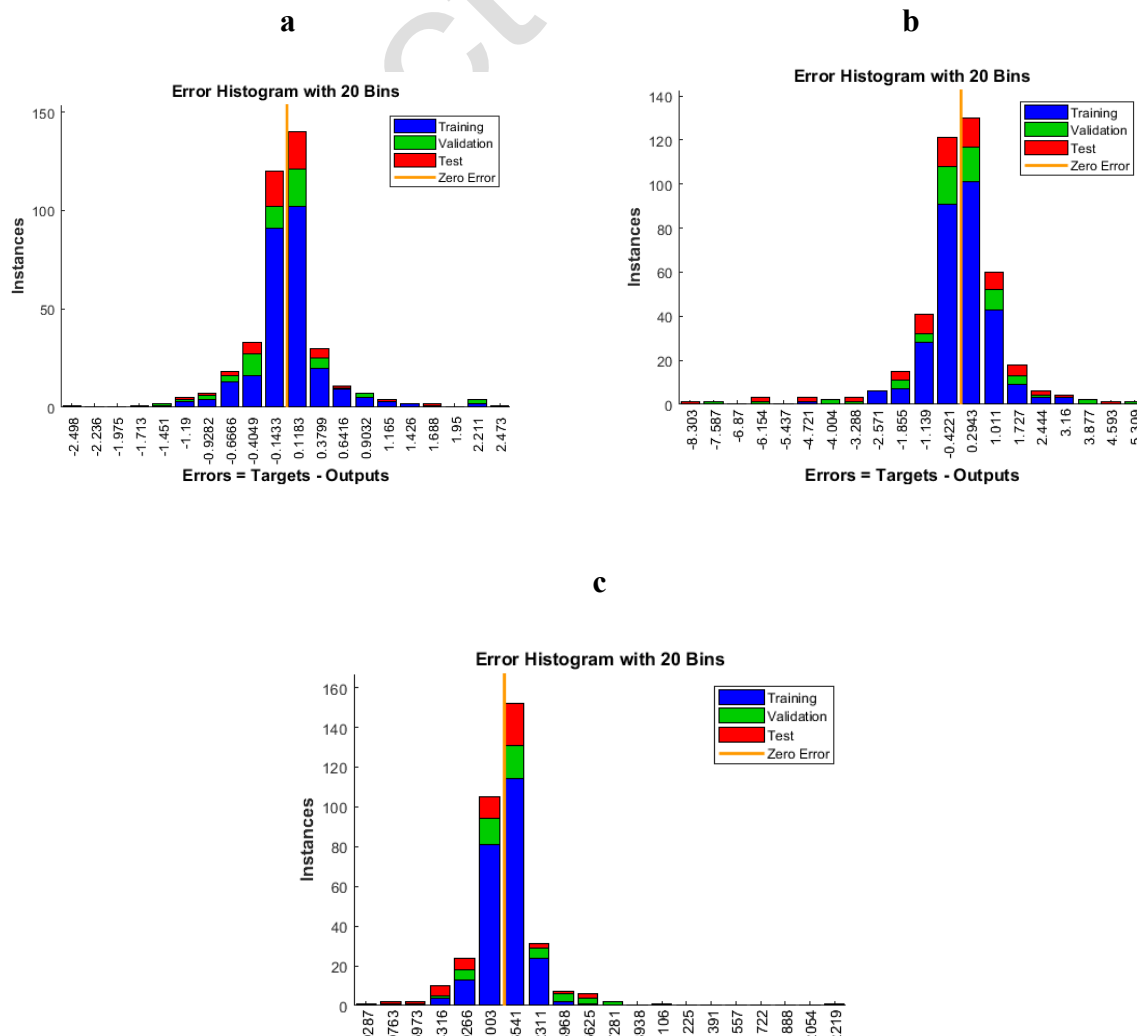


Fig.4 – Demonstration of the error histograms for (a) IET, (b) IQA and (c) IVA

6. Critical zones

Fig.5 demonstrates the collective percentage of WQ monitoring stations in poor and very poor conditions only (see Table 1 in the manuscript), in each zone reported in CETESB's 2017 annual report (CETESB, 2017). CETESB's 2017 data set is chosen as the benchmark year representing the latest condition of the surface WQ (at the time of this project) - that is used by CETESB to plan for interventions - to make cross-comparisons between the rankings of critical zones demonstrated in Fig.6 in the manuscript with CETESB's observations in Fig. 5 here. Overall, these comparative analyses aim to validate the suitability of the method proposed for resilience prediction purposes.

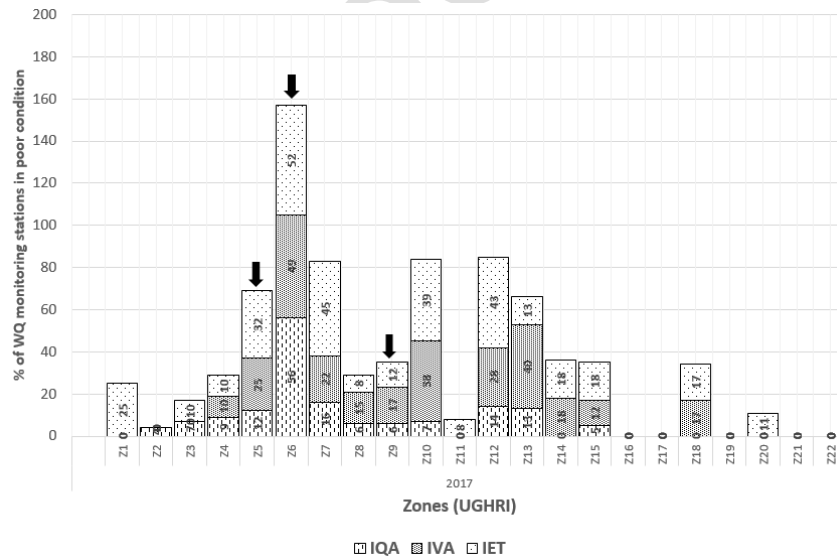


Fig.5 – Percentage of CETESB's WQ monitoring stations (categorised for each WQI), in poor and very poor conditions (see Table 1 in the manuscript) in 22 Zones in 2017

CETESB has reported the poorest IVA condition (based on the max number of stations in critical conditions) in the Zones 6, 10 and 13 which implies a low resilience level leading to aquatic habitat degradation. Also, IET has been reported very high in Zones 5, 6, 7, 10 and 12 indicating high levels of eutrophication mainly due to the trophic climate with high population density adversely affecting surface

water resources in these zones. IQA, overall, has demonstrated a better condition in comparison to IVA and IET but Zones 5 and 6, were still classified in poor condition.

Drawing on the above observations, overall, the critical zones identified by the resilience-driven predictive model shows similarities with CETESB's results in the annual report. This can give a level of confidence that the model is capable of making reasonable predictions of resilience that relates with CETESB's field observations. However, comparisons also show differences between the 'level of criticalities' reported in each zone by CETESB and in this study. This potentially can lead to different zonal prioritisation for interventions. For example, Zone 6 in Fig.5 can be flagged up by CETESB as the most critical zone due to its very high percentage of stations in poor and/or very poor conditions (the conventional approach), while, the resilience model identifies Zone 5 as the least resilient zone. This can be arisen from the fact that adaptive capacities of the system over time (e.g. seasonal self-purification capacity), embraced by resilience approach, is overlooked if decisions are only made based on CETESB's collected data. Another example would be Zone 9 that although its gains a lower priority according to CETESB's observations in comparison to other critical zones but it is the third most critical zone according to the resilience model results. This happened due to prolonged periods of being in poor condition (although in small number of stations) leading to exacerbation of WQ resilience in this zone.

These observations further demonstrate the importance of resilience approach in water management by which the behaviour of the system is studied over time and in a holistic way. Failure in the incorporation of this approach can potentially lead to overestimation and/or underestimation of critical zones. So, the predictive model developed in this study can be characterised as one of the new tools enabling resilience-informed water management and assisting decision-makers with more effectiveness intervention planning.

Tables & Figures

Table 1 - CETESB's WQI (CETESB- Appendix C, 2017)

WQI	Description
IQA	- IQA indicates the introduction of sanitary effluents and domestic sewage into the water body, providing an overview of the quality of surface water. - Variables: Temperature, pH, Dissolved Oxygen (DO), Biochemical Oxygen Demand (BOD), E-Coli, Nitrogen (N), Phosphorus (P), Total Suspended Solid (TSS).
IVA	- IVA is used to assess the quality of water for the protection of aquatic life. - Variables: DO, pH, Toxicity, toxic substances and degree of trophia.
IET	- IET evaluates WQ for nutrient enrichment and its effect related to the growth of Algae. - Variables: Chlorophyll, P.

Table 2 - CETESB's WQI classification and service thresholds (CETESB, 2017)

WQI	Class				
	High quality	Good quality	Average quality	Poor quality	Very poor quality
IQA	$79 < IQA \leq 100$	$51 < IQA \leq 79$	$36 < IQA \leq 51$	$19 < IQA \leq 36$	$IQA \leq 19$
IVA	$IVA \leq 2.5$	$2.6 < IVA \leq 3.3$	$3.4 < IVA \leq 4.5$	$4.6 < IVA \leq 6.7$	$6.8 \leq IVA$
IET	$IET \leq 47$	$47 < IET \leq 52$	$52 < IET \leq 59$	$59 < IET \leq 63$	$63 < IET \leq 67$

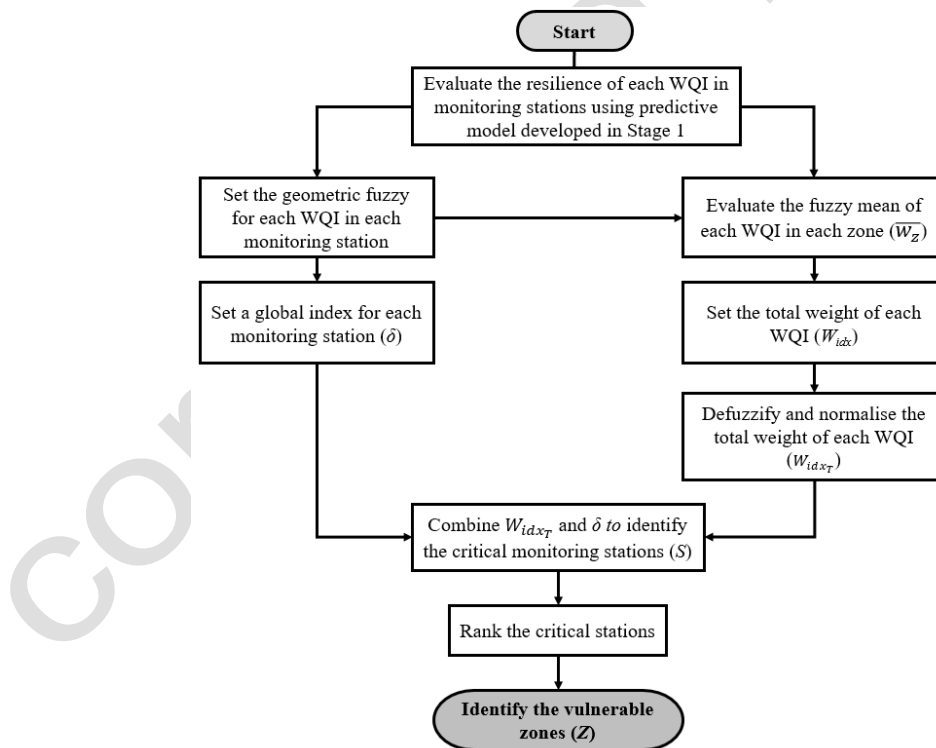


Fig.6 - Flowchart of the predictive model development

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