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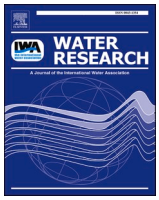

Application of machine learning in groundwater quality modeling - A comprehensive review

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ABSTRACT

Groundwater is a crucial resource across agricultural, civil, and industrial sectors. The prediction of groundwater pollution due to various chemical components is vital for planning, policymaking, and management of groundwater resources. In the last two decades, the application of machine learning (ML) techniques for groundwater quality (GWQ) modeling has grown exponentially. This review assesses all supervised, semi-supervised, unsupervised, and ensemble ML models implemented to predict any groundwater quality parameter, making this the most extensive modern review on this topic.

Neural networks are the most used ML model in GWQ modeling. Their usage has declined in recent years, giving rise to more accurate or advanced techniques such as deep learning or unsupervised algorithms. Iran and the United States lead the world in areas modeled, with a wealth of historical data available. Nitrate has been modeled most exhaustively, targeted by nearly half of all studies. Advancements in future work will be made with further implementation of deep learning and explainable artificial intelligence or other cutting-edge techniques, application of these techniques for sparsely studied variables, the modeling of new or unique study areas, and the implementation of ML techniques for groundwater quality management.

1. Introduction

Groundwater is a rapidly decaying vital resource. Groundwater quality (GWQ) is a rising issue worldwide due to extensive agricultural and industrial activities, and proper management is essential as groundwater provides almost half of all drinking water globally (Water et al., 2016). However, groundwater quality is influenced by a variety of environmental and anthropological factors (Alagha et al., 2014; Liu et al., 2005). Understanding these factors is an important step in developing appropriate management strategies.

Machine learning (ML) is an effective tool for extracting predictive models from data. A subset of artificial intelligence, ML models use inductive hypothesis to analyze and "learn the rules" from data without relying on a determined system of equations. They show great potential in discovering intrinsic patterns from data and making accurate predictions of water quality parameters in freshwater resources, both surface and groundwater. ML techniques are capable of learning features with high dimensionality and nonlinear relationships. With the help of modern computational hardware and architecture (Gupta, 2021; Sze et al., 2017; Zhao et al., 2017) optimized for machine learning algorithms (MLAs), especially for deep learning (Emmert-Streib et al., 2020; LeCun et al., 2015; Shrestha and Mahmood, 2019), data-centric ML methods started to emerge in recent years with a remarkable leap forward in performance. Key parameters extensively collected from groundwater, such as pH, nitrate concentration, etc., can be used to train ML models. Groundwater quality can be predicted or analyzed by inferring the various stages of the trained model.

Although ML has been applied to predict groundwater quality in many studies, there is no modern comprehensive literature review on ML techniques for GWQ modeling. A parallel study exists, a comprehensive survey of artificial intelligence (AI) techniques for surface water quality modeling (Tiyasha et al., 2020b). Some recent reviews for groundwater quality only survey techniques for specific parameters (Che Nordin et al., 2021; Haghbin et al., 2021), or focus on specific models (Kumari et al., 2016; Shen, 2018). Others, while covering a wide range of models and parameter prediction, lack the comprehensiveness owed to the subject (Haghbin et al., 2021; Malakar et al., 2021; Mosaffa et al., 2022).

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In this work, we provide a comprehensive review of ML in GW quality modeling, covering various contaminants for prediction and a broad range of algorithms. The first section is a meta-analysis of the literature, covering topics such as study focus, model inputs, publications years and study areas, and distribution of models. The second part of the paper is a bibliographic review of the literature by ML model category type. As shown in Fig. 1, the model categories were organized by learning type: supervised, semi-supervised, unsupervised, and ensemble. Supervised learning was divided into eight categories: ANN, fuzzy, SVM, decision tree and random forest, linear regression, comparative, deep learning, and optimization techniques. Optimization techniques were further divided into bagging and boosting, genetic algorithms, and wavelet transform. Unsupervised learning was divided into three categories: self-organizing map (SOM), multiple frameworks (MF), and clustering.

Studies were placed into these categories based on the primary algorithm studied. The bibliographic review consists of 1) a theoretical overview of the basic model structure, 2) a brief review of the application of the model in GW quality modeling by topic, and 3) an assessment of the model based on factors such as accuracy, applicability, ease, range of use. These model assessment sections are intended to compare results and summarize the large body of work in each model category. Conflicting case studies are highlighted intentionally as part of this effort. The last section of the paper highlights the results of the general analysis and the bibliographic review and outlines future directions and opportunities for researchers.

1.1. Introduction to the machine learning process and techniques

The training of machine learning models is a process of finding an optimal parameter set of the predictive model through closed-form solutions or iterative updating of its parameters through optimization. Many techniques have been proposed to improve the performance and accuracy of machine learning models.

The input of the machine learning model should be carefully selected for reducing the computational complexity of the machine learning model and improving its predictive performance. Dimensionality reduction techniques can effectively reduce the input features to mitigate the sparsity of the high-dimensional data for better similarity measurement. Feature learning is also beneficial to extracting effective features as the input of the machine learning model for specific tasks.

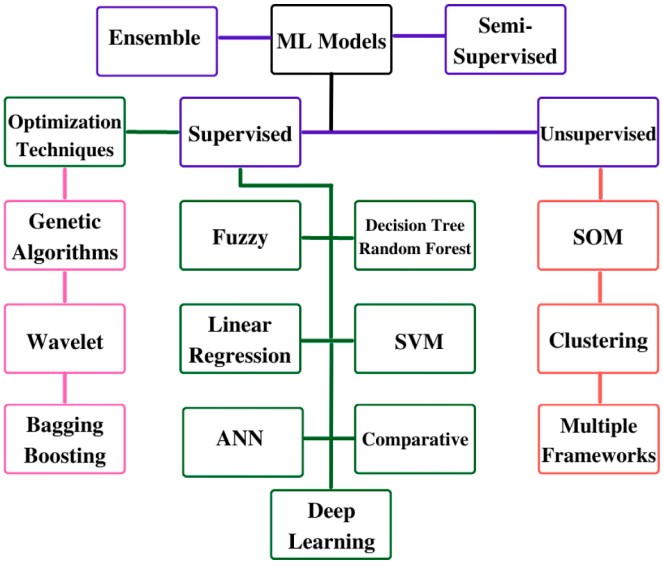

Fig. 1. This study's organization of ML models used for groundwater quality modeling. Learning types are divided into Supervised, Unsupervised, Semi-Supervised, and Ensemble, with the model categories listed under their respective learning type.

Cross-validation, dividing the dataset as a training dataset and a validation dataset, helps to improve the generalization of the predictive model by avoiding overfitting. Data augmentation can be used to increase the amount of training datasets when the size of the collected dataset is small.

Various optimization methods provide ways of finding the optimal model parameters by reaching a global minima of the loss function. Gradient descent is the most popular optimization method for differentiable loss functions. Adaptive learning rate methods help gradient descent find the optimal parameters effectively and efficiently.

2. General analysis of trends

2.1. Study focus (or model prediction)

Fig. 2 displays the study focuses for articles on ML in groundwater quality from 1994 to 2022 based on our literature review from.

Nitrate contamination was the most popular study focus, with 87 articles focusing on this subject. Many of these articles repetitively addressed the same problem; that is, if a certain ML model is viable for nitrate contaminant prediction (See Section 3.1.1.2). Nitrate is a well-monitored compound and has been for decades, especially in the countries with a prevailing focus on this topic, leading to a wealth of data for testing ML models.

Water Quality Index (WQI) is the second-most studied focus, where the authors aim to improve the classification of water quality in a study area. Fuzzy methods are popular for this purpose due to their ability to deal with uncertainties (Vadiati et al., 2016). A variety of other hydrochemical compounds have been studied, such as electrical conductivity (EC), total dissolved hardness (TDH), etc. These parameters are more common as inputs for ML models in many studies, as discussed below in Section 2.2.

2.2. Input parameters and timescales

In total, there were over 300 unique input parameter types used among all studies. Only 26 of these parameters were used by 16 or more studies, as shown in Fig. 3a. The most used parameter was pH, with 70 studies (35%) including it in their input database. Other chemical water properties commonly used were EC and TDS. All DRASTIC parameters were also used by more than 15 studies (See Supplementary Material for DRASTIC model explanation).

Fig. 3b presents an analysis of the number of input parameters of all studies using ML for groundwater quality and provides a useful insight into algorithm optimization. Often, a goal of these studies is to provide an estimation of water quality using easily obtained data while still providing reasonable accuracy (Shekofteh et al., 2012). Many authors have decided 4–6 parameters meets these criteria (26% of all studies used input parameters in this range), as often only a few parameters significantly contribute to a model's performance (Wang et al., 2018; Wheeler et al., 2015). However, physiochemical parameters, such as cations and anions, are easily measured together, resulting in a large amount of hydrochemical parameter inputs for certain studies (Keskin et al., 2015).

Fig. 4 contains the data collection routine timescales for all studies. Over half of all studies did not report the timescale used when collecting data. Often, data was drawn from multiple databases, and so temporal resolution was not reported. The most common collection timescale reported was seasonally, which is useful in areas with seasonal events such as monsoons (Wagh et al., 2017).

2.3. Machine learning models

Publications with a focus on supervised models comprise much of all literature. Unsupervised and ensemble learning techniques make up just

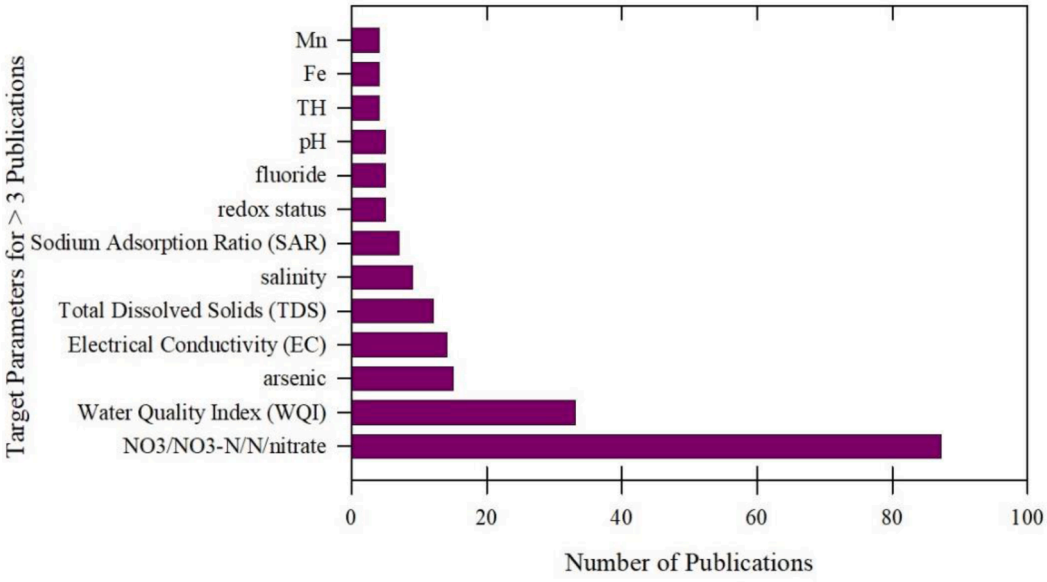

Fig. 2. The study focuses found in > 3 publications for ML in GWQ modeling. (DON: SAR: TH: TDS: EC: WQI).

10% and 7% of all published literature, respectively. Only one paper used a semi-supervised technique (Vesselinov et al., 2018).

Within the supervised models, ANN is the most common model for GW quality modeling. It should be noted that many of these papers used several models, and Fig. 5 only lists the model type focus of the papers.

2.4. Performance metrics

Fig. 6a displays the most common performance metrics used for model analysis for supervised, semi-supervised, and ensemble learning. For unsupervised learning, there are no direct metrics for evaluation and must be analyzed case by case. RMSE is the most used metric, followed by the coefficient of determination (R^2). In total, over 50 different performance metrics were used by studies to assess performance. Most studies used more than one metric to assess performance, as shown in Fig. 6b.

2.5. Historical trends

As with many ML topics, the application to groundwater quality modeling has increased rapidly in the last two decades (Fig. 2). Fig. 7 visualizes the rapid growth that occurred after 2008. Papers were collected by October of 2022, so the number of papers in that calendar year will likely be higher. Uncommon or advanced learning types like unsupervised and ensemble learning have not shown the same growth as supervised learning. Uncommon or advanced learning types like unsupervised and ensemble learning have not shown the same growth as supervised learning.

2.5.1. Geographical trends

The most studied groundwater systems in the world are in Iran, with 50 papers studying aquifers or wells in the country. The United States contains the second-most studied groundwater systems, with 39 papers. Much of Central and South America has not been studied at all, as well as several countries in Europe and Asia. The continent of Africa has been studied twice (Ouedraogo and Vanclooster, 2016; Ouedraogo et al., 2019), but the Democratic Republic of Congo is the only individual country that has been studied (Kihumba et al., 2015).

Iran had one of the most explosive increases of scientific publications in the world since the turn of the century, with a staggering 21% average annual increase in published scientific articles (WorldBank, n.d.). The United States is the next world leader in ML GWQ modeling. The United States Congress started the National Water-Quality Assessment (NAWQA) Program in 1991 to collect surface and groundwater data in a high-quality and consistent manner (U.S.G.S., n.d.), making it an ideal location for groundwater quality modeling.

3. Bibliographic review

3.1. Supervised learning

Supervised learning is one of the modalities of fitting a function from samples of input and output pairs. This review will focus on the most popular supervised learning algorithms in the domain of groundwater quality modeling, including Artificial Neural Network (ANN), Support Vector Machine (SVM), adaptive neuro-fuzzy inference system (ANFIS), deep learning, decision tree and random forest, regression models, comparative studies, and optimization techniques.

3.1.1. Artificial neural network (ANN)

3.1.1.1. Introduction of ANN. ANN (Kleene, 2016; Yegnanarayana, 2009), inspired by biological neural networks, is a unified framework that automatically learns parameters of the predictive model from data. This automatic process of updating parameters is generally achieved by backpropagation. ANNs generally consist of an input layer, a hidden layer, and an output layer. Different ANN models can be created by modifying various architectures, input structures, and layers. Brief descriptions of various ANN models introduced in this section can be found in the Supplementary Materials (S2.2.2).

3.1.1.2. Application of ANN in groundwater quality modeling. Fifteen studies focused on the applicability of neural networks to model groundwater quality, including predicting nitrate leaching, hydrological variables, and groundwater quality. They compared input-output selections, address data gaps or practical applications, or generally contribute to the larger field. These studies reached the conclusion that ANN, back propagation neural network (BPANN), feed-forward neural network (FFANN), multi-layer perceptron (MLP), and Bayesian neural network (BNN) were suitable to model groundwater quality with their choice of model architecture in the specific study area (Beerala et al., 2019; Darwishe et al., 2017; Elhatip and Kömür, 2008; Gemitzi et al., 2009; Heidarzadeh, 2017; Huang et al., 2011; Kheradpisheh et al., 2015;

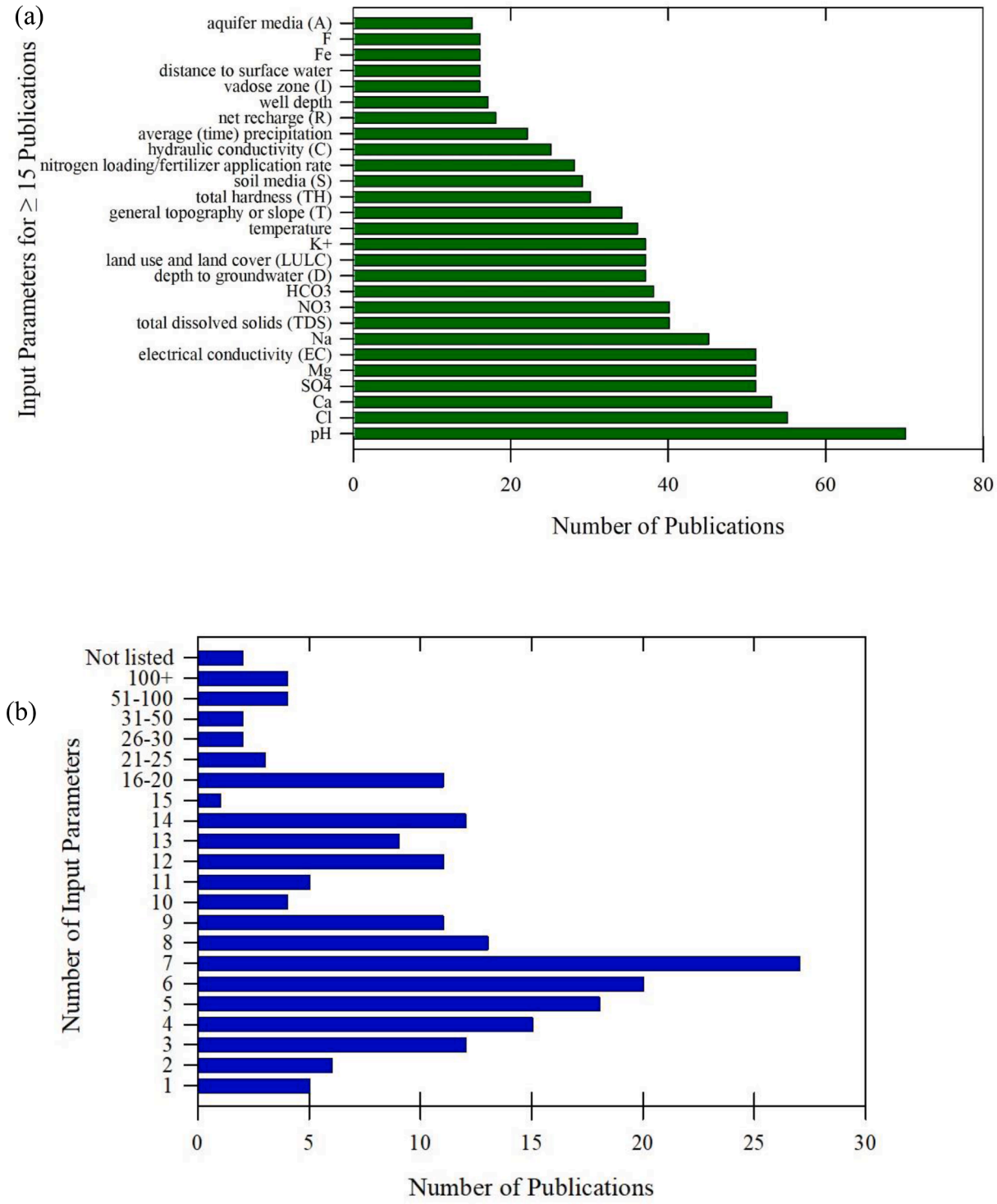

Fig. 3. Graphical analysis of input parameters. a) Input parameters used in ≥ 15 publications. b) The number of input parameters used in each publication.

Maiti et al., 2013; Maria et al., 2022; Modrogan et al., 2010; Mohammadi et al., 2016; Ostad-Ali-Askari et al., 2017; Sirat, 2013; Sunayana et al., 2020; Wagh et al., 2018; Wagh et al., 2017; Wang et al., 2006).

3.1.1.2.1. Nitrate leaching prediction. BPANN or BPNN, which is a type of ANN trained by error-correction learning of backpropagation (Rumelhart et al., 1985, 1986) using stochastic gradient descent, was used to evaluate nitrate leaching potential in agricultural fields (Kaluli et al., 1998), nitrate contamination through drip irrigation systems (Li et al., 2004), and nitrate concentration in a study area with monsoons (Charulatha et al., 2017). Using different variables, most of the work showed reasonable prediction of nitrate concentration, with R^2 values between 0.8 – 0.9. Four separate ANN models (Chittaranjan and K., 2000) were used to predict pesticide and nitrate contamination in different types of rural wells. The models performed very well during training (above 95% for all four) but not during testing, with an accuracy between 80 and 90 percent for drilled and driven wells, but only 50% for predicting nitrate in dug and bored wells.

Another study compared the metamodeling technique multidimensional kriging to radial basis function neural network (RBFNN) for nitrate leaching modeling using simulated data. RBFNN is one type of

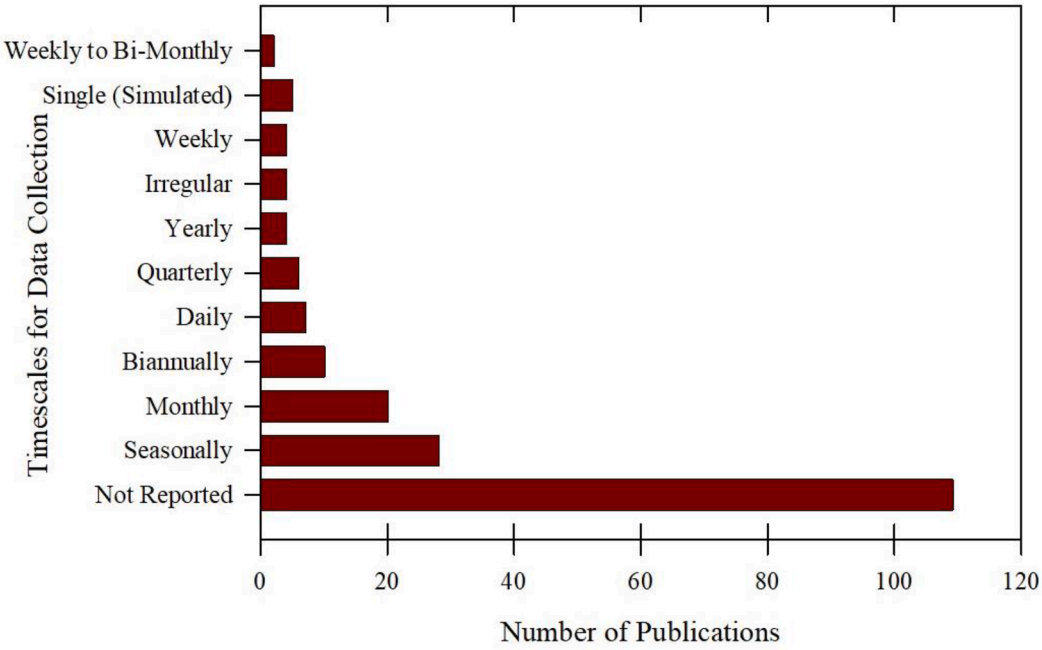

Fig. 4. Data collection timescales reported in each publication. Most studies did not report their data collection timescale.

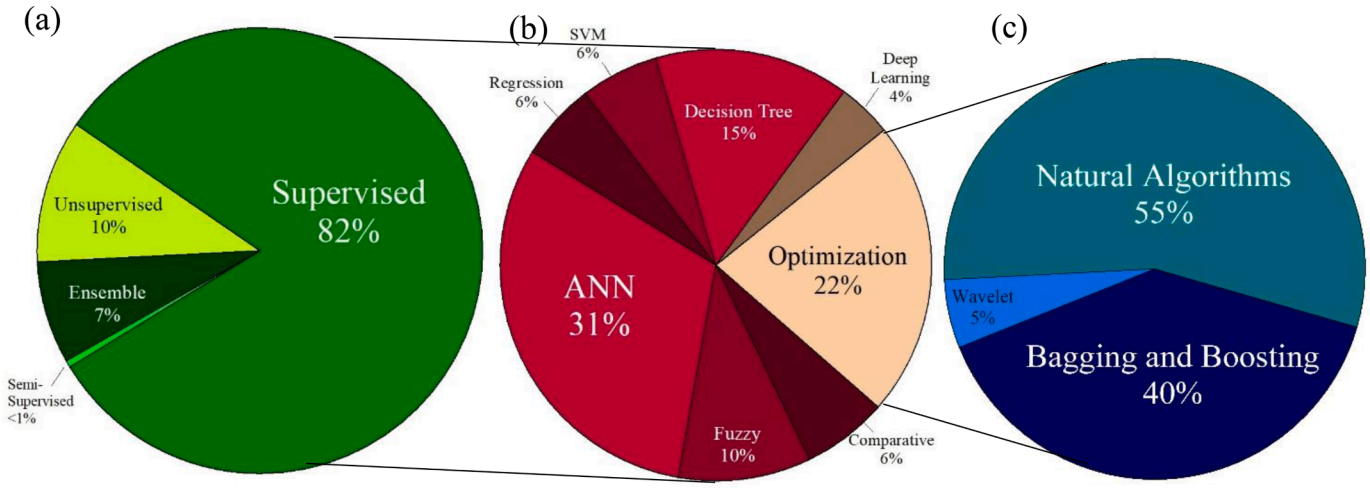

Fig. 5. Study focus of machine learning models used in GWQ modeling. a) The percentage of publications in each learning type. b) The percentage of supervised models by model category. c) The percentage of optimization models by model category.

FFNN, whose connections between nodes do not form a cycle or loop and uses radial basis function (RBF) as activation function. The kriging model performed slightly better than the RBFNN model only in some conditions (Piñeros Garcet et al., 2006). Metamodels made of ANNs were developed to predict nitrate leaching in the unsaturated zone. All performed very well in testing except for the simple model (Nolan et al., 2012).

ANN was used to modify the DRASTIC index. Results were compared to a composite DRASTIC index and a nitrate vulnerability index and found that the ANN had the highest accuracy of the three (Baghapour et al., 2016). Multiple linear regression (MLR), principal component regression (PCR), ANN, and principal component coupled with ANN (PC-ANN) were applied for application to nitrate prediction and found that PC-ANN performed the best for both pre- and post-monsoon (Charulatha et al., 2017). Previously, PC-ANN was found to have a lower mean absolute error in predicting arsenic in southeast Asian countries than MLR or ANN (Cho et al., 2011).

3.1.1.2.2. ANN for modeling hydrogeologic variables and groundwater quality. A multi-layer FFNN was used to estimate unknown groundwater pollution sources and hydraulic conductivity, porosity, and dispersivity (Singh and Datta, 2004). Data for the study was simulated by a physical model, allowing the authors to add varying uncertainty levels. The study found that the model performance decreased as the dataset uncertainty increased. Another work used a Gauss Newton ANN to model pedo-transfer functions. The model was able to work with as little as two variables and was superior to a least-squares fit model (Fuentes et al., 2014).

ANN with quick propagation (QPANN) was evaluated as an option for groundwater salinity mediation (Banerjee et al., 2011). The model was trained with 2 years of real-time field data and used to develop a pumping schedule that can stabilize salinity of groundwater below 2.5% of the seawater for a span of 5 years. A practical study coupled a wireless water quality network (WWQN) with an ANN model to give real-time predictions of groundwater quality (Kılıçaslan et al., 2014). Innovative

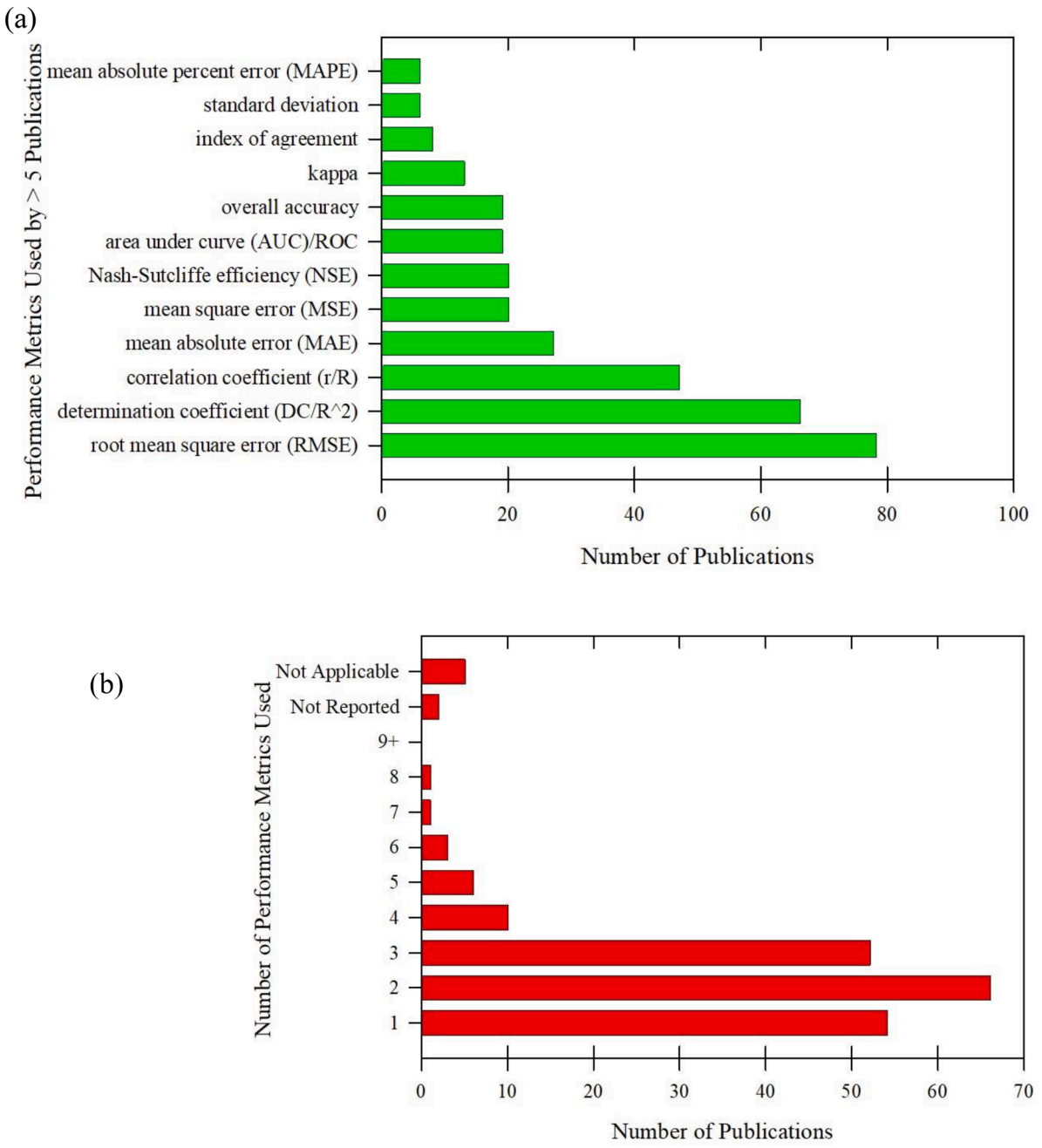

Fig. 6. Graphical analysis of performance metrics used. a) Performance metrics used in > 5 publications. b) The number of performance metrics used in each publication.

ANN architecture, for example, RBFNN coupled with a fuzzy cluster method was found to increase the efficiency for groundwater quality prediction (Azimi et al., 2019). An extreme learning machine (ELM) model, a FFNN that utilizes Moore-Penrose generalized inversion to set its weights without updating them, was found to be most efficient and had the highest predictive performance in comparison to MLP and SVM models when used to predict the level of fluoride contamination in the groundwater (Barzegar et al., 2017). MLP was used as a surrogate model for Bayesian-based Differential Evolution Adaptive Metropolis with Discrete Sampling-Markov Chain to reduce the computational cost for a contaminant source simulation, and was found to reduce simulation time by over 80 percent while keeping model results fairly accurate (An et al., 2022).

3.1.1.2.3. Comparison between ANN and statistical learning methods, and among multiple ANN models. Comparisons between ANN and other statistical learning methods are commonly found. BPNN was found to have lower predictive error for estimating nitrate and electrical conductivity when comparing with linear regression (LR) or MLR in multiple studies (LAAFOU et al., 2016; Ramasamy et al., 2003; Zare et al., 2011). ANN, however, performed the worst in another study, when compared with boosted regression tree (BRT), Bayesian network, MLR and random forest regression (RFR) for nitrate contamination (Nolan et al., 2015). GGAP-RBF network was compared to three sequential learning algorithms for nitrate prediction in groundwater and was found to be more successful at prediction (Wang et al., 2005). ANN performed the best in estimating groundwater electrical conductivity when compared to several kriging and co-kriging models (Maroufpoor et al., 2019).

Comparisons among multiple NN models are also commonly reported in groundwater quality modeling. Modular neural network

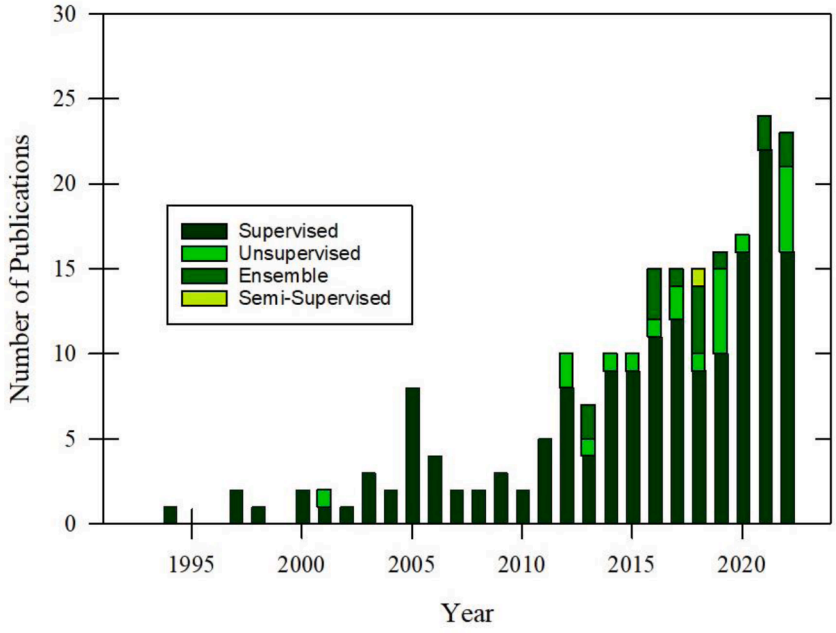

Fig. 7. Total number of studies of ML in GWQ published each year by learning type.

(MNN) and classical ANN models were compared for nitrate prediction and found that the MNN outperformed the best ANN model, but not better than a traditional model developed by MODFLOW for the steady-state ground water flow model and MT3D for nitrate fate and transport (Almasri and Kaluarachchi, 2005b). Twelve different BPNN architectures were compared for predicting nitrate contamination in a shallow aquifer, and the Levenberg–Marquardt algorithm based BPNN was selected as the best with a model correlation coefficient of 0.93 (Yesilnacar et al., 2008). BPNN outperformed RBFNN, and ANFIS models for pesticide prediction in domestic wells (Sahoo et al., 2005), and better than RBFNN for nitrate prediction (Zaqoot et al., 2018). However, another work compared BRNN and RBFNN, and found no statistically significant difference in performance (Ehteshami et al., 2016). BPNN and RBFNN models were compared for both nitrate contamination and drainage flow in agricultural fields, and the RBFNN model outperformed the BPNN model for both inputs that included and excluded field tillage data (Sharma et al., 2003). MLP was found to be the best network with a correlation of 0.9773 when comparing with two other neural network models, i.e., RBFNN, and generalized regression neural network (GRNN) (Al-Mahallawi et al., 2012). MLP was compared to convolutional neural network (CNN) and long short term memory (LSTM) for predicting WQI in Malaysia. LSTM performed the best on the dataset for nearly all performance measures (Sheikh Khozani et al., 2022). LSTM, MLR, and ANN models were compared for prediction of irrigation groundwater quality parameters. For this study, ANN performed the best, since the LSTM model was not very generalizable to the testing data (Kouadri et al., 2022).

3.1.1.3. ANN model assessment. ANN has proven to be a viable method for predicting groundwater quality variables, such as nitrate concentration. As shown in Fig. 5b, ANN models are the most popular algorithm in groundwater quality modeling due to their high accuracy and ease of implementation. Based on the predictions, they have applications for management purposes such as well installation (Chittaranjan and K., 2000) and water remediation (Banerjee et al., 2011; Kılıçaslan et al., 2014).

ANN also has large flexibility in the number of input parameters. It can provide reasonable estimates of nitrate concentrations with as few as 4 input parameters (R^2 > 0.93) (Maria et al., 2022; Yesilnacar et al., 2008) or as many as 41 parameters (MAE (%) < 7) (Nolan et al., 2015). The applicability of ANN with a small number of parameters is especially useful, as comprehensive datasets are rare and difficult to use. Using a few easily measurable parameters makes it feasible for local and municipal governments to apply ANN models.

Often, the performance of the ANN model is highly dependent on selection of input parameters and model architecture. Traditional ANN performs more poorly than BNN and BRT at high numbers of input parameters due to overfitting (Nolan et al., 2015). SVM and ANFIS models have been shown to provide higher accuracy predictions of EC, TDS (Khaki et al., 2015), and arsenic concentrations (Park et al., 2016) than ANNs. However, results are not consistent with model performance due to uncertainties in feature selection and model architecture. ANN has outperformed ANFIS in two studies (Khashei-Siuki and Sarbazi, 2015; Sahoo et al., 2005) and has shown no statistical difference with SVM in two others (Dixon, 2009; Khalil et al., 2005). Many studies found more advanced ANN models, such as RBFNN and RBFNN, performed better than traditional ANN models. Several studies reported opposite results (Ehteshami et al., 2016; Sahoo et al., 2005; Zaqoot et al., 2018). Genetic algorithms have been proven to boost ANN accuracy (Almasri and Kaluarachchi, 2005a; MoasheriP0F and AbadiP4F, 2012), as well as principal component analysis (Charulatha et al., 2017; Cho et al., 2011). In a similar vein, committee neural networks improve the predictive accuracy of multiple types of neural networks (Barzegar et al., 2018; Barzegar and Asghari Moghaddam, 2016). Thus, ANN can be modified to improve performance instead of being replaced with another model altogether. Despite a recent decline, it will likely be the dominant ML algorithm in groundwater and surface water quality for years.

3.1.2. Fuzzy methods

3.1.2.1. Introduction to fuzzy methods. Fuzzy method or analysis is one of the modalities to solve problems with uncertainty where the fuzzy logic (Cintula et al., 2021; Zadeh, 1965) is utilized. Neuro-fuzzy system (NFS) (Berenji and Khedkar, 1992; Buckley and Hayashi, 1994; Buckley and Yoichi, 1995; Halgamuge and Glesner, 1994) combines artificial neural networks and fuzzy logic to learn the parameters in fuzzy sets and fuzzy rules using backpropagation or genetic algorithm or other optimization tools. They are especially useful for classification problems where a WQI is modified or improved through fuzzy methods.

3.1.2.2. Applications of fuzzy methods in groundwater quality modeling

3.1.2.2.1. Viability of neuro-fuzzy methods for groundwater quality modeling and WQI classification. (Dixon et al. 2001) was the reported that a neuro-fuzzy method with the trapezoidal membership function can be used to predict groundwater vulnerability. This model was most sensitive to soil structure properties and land use variables. Another work varied the number of fuzzy sets, the rule weights, and the membership functions, and found that the trapezoidal membership function was the least sensitive to permutations in the model setup (Dixon, 2005).

Adaptive network-based fuzzy inference system (ANFIS) is the most widely used approach of NFS. ANFIS models have been used to predict nitrate contamination in agricultural lands (Jebastina and Prince Arulraj, 2018) and potato fields (Shekofteh et al., 2012) with satisfactory performance. An ANFIS model linked to Latin hypercube sampling to propagate uncertainty of the model parameters was used to estimate global arsenic concentrations, with the highest model performance at an R-square of 0.65 (Amini et al., 2008). ANFIS was found to outperform the traditional TDS-based method for estimating EC (Tutmez et al., 2006) and could estimate how EC affected the water composition of the study area. A study found that the number of parameters was the only significant factor on the performance of ANFIS, and the parameter combination was non-significant (Mousavi and Amiri, 2012). When applied to predict nitrate concentration in an agricultural district of India, the performance of ANFIS increased with the increase of parameters and achieved a determination coefficient of close to 90% with only 5 variables (Jebastina and Prince Arulraj, 2018).

Neuro-fuzzy methods have been used to classify agricultural groundwater pollution (Dahiya et al., 2007; Muhammetoglu and Yardimci, 2006). A Mamdani fuzzy inference model was applied to predict three WQIs and performed well for both wet and dry seasons (Vadiati et al., 2016). ANFIS was used to train models under average climate and extreme temperature conditions to modify a drinking water quality index (RadFard et al., 2019). Another work found weights-of-evidence (WofE), a statistical categorical predictor, 7 classifications provided higher quality results than neuro-fuzzy for WQI prediction (Uhan, 2012).

3.1.2.2.2. Other neuro-fuzzy models. Different types of neuro-fuzzy methods were applied to GWQ modeling. Co-active ANFIS (CANFIS) is an extension of ANFIS with capabilities of taking any number of input-output pairs, and typically performs better when mapping nonlinear function. CANFIS was found to have satisfactory performance for groundwater quality assessment (Gholami et al., 2017), and also performed better than ANN and self-organizing map (SOM) for WQI prediction (Gholami et al., 2022). Catastrophe fuzzy membership functions were used to improve both the general DRASTIC and pesticide DRASTIC methods (Sadeghfam et al., 2016). A fuzzy linear optimization model was applied to find optimal factor weights for the DRASTIC index (Asadi et al., 2017). A fuzzy logic control system was used for improving bioremediation control systems in situ. The system was able to reduce the contamination from "significantly" to "slightly" contaminated (Hu et al., 2003).

3.1.2.2.3. Comparative studies of ANFIS to other ML models. A few works performed comparative studies of ANFIS to other ML models (Al-Mukhtar and Al-Yaseen, 2019; Khaki et al., 2015; Khashei-Siuki and Sarbazi, 2015). The ANFIS (with generalized bell membership function) was found to perform the best for predicting both TDS and EC when comparing with FFNN and a cascade forward network (Khaki et al., 2015). An ANFIS model outperformed ANN and MLR models for all performance metrics for predicting TDS and EC (Al-Mukhtar and Al-Yaseen, 2019). However, another study compared ANN and geostatistical methods for spatial prediction of EC and found that the ANN model outperformed ANFIS and the geostatistical methods (Khashei-Siuki and Sarbazi, 2015).

3.1.2.3. Neuro-Fuzzy model assessment. Fuzzy models are perhaps the most user-friendly models with their linguistic outputs and ability to manage uncertainties. Their usefulness in classification problems makes them a popular choice for WQI problems. In general, fuzzy models are capable of successfully classifying groundwater quality and improving traditional WQIs such as DRASTIC (Asadi et al., 2017; Sadeghfam et al., 2016).

Fuzzy models are not only used for classification problems. ANFIS models can outperform ANN models in predicting TDS and EC if proper types and functions are used (Al-Mukhtar and Al-Yaseen, 2019; Khaki et al., 2015). ANFIS improves on the benefits of ANN with the advantage of fuzzy reasoning, leading to problem simplification and noise reduction and thus, more accurate results (Al-Mukhtar and Al-Yaseen, 2019). However, in one study (Khashei-Siuki and Sarbazi, 2015), ANN was found to be a superior model over ANFIS for EC prediction. The study used only three parameters for the best model, whereas eleven (Khaki et al., 2015) and six (Al-Mukhtar and Al-Yaseen, 2019) parameters were used in other studies. Results likely come from the purely nonlinear approach in parameter optimization and the fuzzy inference system reflecting ambiguity of observed data (Khashei-Siuki and Sarbazi, 2015). Possibly, it is simply a problem of the number of parameters, which lets the fuzzy inference system overcompensate for any errors in the limited data.

Regardless, ANFIS and other fuzzy models are excellent methods for predicting a variety of groundwater contamination parameters and predicting water quality for management purposes. It is also a faster method than ANN (Khaki et al., 2015), giving it a practical advantage in implementation.

3.1.3. Support vector machine (SVM)

3.1.3.1. Introduction of SVM. SVM is a versatile ML model which can solve classification and regression tasks. In its most basic form, SVM is a maximum margin classifier that maximizes the width of the gap between distinct categories. Because the naive maximum margin classifier uses hard margin for separation, it is sensitive to outliers. SVM overcomes this issue by utilizing a support vector classifier or soft margin classifier (Cortes and Vapnik, 1995) that finds the optimal soft margin that gives the best classification score through cross-validation among support vectors within the range of soft margin. SMV can also perform non-linear classification by utilizing a “kernel trick” (Boser et al., 1992). Additional introduction of SVM can be found in the supporting information (S2.2.4).

3.1.3.2. Application of SVM in groundwater quality modeling. SVM has been applied largely to predict nitrate concentrations in groundwater, except for three studies which focused on other contaminants such as sodium and arsenic (Isazadeh et al., 2017; Liu et al., 2020; Park et al., 2016).

The validity of SVM for nitrate contamination prediction was assessed and shown to be satisfactory (Arabgol et al., 2016). A study integrated SVM into the parametric agricultural nitrate hazard index (IPNOA) model (Rizeei et al., 2018). LR was used for weighting/optimization of the SVM before the final prediction was made, which led to a higher accuracy than the regular IPNOA (91.32% and 85.3%, respectively). Liu et al.’s work (J. Liu et al., 2020) marked the first successful effort to apply one-class SVM to groundwater anomaly detection with real-time data.

SVM was compared with ANN models in multiple studies (Dixon, 2009; Isazadeh et al., 2017; Khalil et al., 2005; Park et al., 2016). When compared with a locally weighted projection regression (LWPR) and relevance vector machine (RVM), a method similar to SVM but that uses Bayesian inference to provide probabilistic classification, for nitrate prediction (Khalil et al., 2005), RVM performed the best followed by SVM and ANN, which was attributed to model architecture choices and may not be consistent in all study areas. When compared for nitrate

prediction, SVM and NN performed similarly in the validation phase (0.55 and 0.59 accuracy, respectively). Feature selection did not improve accuracy but did lower the number of necessary variables for prediction (Dixon, 2009). When compared for EC, sodium, and sulfate concentration prediction, SVM had lower uncertainty than FFNN (Isazadeh et al., 2017). ANN and SVM were compared for identifying groundwater arsenic concentrations, and SVM was found to be more accurate (Park et al., 2016).

SVM, along with classification and regression tree (CART) and random forest (RF), was evaluated as part of a wrapper selection study for optimizing feature selection for nitrate prediction models (Rodriguez-Galiano et al., 2018). The highest performing SVM model was sequential forward selection-SVM. However, the best CART and the best RF model were superior to SFS-SVM.

3.1.3.3. SVM model assessment. SVM models have been found to accurately predict nitrate concentration (Arabgol et al., 2016; Khalil et al., 2005) and other hydrochemical compounds (Isazadeh et al., 2017; Park et al., 2016). Additionally, they have advantages over ANN models. For example, SVM models do not rely critically on network structure selection, the biggest weakness of ANN. They are also less prone to overfitting because there is no need for iterative training. In addition, they are faster (Khalil et al., 2005).

Despite these advantages, results are not conclusive on SVM superiority over ANN for groundwater quality modeling. SVM models still rely on kernel function selection, which may affect results as they use different methods to map data into higher dimensions. Researchers should expect results of these comparisons to be dependent on model architecture, area-specific, and not generalizable to other research areas (e.g., surface water). SVM was shown to be inferior to CART and RF for feature selection (Rodriguez-Galiano et al., 2018), but superior to BRT and multi-discriminant analysis (MDA) for nitrate contamination prediction (Sajedi-Hosseini et al., 2018). As with all models discussed here, an ensemble approach was able to improve SVM individual performance (Sajedi-Hosseini et al., 2018). Regardless, SVM is a sturdy model capable of achieving low uncertainty under reasonable computational demands (Isazadeh et al., 2017). Most studies on SVM are recent, and there is clearly still work left on this topic.

3.1.4. Regression models

3.1.4.1. Introduction to regression models. The regression model predicts the dependent variable from one or more independent variables through a function that estimates their relationships. Regression analysis is generally used for predicting the target value of missing input other than the training samples.

3.1.4.2. Application of regression models in groundwater quality modeling. Several of the earliest studies used a ML logistic regression model to accurately predict nitrate contaminations (A. Liu et al., 2005; Nolan et al., 2002), Selenium thresholds (Nolan and Clark, 1997), and groundwater vulnerability (Teso et al., 1996). These models are now often used as a benchmark comparison to demonstrate alternate model superiority. More advanced regression models such as multivariate regression, multiple linear regression (MLR), and regression trees were later introduced to study nitrate contamination and source pollution (Boy-Roura et al., 2013; Kihumba et al., 2015; Mattern et al., 2009; Nolan, 2001). MLR is still a useful modern tool; MLR outperformed ANN for predicting water quality index types in Nigeria (Akakuru et al., 2022).

3.1.4.3. Regression model assessment. LR and MLR have been shown repeatedly to be superior to computationally costly physical models, but in the current research meta they are the benchmark for the lowest acceptable accuracy. For example, RF models are highly superior to LR models (Ouedraogo et al., 2019; Tesoriero et al., 2017; Wheeler et al., 2015).

3.1.5. Decision tree and random forest

3.1.5.1. Introduction to decision tree and random forest. Decision trees (DT) are a type of supervised ML where the data is continuously split according to a certain parameter, and trees consist of decision nodes and leaves. The random forest (RF) is a classification algorithm consisting of many DTs. RF randomly selects observations and features to build each individual tree to create an uncorrelated forest of trees (Biau and Scornet, 2016).

3.1.5.2. Application of decision tree and random forest in groundwater quality modeling. One study used only DT to predict water quality classifications, which was found to be more precise and efficient than principal component analysis (Saghebian et al., 2014).RF was used to predict nitrate and arsenic concentrations and allowed for a general assessment of the vulnerability of basin-fill aquifers (Anning et al., 2012). When used to predict pollution in agricultural groundwater, an RF model only needed four explanatory variables when driving forces, such as anthropological effects, were added to water quality parameters (V. Rodriguez-Galiano et al., 2014). RF was used to locate the sources and flow paths of dissolved organic nitrogen (DON) in groundwater based on landscape characteristics (B Wang et al., 2018). In conjunction with a fuzzy method, RF was able to determine the WQI and groundwater quality index (GQI) (Norouzi and Moghaddam, 2020). RF has shown satisfactory performance for fluoride modeling in India (J. E. Podgorski et al., 2018) and arsenic modeling in Uruguay (Wu et al., 2021). RF was supplemented with Global Information System (GIS) for spatiotemporal assessment and prediction of groundwater nitrate contamination, with a high accuracy (Judeh et al., 2022).

At a large scale, RF and quantile RF were used with the European Water Framework to estimate national redox and nitrate groundwater conditions at high resolution (Knoll et al., 2020). A methodology was proposed to accommodate the computational demands of large datasets using RF, and national-scale predictions of groundwater redox class for New Zealand were presented (Wilson et al., 2020). RF with Shapley Additive exPlanations (SHAP) was compared to kriging to derive insight on nitrate modeling was found to be more accurate than the traditional method (W. Li et al., 2022). RF and a generalized boosted regression model were combined into a final model for analysis of physiochemical parameter relationships by creating spatial maps showing relationships between manganeses, iron, and arsenic (Podgorski et al., 2022). Classification and Regression Tree (CART) model was used for prediction of GWQI assessment in India, which achieved low error and produced results for the soil types by GWQI (Singha et al., 2022).

RF performed better for nearly all benchmarks when comparing to linear regression for predicting the occurrence of redox-active constituents in groundwater (Tesoriero et al., 2017). RF has been found to be superior to MLR, regression tree, linear regression, kriging models, generalized additive model (GAM), CART, BRT, RF, SVM, Naïve Bayes, and C4, a tree-based algorithm for modeling nitrate in private wells in rural areas (Wheeler et al., 2015), at the continental scale (Issoufou Ouedraogo et al., 2019), in the Arab Emirates (Khan et al., 2021), and using exclusively spatial predictors (Knoll et al., 2019). RF has also been found to be superior Multiple Discriminant Analysis (MDA) and BRT for susceptibility prediction of groundwater hardness (Mosavi et al., 2020) and ANN for prediction of WQI in an urban area (Anjum et al., 2021). Five tree-based models were used for arsenic risk prediction in a region in India, RF, Optimized Forest, cost-sensitive Forest (CS Forest), Split-Point and Attribute Reduced Classifier (SPAARC), and Reduced Error Pruning (REP) Tree. The most accurate was Optimized Forest, with RF close behind, while the least accurate was CS Forest and REP Tree (Kumar and Pati, 2022). Random forest was found to have the best

classification performance for groundwater arsenic prediction compared to DT, MLP, and Naïve Bayes algorithm (Siddharth Kumar and Pati, 2022). RF and a k-nearest neighbor (kNN) model had the highest accuracy for prediction of water quality class in India compared to linear discriminant analysis, CART, and SVM models (MOGARAJU, 2022).

A study used numerical model outputs as predictors to create a hybrid boosted regression tree model (i.e. DTs with continuous outcome) for predicting nitrate concentration (Ransom et al., 2017). A conditional inference forest (CIF), a DT that utilizes unbiased recursive partitioning of dependent variables based on the value of correlations, was paired with a physical model in a groundwater vulnerability analysis. The metamodel allowed for multiple simulations of the computationally expensive physical model, with a higher than 60% agreement in GW sites for predicted classes (Soriano et al., 2021).

3.1.5.3. Decision tree and random forest model assessment. RF models are less of a "black box" than other ML models; that is, researchers may glean information about parameters connections (B Wang et al., 2018). However, RF models can struggle with accuracy and availability of anthropologic data (Knoll et al., 2020; V. Rodriguez-Galiano et al., 2014). Additionally, the size of the tree-based algorithm can be a restriction.

3.1.6. Comparative studies

3.1.6.1. Introduction to comparative studies. Some studies compare models without intention of selecting a "best model" and optimizing it for the study area, or without intention of comparing a novel model to a base model. These studies are collected in this section.

3.1.6.2. Application of comparative studies in groundwater quality modeling. Four algorithms, MLP, ANFIS, SVM, and gene expression programming (GEP) were compared for estimating TDS, and GEP was found to be superior (Jafari et al., 2019). RF demonstrated a slightly lower error than ANFIS, logistic regression mode (LRM), fuzzy, and adaptive fuzzy regression (AFR) for groundwater arsenic prediction (Bindal and Singh, 2019). BPNN, evolutionary polynomial regression (EPR) and the naive Bayes model (NBM) were compared across seven performance metrics for predicting nitrogen concentration on a weekly basis. No single model significantly outperformed any of the others in all analysis (Markus et al., 2010). Additive regression (AR) surpassed the accuracy of SVM, M5P tree model (M5P), and random subspace (RSS) for WQI prediction in India (Elbeltagi et al., 2022).

Thirteen ML algorithms were compared for dissolved organic nitrogen prediction in an urban setting. Bagged MARS, RF, and cubist, a rule-based model that utilizes decision tree and regression (Quinlan and others, 1992), were the most optimal models with the most generalizability (Benya Wang et al., 2016). For comparison of seven ML algorithms for arsenic prediction, Cubist performed the best in training; however, RF and bagged tree were the best models for internal validation (de Menezes et al., 2020).

SVM was found to have superior performance to RF, flexible discriminant analysis (FDA), mixture discriminant analysis (MDA), BRT, and MARS for groundwater salinity mapping (Mosavi et al., 2021). Hosseini et al. found that instance-based K-nearest neighbors outperformed KStar, M5P, locally weighted learning, and regression by discretization for fluoride contamination prediction (Khosravi et al., 2020).

3.1.6.3. Comparative studies assessment. Comparative studies contain models that have only appeared once in ML GWQ modeling literature. These studies serve the purpose of assessing less-common models for completion of the literature. However, it is important to note that these studies do not necessarily agree on model superiority and should be taken on a case-by-case basis. For example, one study concluded that SVM was the most accurate of six models, including MARS, for groundwater salinity mapping (Mosavi et al., 2021). However, another found that of their thirteen models tested for dissolved organic nitrogen prediction, MARS was among the top three, whereas two different SVM models were not (Benya Wang et al., 2016). This example reinforces the danger of generalizability in comparative studies.

3.1.7. Optimization techniques

Optimization techniques are practices of optimizing the performance of the predictive model from various aspects. Widely used techniques include efficient searching for the optimal parameter set of the model, feature engineering for effective feature learning, and improving the stability and accuracy of learning algorithms.

3.1.7.1. Introduction to genetic algorithms. Genetic algorithms (GAs) (Katoch et al., 2021; Lambora et al., 2019; Yang, 2020), inspired by natural selection, are part of evolutionary algorithms (EAs) which are generic population-based metaheuristic optimization algorithms. Genetic algorithms utilize biologically inspired operations like mutation, crossover, and selection to provide solutions for optimization and search. Genetic algorithms can deal with complex problems across diverse types of optimizations. To make genetic algorithms converge, the parameters of the specific genetic algorithm need to be carefully selected, and a wide range of options exists. A brief description on GAs, particularly on variations of GAs mentioned in the sections below, can be found in the Supporting Information (Section 2.2.5).

3.1.7.2. Application of genetic algorithms in groundwater quality modeling

3.1.7.2.1. Improving model performance with GA. BPNN and GA have been integrated and was found to perform better than other ANN models for nitrate prediction (Almasri and Kaluarachchi, 2005a; MoasheriP0F and AbadiP4F, 2012). The bee algorithm (BA), a population-based algorithm that mimics the food foraging behavior of honeybee colonies with good convergence to the global optimum, was used with BPNN for prediction of water pollution sources, which showed significantly higher accuracy than the unmodified BPNN (Keskin et al., 2015). An FNN-SVR hybrid model was optimized with GA and needed less parameters than MLR (Hosseini and Mahjouri, 2014). The viability of ELM modified by crow search algorithm (CSA) for predicting groundwater quality was evaluated and found to be more accurate than the unmodified ELM (Liu et al., 2017) and to raise the accuracy of ANFIS for prediction of specific conductance (Zounemat-Kermani et al., 2022). PSO and GA optimization of ANFIS were not found to be statistically different for modeling EC, pH, and Cl (Jalalkamali, 2015). For WQI prediction, a PSO-naïve Bayes classifier slightly outperformed a PSO-SVM model (Agrawal et al., 2021). PSO was also used with NN and Empirical Bayesian Kriging for prediction of physiochemical and metallic parameters in an island area (De Jesus et al., 2021; Senoro et al., 2022). The firefly algorithm (FFA), a global optimization algorithm inspired by flashing behavior of firefly insects, was shown to improve performance in ANN, ANFIS, SVM, MARS, and RF models for prediction of groundwater parameters, of which SVM-FFA and ANN-FFA were the most robust. A combination of PCA, PSO, and SVM was optimized to evaluate water quality category. The PCA-PSO-SVM model performed better than the PSO-SVM, the SVM, and a BPNN model and had a 99 percent accuracy (Ni et al., 2022).

3.1.7.2.2. GA comparative studies. Several studies compared the performance of multiple genetic algorithms against each other (Banadkooki et al., 2020; Kisi et al., 2019; Ritzel et al., 1994). Pareto GA was found to be superior to a vector-evaluated GA for solving a multi-objective groundwater pollution containment problem (Ritzel et al., 1994). Continuous genetic algorithm (CGA) was found to be overall superior to PSO and ant colony optimization for continuous domains (ACOR)for training and optimization of ANFIS for modeling EC, total hardness, and sodium adsorption ratio (SAR) in groundwater (Kisi et al., 2019). Moth flame optimization (MFO) and cat swarm

optimization (CSO) have also showed better performance in optimization of ANFIS for TDS compared to PSO and three other GAs (Banadkooki et al., 2020).

Three studies compared GAs against other algorithms (Aryafar et al., 2019; Najafzadeh et al., 2022; Wu et al., 2017). GA was compared to generalized linear regression, decision tree, and gradient boosted tree for nitrate prediction (Wu et al., 2017). While the GA did the least over/underestimating of the models, it was not very robust. When comparing genetic programming (GP) to ANN and ANFIS for estimating TH, TDS, and EC, the GP model was superior (Aryafar et al., 2019). Evolutionary Polynomial Regression (EPR) and gene-expression programming (GEP) were compared against M5 model tree and Multivariate Adaptive Regression Spline (MARS) for WQI prediction, and EPR had the highest accuracy (Najafzadeh et al., 2022). GEP was also used to predict salinity and EC in Iran (Khalaj et al., 2019).

3.1.7.3. Genetic algorithm model assessment. GA is a popular method for improving model results with a wide range of options. They provide advantages over ANN and ANFIS models by structural independence and protection from over-fitting and early convergence due to their crossover and mutation operators (Aryafar et al., 2019). They are also remarkably consistent; every study that modified existing algorithms found that GAs improve model performance. Additionally, they can work with as few as three parameters (Banadkooki et al., 2020; Jalalkamali, 2015) or more than 10 parameters (Hosseini and Mahjouri, 2014; Ransom et al., 2017).

More evolutionary models have been tested in recent years, such as CSA and PSO. There is not a clear consensus from the literature if these newer models have an advantage in groundwater quality modeling (Jalalkamali, 2015; Kisi et al., 2019). However, the new models are just as viable for predicting groundwater quality (Keskin et al., 2015; Liu et al., 2017). Because of their consistency, flexibility, and compatibility with other models, GAs will continue to be a useful tool for researchers.

3.1.7.4. Introduction to wavelet transform. Wavelet transform (Chui, 1992; Daubechies, 1992; Debnath and Shah, 2002) was proposed to solve constant time and frequency resolution caused by the fixed length of the window used in short-time Fourier transform (STFT). Wavelet transform uses wavelet as the basis function rather than the window function to realize multiresolution analysis by controlling the width of the wavelet and its central frequency. Wavelet transform and its discrete version, discrete wavelet transform (DWT) (Akansu and Haddad, 1992), are effective tools of doing feature engineering to select optimal features from raw data as training data. Wavelet transform can also be directly used in ML architectures like wavelet neural networks (WNN) (Alexandridis and Zapranis, 2013) which combine wavelet analysis with neural networks to approximate deterministic functions.

3.1.7.5. Application of wavelet transform in groundwater quality modeling. Wavelet transform is a common surface water modeling technique, but few studies have used wavelet transform techniques for groundwater quality modeling. A study used electromagnetic sensor arrays as input for a MLP with wavelet transform for feature selection to estimate groundwater quality. The model could predict nitrate and sulfur concentration even in the presence of other contamination (Nor et al., 2015). Another study optimized a MLP with a wavelet neural network (WNN) and BPNN for assessing shallow groundwater quality (Yang et al., 2017). Wavelet transform, along with self-organizing map (SOM) and mutual information (MI) was used to extract features for modeling nitrate time series with FFNN. The hybrid coupling improved the performance of the FFNN by up to 39% and was able to predict nitrate load in the study area's sub-basins and outlet (Nourani et al., 2017).

3.1.7.6. Wavelet transform model assessment. Wavelet transform can decompose non-stationary data (Nourani et al., 2017). This temporal preprocessing can improve models as it can find trends, discontinuities, and other data anomalies that other preprocessing techniques might miss (Yang et al., 2017). Thus far, it has only been applied to improve an MLP model and ANN models and used in preprocessing for a hybrid FFNN model. While wavelet transform has some flexibility in selection of the mother wavelet, this does affect results and can compound on ANN model architecture selections (Yang et al., 2017). However, wavelet transform is a useful tool for improving results if the complexity of application is not an issue.

3.1.7.7. Introduction to bagging and boosting. Boosting is an ensemble learning method for reducing variance and overfitting in a sequential way by adjusting the weight of sample as each base model is evaluated (Hastie et al., 2009). Gradient boosting (GBT), or boosted regression tree (BRT), (Friedman, 2002; Hastie et al., 2009) is an ensemble learning model using decision trees as base models.

3.1.7.8. Application of bagging and boosting in groundwater quality modeling. BRT has been used for predicting arsenic (Chakraborty et al., 2020; M L Erickson et al., 2018; Lombard et al., 2021), manganese (Melinda L Erickson, Elliott, Brown, Stackelberg, Ransom, Reddy, et al., 2021), pH (Stackelberg et al., 2021), redox conditions (Melinda L Erickson et al., 2021) and nitrate concentration (Ransom et al., 2022) in various glacial aquifer systems in the United States. BRT was found to be a cheap and reliable method for real-time groundwater level and nitrate concentration predication (Mettu and Latifi, 2021).

Extreme gradient boosting (XGB), a specific implementation of gradient boosting with regularization to improve the generalization of the model, was found to be superior to DNN and MLR for mapping groundwater salinity (Sahour et al., 2020) and ANN and SVM for nitrate and pesticide prediction (Bedi et al., 2020). XGB performed the best for improving a groundwater vulnerability prediction framework, when compared with AdaBoost, RF, Light Gradient Boosting Machine (LGBM), and Categorical Boosting (CatBoost) (Barzegar et al., 2021). Adaptive boosting (Adaboost) was found in two instances to have higher predictive performances than RF, ANN, and SVR for predicting irrigation water quality, although the SVR and ANN models showed higher generalization potential (El Bilali et al., 2021; Trabelsi and Ali, 2022). Random Forest Regression (RFR), the Extreme Gradient Boosting Regression (XGBR), the CatBoost Regression (CBR), and the Light Gradient Boosting Regression (LGBR) were compared for salinity prediction in coastal aquifers, with the CBR model reaching the best accuracy and stability (Tran et al., 2021). However, for arsenic prediction, RF was found to have better capabilities (Chakraborty et al., 2020); for nitrate, XGBoost showed superior performance (Ransom et al., 2022).

3.1.7.9. Bagging and boosting model assessment. The robustness and computational restrictions of a model can be addressed with boosting. A popular method is XGB, although others exist and have been studied for GW quality modeling. XGB has been shown to have higher accuracy than ANN, DNN, and MLR models for prediction of nitrate, salinity, and pesticides in groundwater (Bedi et al., 2020; Sahour et al., 2020). It is also comparable to SVM (Bedi et al., 2020), although generalized boosted models (GBM) and BRT are not as accurate (Mosavi et al., 2021; Benya Wang et al., 2016).

3.1.8. Deep learning

3.1.8.1. Introduction to deep learning. Deep learning is part of ANN-based machine learning algorithms, whose network architecture is constructed with multilayer perceptron (MLP) to achieve better predictive capability while maintaining a moderate complexity of the network. Deep learning methods are capable of effectively modeling complex relationships from observations. Its training and inferencing

performance can be improved by leveraging modern hardware-accelerated parallelization.

3.1.8.2. Application of deep learning in groundwater quality modeling. The deep neural network (DNN) emulator was found to be able to model simple contaminant transport much faster than MLP for contaminant transport modeling (Yu et al., 2020). Recently, DNNs have been compared to several models for both ammonium (Perović et al., 2021) and WQI (Singha et al., 2021) prediction, and provided remarkably high predictive performance ($R^2 = 0.996$) (Singha et al., 2021). A DNN model showed significant improvement over ANN and SVR models for ammonium prediction in alluvial groundwater (Perović et al., 2021). For prediction of WQI and Entropy Water Quality Index (EWQI), DNN performed better than GBM and extreme gradient boosting (XGB). Results for the boosting methods are mixed for the two indices (Raheja et al., 2022). CNN and DNN outperformed RF and XGB for estimation of groundwater quality parameters such as TDS, potential salinity, sodium adsorption ratio, and chloride in a coastal aquifer using only EC and pH as input parameters (Taşan et al., 2022). However, for nitrate prediction in an unconfined aquifer, XGB was more accurate than a DNN and MLR model (Gholami and Booij, 2022).

A DNN was used for point source identification in a simulated groundwater quality scenario. The authors projected the high dimensional problem into a lower dimension, and so the proposed network provided a good surrogate of a transport system without losing accuracy, with the autoregressive strategy reducing the DNN computational time (Mo et al., 2019).

3.1.8.3. Deep learning model assessment. Deep learning is a promising field of study in computer science, and especially in groundwater quality modeling. While the number of case studies is still small, deep neural networks have consistently performed better than conventional ML models such as ANN for supervised groundwater quality modeling (Perović et al., 2021; Singha et al., 2021; Taşan et al., 2022). Although deep-learning network is an effective type of predictive model with capability of modeling complex functions on high-dimension input, several aspects have to be taken care of while training the network. For example, a larger amount of training data is needed to train a complex deep-learning network with good generalizability. Practices like regularization are also necessary to prevent the model from overfitting.

3.2. Semi-Supervised

3.2.1. Introduction to semi-supervised ml models

Semi-supervised learning (Chapelle et al., 2009; Zhu and Goldberg, 2009; Zhu, 2005) is a combination of supervised learning and unsupervised learning and it utilizes a small amount of labeled data and a large amount of unlabeled data for training. The success of semi-supervised learning depends on the critical assumptions which are continuity, cluster, and manifold. Popular semi-supervised learning includes self-training, mixture models, co-training, multi-view learning, graph-based methods, low-density separation, and semi-supervised support vector machines.

3.2.2. Application of semi-supervised ml models in groundwater quality modeling

A study proposed a new groundwater contaminant source identification method, which used a non-negative Matrix Factorization (NMF) method for Blind Source Separation (BSS), coupled with a custom semi-supervised clustering algorithm (Vesselinov et al., 2018). The authors had previously applied this method to identify the sources of pressure fluctuations in water (Alexandrov and Vesselinov, 2014). The semi-supervised k-means clustering algorithm could unmix the geochemical signatures in the observations and identify the contaminant sources and was found to be capable of identifying both the number of groundwater types and the original concentration of the contaminant sources from mixtures without any mixing ratio or site information.

3.2.3. Semi-Supervised model assessment

Semi-supervised algorithms are rare in water quality modeling. As of 2020, they had not been used for river water quality modeling (Tiyasha et al., 2020a) and have been only used once for GWQ modeling as of 2022. The method provided promising results and could be an emerging topic for researchers focused on contaminant source identification.

3.3. Ensemble learning

3.3.1. Introduction of ensemble learning

Ensemble learning (Haykin and Network, 2004; Opitz and Maclin, 1999; Polikar, 2006) is a modality of ML where multiple base learning models (weak learners) are aggregated to obtain better predictive performance than any of the base learning models alone. The aggregation is achieved by using meta-algorithms like bagging, boosting, and stacking. In this review, models are grouped into committee neural networks (CNN), ensemble fuzzy models, and others.

3.3.2. Application of ensemble learning in groundwater quality modeling

3.3.2.1. Committee neural networks. Committee machine or committee neural network (CNN) (Haykin and Network, 2004) is a type of ensemble learning utilizing multiple neural networks as base models and combining the predictions of base models into a final prediction with higher accuracy. A CNN of three NN models (i.e., MLP, RBFNN, and GRNN) were compared for groundwater salinity prediction, and the CNN outperformed any individual model in RMSE and R^2 (Barzegar and Asghari Moghaddam, 2016). A CNN was used with ELM, MARS, M5, and SVR for improving DRASTIC predictions. In terms of the correlation coefficient (r) and Willmott index (d), CNN was clearly superior to any individual method (Barzegar et al., 2018). Ensemble of ANNs was compared to ANN with early stopping and ANN with Bayesian regularization for prediction of WQI but did not higher correlation coefficient in both training and testing data set than the Bayesian regularization algorithm (Sakizadeh, 2016).

3.3.2.2. Ensemble fuzzy models. Ensemble fuzzy models (Yang et al., 2006) combine various fuzzy logic methods with ensemble learning for better performance. Ensemble fuzzy models have been applied exclusively to improving DRASTIC method performance. A few studies (Barzegar et al., 2016; Fijani et al., 2013; Nadiri et al., 2013) used supervised committee machine with artificial intelligence (SCMAI) to predict fluoride concentration and improve the DRASTIC method. Each study ran Sugeno fuzzy logic (SFL), Mamdani fuzzy logic, ANN, and neuro-fuzzy (NF) individually for the problem before testing the SCMAI. Some results showed that they each fit the data for fluoride prediction similarly (Nadiri et al., 2013). NF was shown to be the best of the individual models in one study area (Fijani et al., 2013), and in another both NF and SFL performed very well (Barzegar et al., 2016). All studies observed that the SCMAI was able to further improve on any individual model's performance. Another study found that in the validation phase for improving DRASTIC performance, supervised committee fuzzy logic (SCFL), and committee fuzzy logic (CFL) had higher correlation coefficients than three individual fuzzy logic models (Nadiri et al., 2017).

3.3.2.3. Other ensemble models. Three different ML types, BRT, MDA, and SVM, and an ensemble of these three models were compared for groundwater risk assessment for a region in Iran., and the ensemble approach surpassed all individual models (Sajedi-Hosseini et al., 2018). Two similar studies reached the same conclusion for an area of Pakistan (Awais et al., 2021) and a different Iran region (Rokhshad et al., 2021). Radial Basis Neural Networks (RBNN), Support Vector Regression

(SVR), and ensemble Random Forest Regression (RFR) were compared for nitrate contamination evaluation; the ensemble model performed the best (Elzain et al., 2022). RF, gradient boosted machine, SVM, and ANN, along with bagging ensemble model were used to model nitrate concentration in private wells. No model performed well ($R^2 < 0.33$), and final RF model outperformed the bagging ensemble models (Messier et al., 2019). A 2022 study compared bagging (Bagged Decision Trees, Random Forest, and Extra Trees), boosting (AdaBoost and Stochastic Gradient Boosting), and ensemble methods (Logistic Regression, kNN, Decision Tree, SVM, and Naïve Bayes) for WQI prediction. The highest accuracy was achieved by the ensemble model, bagged decision trees, and gradient boosting (Shrivastava et al., 2022).

3.3.3. Ensemble model assessment

Ensemble models are a powerful tool for GW quality prediction. Virtually all ensemble modeling studies have shown that CNNs, ensemble fuzzy models, and ensemble models of other ML algorithms can improve predictive capabilities. An ensemble approach can eliminate weaknesses of each individual model and provide a more robust prediction. However, ensemble models are not always perfect advancements. For example, one study found that an RF model had a higher R^2 value than the bagging ensemble model, which used R^2 as the only performance metric (Messier et al., 2019). Another study found that the CNN had the lowest RMSE but not the highest R^2 value, but it also outperformed any individual model in terms of correlation coefficient r and Willmott index of agreement (Barzegar et al., 2018). In general, ensemble models outperform other models in various performance metrics (Barzegar and Asghari Moghaddam, 2016; Elzain et al., 2022), although they may have lower R^2 values.

3.4. Unsupervised learning

Unsupervised learning (Barlow, 1989; Hinton et al., 1999) is an algorithm that can discover hidden patterns and insights from the dataset without labels. Common unsupervised learning tasks include clustering, association, and principal component analysis (PCA).

3.4.1. Self-Organizing maps (SOM)

3.4.1.1. Introduction of som. Self-organizing map (SOM), also known as self-organizing feature map (SOFM) or Kohonen self-organizing feature maps (KSOFM) (Kohonen, 1982; Kohonen et al., 1996; Kohonen and Honkela, 2007), is an unsupervised neural network that clusters high-dimensional data and transforms high-dimensional features into low-dimensional (two-dimensional) features while preserving symmetrical relationships between samples.

3.4.1.2. Application of self-organizing maps in groundwater quality modeling. SOMs have been used for point source identification, modification of neural networks, prediction of hydrochemical parameters, and in conjunction with clustering (Hong and Rosen, 2001; Nakagawa et al., 2016; Nourani et al., 2015). The first study to use SOM generated U-matrix maps which allowed the authors to find site-specific correlations between variables by comparing these maps to the real world (Hong and Rosen, 2001). SOM was able to provide high quality, area-specific interpretable results to classify the groundwater data (Choi et al., 2014). When SOM was used with a FFNN to model, the SOM-FFNN method improved the accuracy of predictions 84.5% and 17% for modeling EC and TDS, respectively, on average with regard to the MLR model (Nourani et al., 2015). A modified SOM (MSOM) was found to perform better than three supervised MLAs (i.e., LDA, BRT, and RF), in predicting oxic, mixed, and anoxic conditions for a groundwater redox condition study in an agriculturally dominant region (Friedel et al., 2020). SVM with PCA and hierarchal clustering analysis (HCA) was used for identifying hydrological pathways and ion sources in aquifer systems in Japan (Rahman et al., 2022).

SOM was coupled with clustering algorithms in several studies. A study used SOM with k-means and Ward's algorithms for clustering to identify surface and groundwater chemistry classes and determined pathways for certain chemicals (Nakagawa et al., 2016). SOM and fuzzy c-means (FCM) clustering were able to identify distinct and interpretable clustering groups when evaluating urban (Lee et al., 2019) and SOM with hierarchal clustering (HCA) achieved this for regional groundwater quality (Zhong et al., 2022).

3.4.1.3. SOM model assessment. SOMs offer insights into parameter connections and point source identification, as well as improvements on predictions of GWQ parameters. They can capture insight on complex variable relationships with no a priori knowledge of physical transport mechanisms. The application of SOM in groundwater quality modeling is still an emerging field and has little generalizability. Overall, SOMs can be useful tools for local or regional groundwater management.

3.4.2. Clustering

3.4.2.1. Introduction to clustering. Clustering (Rokach and Maimon, 2005; Xu and Wunsch, 2008) is an unsupervised ML task that automatically separates data into groups according to the similarities of samples specified by certain type of distance metric. Clustering has been used to identify unknown connections among parameters and improve other ML techniques. K-means algorithm (Forgy, 1965; Lloyd, 1982; MacQueen and others, 1967) is a centroid model for partitioning data into k clusters through iteration where each cluster is represented by a single mean vector.

3.4.2.2. Application of clustering in groundwater quality modeling. Clustering, such as factor analysis (FA), cluster analysis (CA), and K-means clustering, was used to understand variable relationships. Factor analysis (FA) and cluster analysis (CA) were used along with a hydrochemical model package (PHREEQC) to model hydrochemical properties of a small island aquifer. Inspecting the elements of each cluster led to explain the three most significant processes affecting the groundwater aquifer (Aris et al., 2011). K-means clustering was used to understand spatial variations in groundwater chemistry to identify pathways and study the effects of industrial and agricultural activities on two aquifers (Fabbrocino et al., 2019). Hybrid BN was used to apply probabilistic clustering for assessing groundwater quality and predictive uncertainty, which optimized the number of samples needed for an accurate estimate by ignoring samples with high error probability (Aguilera et al., 2013). Hierarchal clustering analysis (HCA) method was used in a similar manner to visualize hydrochemical links in Algeria. HCA identified three water quality groups and allowed the authors to draw links between hydraulic pathways and geology (Selmane et al., 2022). Clustering was also used to improve existing ML methods. The effect of k-means clustering on two ML techniques, ANN and SVM, was evaluated for predicting nitrate concentration. The clustered aggregate SVM performed slightly better than the clustered ANN (Alagha et al., 2014). Quantile regression (QR) and uncertainty estimation based on local errors and clustering (UNEEC) were applied to ML models SVM, RF, and k-NN in groundwater nitrate contamination prediction. The UNEEC methods had similar predictive performance statistics as RF, but better than SVM.

3.4.2.3. Clustering model assessment. Clustering methods for studying relationships among parameters is a useful tool. They have been shown to provide information on processes affecting aquifers (Aris et al., 2011; Fabbrocino et al., 2019), but much like SOM, the results are not generalizable to other study areas. However, clustering can be an excellent preprocessing tool for other ML algorithms, such as ANN and SVM (Alagha et al., 2014) or for assessing uncertainties (Rahmati et al.,

2019). While it is difficult to compare methods, there are more user-friendly parameter assessment methods (SOM) and more rigorous model enhancement methods (ensemble, GA) than clustering. However, it can be an appropriate tool where uncertainties are an important aspect of a study.

3.4.3. *Artificial intelligence with multiple frameworks (AIFM)*

A few studies used multiple ML frameworks in parallel or sequential to construct a comprehensive unsupervised learning pipeline for better data analysis and pattern discovery for specific domains to improve the basic DRASTIC framework (BDF) (See Section 2.2 for a brief explanation of the DRASTIC framework). One study used BDF parallel to AIMF with least-squares SVM (LS-SVM) and fuzzy catastrophe framework (FCF) to map aquifer vulnerability. Both frameworks were weak on their own when using N as measure of vulnerability. However, the AIMF strategy with LS-SVM produced a high accuracy in testing. Another study used four DRASTIC variations with SVM for the AIMF. The AIMF was able to enhance the correlation of coefficient value to nearly double of the best DRASTIC variation (Nadiri et al., 2018).

Various combinations of ANN, neuro-fuzzy, fuzzy logic, GEP, SVM, GA, BDF, and FCF were used in supervised and unsupervised ensemble techniques for modeling a tropical island aquifer. The best model combined the unsupervised BDF and BDF-FCF with the supervised BDF-GA and BDF-GEP using LS-SVM, displaying the advantage of both supervised and unsupervised learning types (Nadiri et al., 2019).

Unsupervised combinations of GQI and GWQI indexes were applied twice to predict Iran groundwater quality, and this combination performed better when compared to nitrate-arsenic maps in that regions (Najib et al., 2022; Sedghi and Nadiri, 2022).

Like supervised ensemble models, multiple frameworks combine several models at once. However, the models combined are variations of the BDF, which are unsupervised. The models can also be combined in some supervised method (Nadiri et al., 2018, 2018). Multiple frameworks can clearly enhance the performance of the unsupervised frameworks for prediction of groundwater quality parameters (Nadiri et al., 2018, 2018). For problems with an unsupervised problem set, multiple frameworks can be a powerful tool for the enhancements of weaker frameworks.

4. Conclusions and future work

Groundwater quality modeling using ML continues to grow as a field. This review covered over 200 papers on ML water quality modeling for prediction and management of groundwater as concise and accessible as possible without risking oversimplification. The first part of the study analyzed the literature as a group and uncovered important trends. The amount of work on this topic increased rapidly in the early 2010′s and continues to grow in recent years (Fig. 2). The world leaders in publications in this field are Iran and the United States (Fig. 8). Nitrate is by far the most studied groundwater quality parameter (Fig. 2). A great many parameters are viable for these types of prediction (Fig. 3a), although the number of parameters used often hovers between 3 and 8, to take advantage of readily available data, or 13–20, to take advantage of common hydrochemical parameters (Fig. 3b).

A wealth of models has been applied to groundwater quality modeling. For supervised learning models, ANN is the most common, followed by fuzzy, natural, and SVM (Fig. 5b). Additionally, interest in unsupervised and alternative supervised models has increased rapidly in the last 12 years.

The second part of the assessment focused on the results from each publication by model type. A brief description of the basic model type gave a basic understanding of the use. Then, an in-depth bibliography and a model assessment focused on the strengths and weaknesses of each model. ANN models are the most popular algorithm due to their high accuracy, ease of implementation, and flexibility in number of input parameters. The performance of ANN models are highly dependent on selection of input parameters and model architecture. As such, performance of ANN models compared to other model types such as SVM or ANFIS or other ANN model types such as RBFNN is not consistent. SVM and fuzzy methods are also heavily dependent on architecture and hyperparameter selection, increasing the likelihood of conflicting results. Model optimization techniques such as wavelet transform and genetic algorithms intend to eliminate some heuristic error in the base models, but don't always achieve this.

Methods such as random forest and deep learning show more constant results when compared to other model types. The random forest model achieves high accuracy from its model structure, and can manage

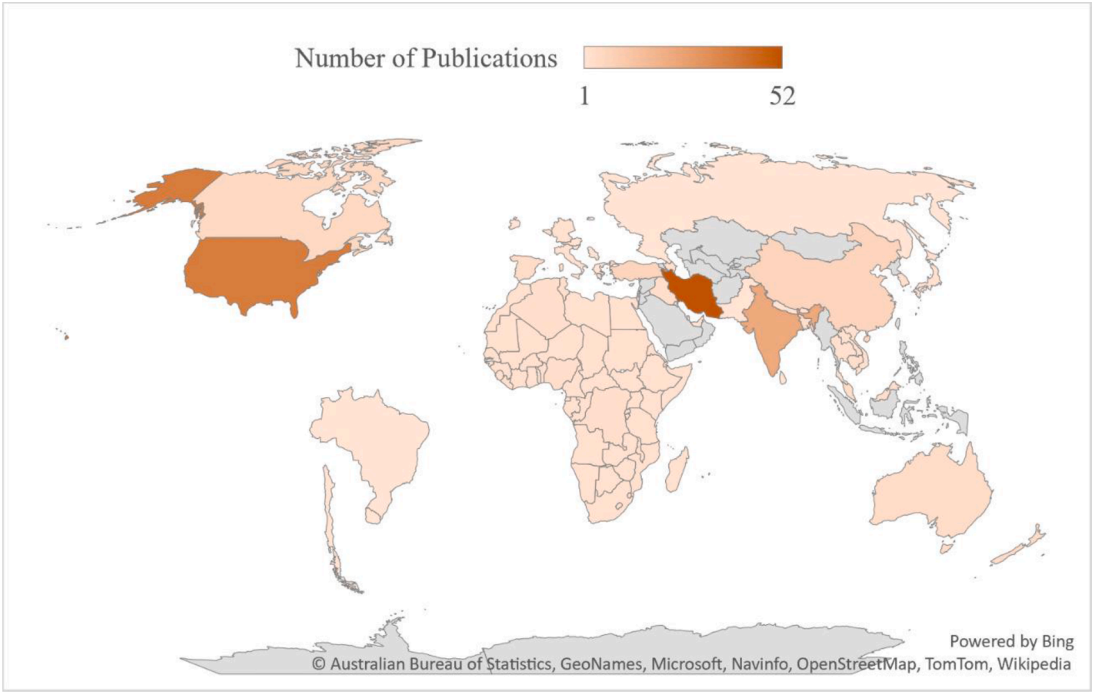

Fig. 8. Geographical locations of study areas by country.

large, missing, and outlier data well. Ensemble learning attains this as well and is another promising avenue for groundwater quality modeling. Deep learning can also achieve high accuracy and can manage unstructured data well. However, these models are all "black box" models. While potentially highly useful for GW quality management, they do not offer much insight for researchers.

As groundwater modeling through ML continues to expand, there are several areas for future researchers that should be addressed, which are discussed in the following section.

4.1. Future work

4.1.1. Implementation of best practices

Machine learning for hydrology, especially forecasting methods, is facing a modern evaluation of historical misapplication (Gharib and Davies, 2021; Zheng et al., 2018). Wavelet transform especially is prone to error often resulting from data preprocessing and handling (Du et al., 2017; Quilty and Adamowski, 2018). As the interest in ML for managing and forecasting GW quality grows, it is important to understand the missteps and limitations of these models, especially when related to data selection and handling. Without proper implementation of current standards and best practices for steps like data splitting, model architecture, and model evaluation, results from the expanding field will be muddied with errata.

4.1.2. Cessation of duplicate studies

Many papers on ANN only described how an ANN model may be applied to a certain study area. They did not provide any innovate data pre- or postprocessing ideas or amplify or modify the model to a degree that contributed significantly to the literature. This repetition is a trap for authors to avoid.

4.1.3. Application of deep learning

Deep learning is a rapidly developing field of machine learning that shows promise in hydrology (Shen, 2018). So far, it has been applied minimally to GW quality modeling (Mo et al., 2019; Perović et al., 2021; Singha et al., 2021), making this one of the biggest and most exciting opportunities in groundwater research. With the growth of GW water data collection, lifelong learning (LL) (Parisi et al., 2019) is a promising direction to solve the catastrophic forgetting issue when training an existing network on newly collected data. Meta-learning (Hospedales et al., 2022) gives a systematic solution to automatically learn a learning model from datasets with good optimization on the hyperparameters for higher prediction accuracy with a cheaper training process. This will generally help researchers discover insight for designing suitable learning algorithms in GW water research.

4.1.4. Explainable AI

Explainable AI (XAI) is another emerging tool in machine learning. Unlike many models discussed in this paper, such as ANN, which are "black box" models, XAI is a theory that aims to provide interpretation and visualization to users on the processes studied through various techniques (Samek et al., 2019). A big weakness of current ML studies right now is the caveat that all results may only hold in the specific study area, which has led to several discrepancies among model performance results. For practical studies to make an impact, they must be applicable outside of the study area, and XAI will be a useful tool for this purpose, as human-explainable results will allow for larger generalizability.

4.1.5. Exploration of underrepresented models

Many models have only been studied once for GW quality modeling, and the highest performers, along with models that have never been applied to the subject, should be explored further. Similarly, model enhancement techniques, such as genetic algorithms, have not been applied to all models and implemented in GWQ modeling.

4.1.6. Accessibility of supplementary materials

To allow for greater standards and stricter benchmarks, it is suggested that more researchers allow materials such as code and data to be open-source and available to the public. The advantages of more databases are clear, but freely available code would allow for validation across multiple study areas, and potentially provide insights from one group to another.

4.1.7. Application to new study areas

Many studies took advantage of the massive and historical datasets available in areas such as Iran and the United States. There are large areas of the world that have not had groundwater quality assessment through ML and could benefit from the analysis. The models will also be tested for robustness through this method.

4.1.8. Inclusion of infrequently used parameters

Many parameters, such as anthropological effects or long-term climate conditions, are difficult to obtain or estimate for a dataset. However, they can be powerful indicators in the present, and their exclusion in a dataset may invalidate the model after future changes in the study area. Researchers should consider a wide variety of input parameters to account for this.

4.1.9. Practical application of machine learning for groundwater quality management

This review has displayed overwhelming evidence of the power of machine learning for groundwater quality modeling. Groundwater quality management is short in this area. Application of machine learning for this purpose would reduce the cost in both time and resources of testing for groundwater quality. The bulk of literature aims to evaluate the viability of machine learning for groundwater quality forecasting to increase the accuracy and accessibility of groundwater quality prediction, but the literature does not provide clear steps to bridge the gap between academia and industrial and governmental management. An increased cooperation between data scientists and municipal authorities, such as increased open-source machine learning code and results, adaptation of water quality monitoring systems with machine learning in mind, and increased local funding for machine learning projects is necessary so that the proper evaluation and management of groundwater can be guided by machine learning.

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.

Data availability

No data was used for the research described in the article.

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Supplementary materials

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