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*CORRESPONDENCE

⊠ igul@iese.nust.edu.pk

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Groundwater estimation and determination of its probable recharge source in the Lower Swat District, Khyber Pakhtunkhwa, Pakistan, using analytical data and multiple machine learning models

Imran Ahmad¹, Ibrar Ul Haq¹, Mansoor Ahmad², Iram Gul³*, Mursaleen Khan¹, Khushnuma Khushnuma¹, Ubaid Ullah¹, Maqsood Ur Rehman⁴ and Mohamed Metwaly⁵*

¹Department of Geology, University of Malakand, Chakdara, Pakistan, ²Department of Software Engineering, University of Malakand, Chakdara, Pakistan, ³Institute of Environmental Sciences and Engineering (IESE), School of Civil and Environmental Engineering (SCEE), National University of Sciences and Technology (NUST), Islamabad, Pakistan, ⁴Institute of Advanced Marine Research, China University of Geosciences, Guangzhou, China, ⁵Archaeology Department, College of Tourism and Archaeology, King Saud University, Riyadh, Saudi Arabia

This study addresses the lack of integrated hydrogeochemical and machine learning approaches in groundwater assessment, particularly in complex mountainous terrains like the Lower Swat District, Pakistan. It aims to identify recharge sources using a combination of analytical data and advanced machine learning (ML) algorithms. Groundwater recharge sources and demarcation of feasible exploration sites via actual field data and machine learning-based approaches in the Lower Swat District were carried out. Based on variations in subsurface lithological composition (e.g., relative proportions of gravel, clay, silt, and bedrock) and the varying distances of selected well sites from the Swat River, the study area was divided into seven zones. Water samples were collected from surface runoff (river and canals) and groundwater (wells and springs) and analyzed for various physicochemical parameters, including major and trace elements, to identify the probable recharge source in the floodplain area of the Swat River. X-ray fluorescence (XRF) analysis of rock samples collected from the spring hosts was also performed to compare their mineral constituents with the dissolved load of the analyzed groundwater samples. Analytical data interpretation reveals that the recharge source for groundwater in the floodplain regime is the Swat River, while infiltration and percolation of rainwater act as probable recharge sources in the mountainous and elevated areas. Acceptable similarities were observed in the geochemical composition of the rock samples, spring water samples, and representative wells in their immediate neighborhood. A linear relationship was observed between the water table and distance from the Swat River, illustrating that water depth in wells increases with increasing distance from the main recharge source. The study applied six ML models, including random forest, support vector machine (SVM), and ridge Regression, to predict groundwater zones, with random forest achieving the highest accuracy (R^2 =

0.95, root mean square error (RMSE) = 8.49, and mean absolute error (MAE) = 4.03), followed by decision tree (R^2 = 0.93). These metrics validate the precision of our groundwater mapping and recharge zone predictions. This integrated approach improves groundwater exploration strategies and supports sustainable water resource management. Furthermore, predicted zones for potential water wells were marked in model wells using artificial intelligence (AI) and machine learning techniques.

KEYWORDS

water table, groundwater, recharge source, flood, machine learning algorithms

1 Introduction

Groundwater is essential for sustainable development and the provision of a steady, renewable supply of drinking water as it provides freshwater to one-third of the world's population (Carrard et al., 2019; Li et al., 2021). It is primarily recharged through natural processes such as precipitation and the infiltration of river water into aquifers (Zhang and Wang, 2021; Zhang et al., 2023). In Pakistan, the dependency on groundwater is steadily increasing, yet systematic assessments of recharge mechanisms remain scarce, particularly in mountainous terrains like Swat. The improper selection of drilling sites and lack of coordinated exploration often led to ineffective well placement. This study attempts to bridge the gap between geochemical data interpretation and machine learning-based groundwater modeling to offer a replicable framework. However, in urban areas, groundwater resources are increasingly threatened by overexploitation and contamination resulting from industrial activities and unregulated human development, which significantly degrade water quality (Li et al., 2021; Karunanidhi et al., 2022; Akhtar et al., 2021). An additional factor contributing to the significant decrease in aquifer levels is the unrelenting urban demand for water. In order to meet the present water resource demands and supply chain requirements, groundwater exploration using modern hydrological and geophysical techniques is crucial.

The rationale for selecting the Lower Swat District lies in its lithological diversity, unregulated groundwater usage, and increasing population pressure.

Groundwater recharge is the process through which surface water percolates into the earth and replenishes the saturated zone (Boerner and Weaver, 2012). Aquifer recharge can be estimated using a variety of techniques; however, they are primarily dependent on the baseline information that is readily available, including geology, rainfall data, precise topographical information, and climate data across a wide range of temporal and spatial scales. There are several techniques for estimating groundwater recharge, such as groundwater modeling (GM), saturated volume fluctuation (SVF), cumulative rainfall departure (CRD), the extended model for aquifer recharge and moisture (EARTH), water-table fluctuation (WTF), and chloride mass balance (CMB). Among these methods, the CMB method is the most widely used/applied globally to estimate recharge in the aeration and saturation zones (Healy, 2010). According to Marei et al. (2010), due to its conservative nature, the chloride ion is considered to be a good environmental tracer with high solubility in aqueous solutions. Xu and Beekman (2003) concluded that the CMB method is a good technique for recharge estimation in southern Africa after reviewing 30 years of studies on the subject.

Fluctuations in groundwater levels are highly variable in both space and time and are influenced by a number of factors, including geography, climate, and anthropogenic activity (Manna et al., 2019). Although rainfall is often a key driver of groundwater recharge, particularly in shallow unconfined aquifers (Abdullahi and Garba, 2015), human activities such as excessive groundwater extraction for irrigation, urban wastewater infiltration, and land use changes can also significantly influence groundwater dynamics (Ndehedehe et al., 2021; Youssef et al., 2021; Baart et al., 2024). As a conjunctive water management tool, the groundwater table analysis in the spatial-temporal patterns can be used (Vasconcelos et al., 2017). The water-table fluctuation (WTF) method is one of the physical techniques and is based on the idea that groundwater recharge occurs as a result of an increase in the groundwater level caused by earlier rainfall. This method is the most accurate method for estimating groundwater recharge when compared to studies conducted in laboratories to estimate water retention curves and pumping tests (Crosbie et al., 2005). This method is most suitable for calculating groundwater recharge in shallow unconfined aquifers where rainfall has a significant impact on the groundwater level.

With the advancement of remote sensing (RS) and geographic information systems (GIS) over the past few decades, numerous models and algorithms have been developed worldwide (Murasingh et al., 2018; Lee et al., 2018). Different types of lithological and geomorphological units serve as a base for the identification of groundwater potential zones (GWPZs). The integration of RS and GIS is considered to be a flexible tool that increases GWPZ accuracy. Researchers in different regions employ diverse methodologies to ascertain the GWPZs. Certain studies demarcate GWPZs using simple standard mathematical models-for instance, logistic regression (Chen et al., 2018), frequency ratio (Guru et al., 2017; Pourtaghi and Pourghasemi, 2014; Naghibi et al., 2015; Das and Pal, 2019), and weights of evidence (Tahmassebipoor et al., 2016; Chen et al., 2018). However, these necessitate expert-based knowledge, which means that long-term groundwater knowledge is required for the same geo-environmental factor or precise location, which is frequently unavailable. Since the statistical method can map the GWPZ on a scale of 1: 20,000 or 1: 50,000, it can map spring and well locations scientifically (Singh et al., 2013; Jha et al., 2010). However, it disregards non-linear relationships. Thus, a machine learning technique based on AI has been developed. Previous studies on groundwater prediction can broadly be categorized into (i) analytical methods such as chloride mass balance and water table fluctuation, (ii) remote sensing and GIS-based spatial models, and (iii) datadriven machine learning models. Our study builds on the third

category, integrating it with geochemical data for enhanced reliability. Despite numerous studies on groundwater recharge and potential zone mapping, few have integrated field-based chemical analysis with multiple machine learning (ML) algorithms in high-grade metamorphic regions like Lower Swat. This study addresses that gap by combining geochemical compatibility analysis and model-based well prediction.

The ML technique relies on data mining, which is necessary for enhancing groundwater capacity (Naghibi and Pourghasemi, 2015; Rahmati et al., 2016; Naghibi et al., 2016; Golkarian et al., 2018; Arabameri et al., 2019). Most studies that evaluate GWPZ use techniques like classification and regression trees (CART) (Naghibi et al., 2015; 2016; Kordestani et al., 2019), random forest (RF) (Youssef et al., 2016; Naghibi and Dashtpagerdi, 2017a; Kim et al., 2018), support vector machines (SVMs) (Naghibi and Dashtpagerdi, 2017a; Lee et al., 2018), and artificial neural networks (ANNs) (Lee et al., 2018). These techniques provide an accurate estimation of a region's potential for groundwater in the future (Naghibi and Pourghasemi, 2015; Chen et al., 2018). Complex classification and mapping issues are resolved through the use of hybrid machine learning techniques. This method is more effective than a single method because it addresses the shortcomings of individual models (Naghibi et al., 2017b; Kordestani et al., 2019). Researchers propose to design and evaluate new techniques for mapping the groundwater potential zone based on this integrated or hybrid model. Based on the recent literature emphasizing datadriven groundwater potential mapping (Naghibi et al., 2017b; Lee et al., 2018), the present study employs a hybrid AI/ML modeling framework for enhanced predictive accuracy. The reviewed methods directly informed our choice of regression-based and ensemble learning models.

Recent studies have extended the use of machine learning in hydrological assessments. For example, groundwater source identification through unsupervised ML in New Mexico (Hobbs et al., 2025) provides a model for our recharge source detection approach. Similarly, the impact of the Chamravattam regulator on Bharathapuzha River (Ajith and James, 2016) exemplifies the regional hydrological influence of man-made structures. The objectives of this study are (i) to determine groundwater recharge sources using chemical and lithological data; (ii) to apply and compare ML models for well site prediction; and (iii) to evaluate the relationship between geochemistry and distance from the recharge source. Despite extensive studies on groundwater estimation, few have explored the integration of machine learning algorithms with geochemical field data in high-relief terrains. This lack of interdisciplinary methodology limits the reliability of groundwater zone predictions.

2 Materials and methods

2.1 Study area

The study area lies in the Lesser Himalayas, an integral part of the Himalayan Tectonostratigraphic Basin, which is tectonically active and hydrogeologically diverse. The Lesser Himalayas are bounded in the south by a regional tectonic boundary, Main Boundary Thrust (MBT), and in the north by Main Mantle Thrust (MMT), offering a unique combination of metamorphic rocks, igneous intrusions, and unconsolidated glacial and fluvial deposits. The MBT is the southernmost thrust, which places metasedimentary rocks of the Lesser Himalayas over the unmetamorphosed clastic rocks of the Himalayan foredeep (Figure 1).

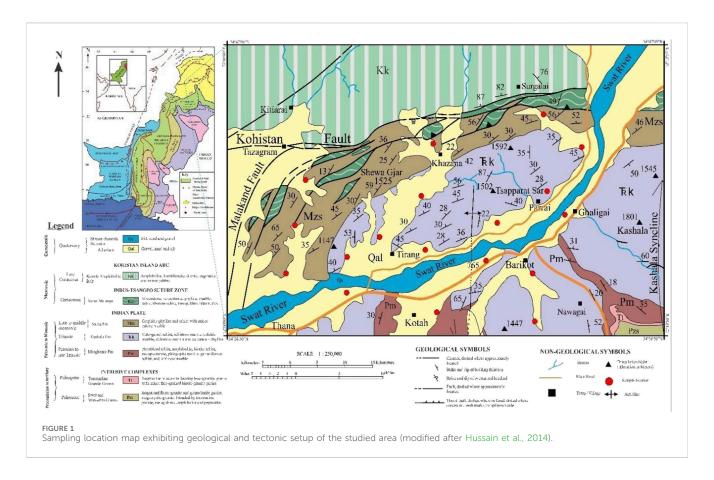
Swat District, located in the Lesser Himalayas, is a mountainous terrain composed mainly of metamorphic rocks intruded by several igneous intrusions. Intermontane basins of the study area are filled with unsorted glacial and sorted fluvial deposits. Glacial deposits have capped most of the bedrock units in the Upper Swat District, while fluvial deposits are common in the Lower Swat District. Fluvial deposits are mostly composed of sorted layers of boulders, pebbles, cobbles, sand, silt, and clay. These materials are eroded and transported by multiple perennial and seasonal contributory channels originating from the surrounding mountains. The coarse alluvial deposits comprising sand, gravel, pebbles, and boulders are found along mountain fronts (Figures 2, 3).

The study area was selected due to its increasing reliance on groundwater for domestic and agricultural purposes, increasing urban demand, and lack of systematic groundwater assessments. Its hydrogeological complexity, characterized by varied lithologies and dynamic recharge patterns, makes it an ideal case for assessing groundwater potential and quality. The area's significance also stems from the presence of multiple perennial and seasonal tributaries that influence sediment distribution and aquifer characteristics, offering valuable insights into groundwater dynamics in mountainous terrains.

2.2 Field survey and sample collection

Extensive fieldwork activity was conducted to collect field data and rock/water samples and mark the inspected area on a map. During this field visit, data including well depth, water level, location, well logs, distance from the Swat River, variations in the water level, and the diameter of the wells (whether they are bore wells or dug wells) from approximately 500 points were collected. Maximum data were acquired through structured interviews with well owners/local residents and field observations. Additionally, the installation dates and the current status of wells along with fluctuations in the water table were also recorded as a basic part of the data collection process. These diverse data points provide a comprehensive overview of the wells in the area, enabling us to analyze and draw meaningful conclusions about the water resources and their associated hydrogeological characteristics.

After an extensive field visit, a total of 15 water samples were collected from various locations and sources (the river, canals, springs, hand pumps, boreholes, open wells, dug wells, and water-logged areas) within the study area and subsequently analyzed (Figure 1). The area was divided into seven zones based on the distance of samples from the Swat River, namely, Group A (0–250 m), Group B (251–500 m), Group C (501–1,000 m), Group D (1,001–1,500 m), Group E (1501-2000 m), Group F (2001–2,500 m), and Group G (2,501–3,000 m). In order to ensure representative sampling, 1–2 samples from each zone were collected. This approach allowed for a diverse range of water sources to be included in the analysis, providing a



comprehensive understanding of the water quality and characteristics in the study area.

Sampling locations were selected to reflect spatial heterogeneity in terms of altitude, proximity to surface water bodies, lithological differences, and land use. This strategy aligns with established groundwater sampling guidelines, ensuring comprehensive spatial coverage (APHA, 2017).

Water samples were collected using sterilized polyethylene bottles, labeled properly, and transported within 24 h to the Pakistan Council of Research in Water Resources (PCRWR) laboratory for analysis.

Additionally, four rock samples were specifically collected from the vicinity of springs and wells to complement the water sampling and provide valuable insights into the geological composition and context of the surrounding areas. The rock samples were analyzed at the Centralized Resource Laboratory (CRL), University of Peshawar.

2.3 Sample analysis

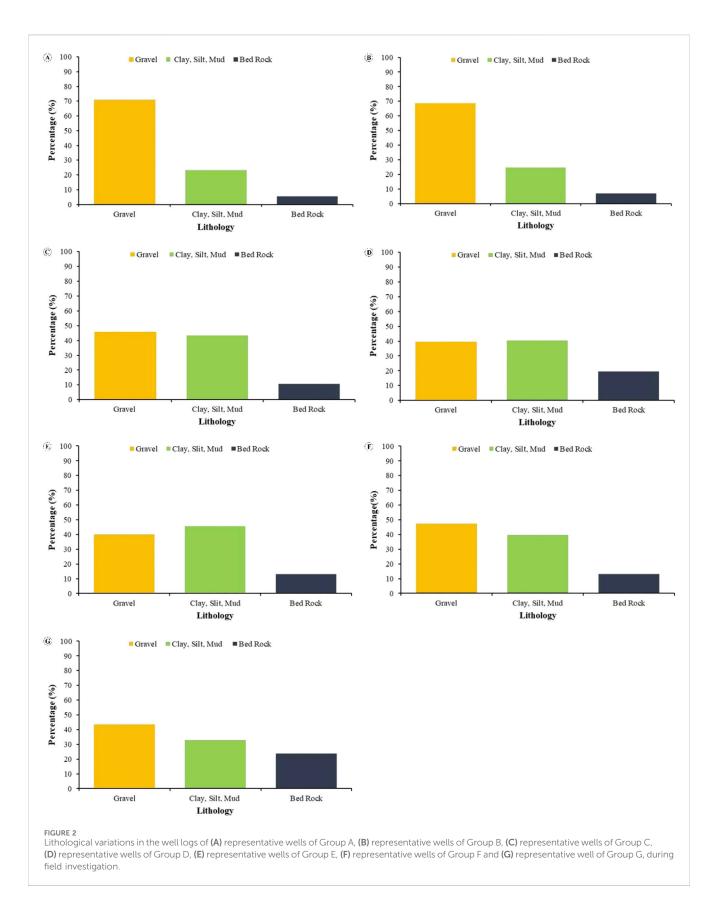
The physicochemical characteristics of the water samples, including alkalinity, hardness, total dissolved solids (TDS), carbonates, bicarbonates, calcium (Ca), magnesium (Mg), chloride (Cl), potassium (K), sodium (Na), sulfate (S), and nitrate (N), were determined using standard procedures (APHA, 2017).

The elemental composition (both major elements, i.e., Mg, Ca, Fe, and Si, and minor/trace element, i.e., Mn within the rock samples) of rock samples was analyzed using X-ray fluorescence (XRF) spectroscopy. First, the rock samples were crushed into

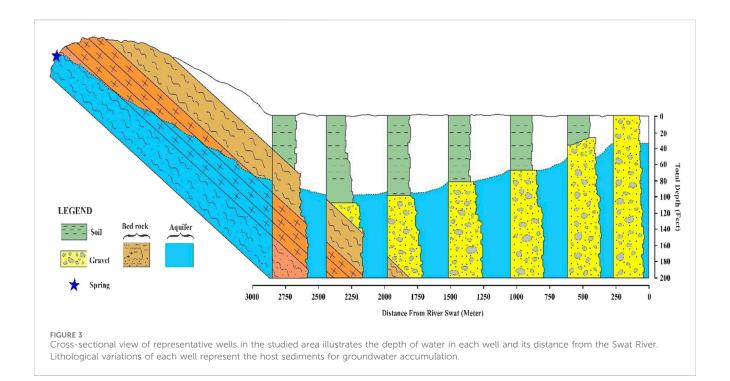
powder using a crushing machine; afterward, 0.5 g of powdered samples was digested in an aqua regia solution (HNO₃: HCl in a 1: 3 ratio) on a hot plate at 200°C for 2 h. After complete digestion, samples were diluted to 100 mL with deionized water, mixed well, and filtered. The major and trace elements including aluminum (Al), silicon (Si), calcium (Ca), iron (Fe), potassium (K), titanium (Ti), sulfur (S), strontium (Sr), zirconium (Zr), vanadium (V), zinc (Zn), copper (Cu), iridium (Ir), and yttrium (Y) in the digested samples were analyzed through XRF.

2.4 Machine learning

ML is a branch of artificial intelligence (AI) that primarily focuses on creating algorithms and statistical models that enable systems to learn from data and make decisions without being explicitly programmed. Huge amounts of data can be used by ML systems for finding patterns, predicting outcomes, or improving performance through experience over (Domingos, 2012). This technology has made possible the automation of complex processes in several industries, facilitating decision making and generating insights that were hitherto impossible (Jordan and Mitchell, 2015). The heart of machine learning is to create models that generalize well from training data to unseen examples, thus enabling accurate prediction or classification (McAfee and Brynjolfsson, 2017). Various techniques such as supervised learning, unsupervised learning, and reinforcement learning are employed for this purpose in different situations (Bishop, 2006). Machine learning technologies



have been expanding their capabilities due to the exponential growth of data and increased computing speed, resulting in innovations such as condition monitoring tools in the healthcare industry; fraud detection algorithms in the financial sector; personalized product development based on customer preferences in marketing; and autonomous navigation systems in drones, among other



applications within these fields (Goodfellow et al., 2016). Recent studies continue to show innovative uses of AI/ML in hydrology. For instance, lean construction AI in Iran (Ugural et al., 2024), groundwater potential zone mapping in Kohat (Faheem et al., 2023), and GIS-based recharge studies in Swat (Hussain et al., 2022) support the relevance of hybrid geospatial and machine learning approaches.

2.4.1 Linear regression

Linear regression is a technique in statistics that explains the relation between the dependent variable and one or more independent variables. It is meant to identify the linear equation that best forecasts the dependent variable from other independent variables. The mathematical expression of a simple linear regression line is given by $y = \beta 0 + \beta 1x + \epsilon$, where y represents the dependent variable, x represents the independent variable, $\beta 0$ is the y-intercept, $\beta 1$ denotes the slope of the line, and ϵ represents the error term, which accounts for variability in y that cannot be explained by its linear relationship with x. The parameters $\beta 0$ and $\beta 1$ are estimated using methods such as the least squares procedure, which minimizes the sum of squared differences between the observed values and those predicted by the model (Weisberg et al., 2013; Seber and Lee, 2012).

2.4.2 Decision tree

The decision tree is a flexible machine learning model that can be used for classification and regression. It splits data into subsets based on input features recursively to form a tree-like structure, with each node representing a decision made based on a feature and each leaf node standing for the predicted outcome. The objective in regression is to make predictions about continuous dependent variable y using one or more independent variables x_1, x_2, \ldots, x_p . Usually, the splitting criterion at each node is the

mean squared error (MSE), which is calculated as shown in Equation 1:

$$MSE(t) = \frac{1}{N_t} \sum_{i \in t} (y_i - \hat{y}_t)^2, \qquad (1)$$

where N_t is the number of observations in node, y_i is the actual value, and \widehat{y}_t is the mean target value in node t. The selection of features and thresholds for split is done to maximize the reduction in MSE, which is defined as shown in Equation 2:

$$\Delta MSE = MSE(t) - \left[\frac{N_t^L}{N_t} MSE(t^L) + \frac{N_t^R}{N_t} MSE(t^R) \right], \qquad (2)$$

where t_L and t_R are child nodes. Stopping criteria, such as maximum depth or minimum samples per leaf, determine when the tree stops growing. Predictions for new observations are based on their average values.

2.4.3 Random forest

Random forest for regression involves building multiple decision trees on various bootstrap samples of the training data and then averaging their predicted values to improve accuracy and reduce overfitting. Mathematically, for an input x, the predicted value \hat{y} is calculated as shown in Equation 3:

$$\hat{y} = \frac{1}{B} \sum_{b=1}^{B} T_b(x), \tag{3}$$

where $T_b(x)$ is the prediction from the bth tree and B is total number of trees in the forest (Breiman, 2001). By aggregating outputs of several trees, random forest can provide robust predictions that capture complex patterns in data (Liaw and Wiener, 2002).

2.4.4 Support vector machine

SVM for regression, also referred to as support vector regression (SVR), searches for a function that approximates with minimum errors of prediction how input features relate to the target variable. The aim is to find a function $f(x) = w^T x + b$ that deviates from the actual target values y_i by at most ϵ while maintaining the smallest possible margin. Mathematically, the optimization problem is defined as follows (Equation 4):

$$\min_{w,b,\xi} \quad \frac{1}{2} |w|^2 + C \sum_{i=1}^n \xi_i \tag{4}$$

2.4.5 Ridge regression

Ridge regression is a method used to tackle multicollinearity and overfitting in linear regression by supplementing the loss function with a regularization term. The main aim is to minimize the sum of squared residuals with an additional penalty that is proportional to the square of the size of the coefficients. Mathematically, ridge regression can be described as shown in Equation 5:

$$\min_{w} \left\{ \frac{1}{2} \sum_{i=1}^{n} (y_i - x_i^T w)^2 + \lambda |w|^2 \right\}, \tag{5}$$

where w represents a vector of coefficients, y_i represents target values, x_i represents input features, and λ is a regularization parameter that specifies how strong this penalty term should be (Hoerl and Kennard, 1970; Tikhonov and Arsenin, 1977). By introducing $\lambda |w|^2$, ridge regression can balance between model fit and coefficient complexity, leading to more robust and interpretable predictions (Hastie et al., 2009).

2.4.6 Multi-layer perceptron

An artificial neural network named multi-layer perceptron (MLP) is employed, in general, for classification and regression. It is made up of several layers of neurons, consisting of an input layer or an output layer and one or more hidden layers. Every neuron calculates a weighted sum of its inputs, followed by a non-linear activation function. The mathematical form for the output \hat{y} of an MLP is provided in Equation 6 as follows:

$$\hat{y} = f(W_L \sigma(W_{L-1} \cdots \sigma(W_1 x + b_1) \cdots + b_{L-1}) + b_L), \tag{6}$$

where W_l and b_l are the weights and biases of the lth layer, σ is a non-linear activation function (like ReLU or sigmoid), and f is the output activation function (Bishop, 2006). MLP learns to adjust the weights W_l and biases b_l through backpropagation to minimize the loss function, thereby improving its predictive performance (Goodfellow, Bengio and Courville, 2016; Rumelhart, Hinton and Williams, 1986; LeCun et al., 1998).

3 Results

3.1 Lithological variation

The lithological variations observed in wells within various zones at distinct distances from the Swat River are presented in Figure 2. One of the essential parameters in data collection was the well log, which provides valuable insights into the subsurface

lithology. To obtain lithological data, we directly interviewed well owners or well constructors during field visits. They were asked to describe the sequence of materials encountered during well construction such as the order and thickness of gravel, clay, silt, mud, and bedrock layers. This local knowledge was systematically recorded and cross-compared among wells in each group. For each group, this information was carefully examined to identify the prevailing lithological composition, including gravel (a combination of pebbles, cobbles, and sand), clay, silt, mud, and bedrock. The maximum percentage of gravel was observed in group A, followed by groups B, C, F, G, E, and D. The results showed that the wells located in Zone A contain a higher amount of gravel than those located in other zones. The gravel in wells of groups A, B, C, D, E, F, and G was 71%, 68%, 48%, 39%, 40%, 46%, and 42%, respectively. The maximum percentage of clay, silt, and mud (32%) was found in Group E, while the minimum (22%) was found in Group A. Moreover, bedrock was most prevalent in Group G (24%) and least prevalent in Group A (8%).

3.2 Geochemistry of water samples

The physicochemical characteristics of water samples collected from different zones of the study area are presented in Table 1. Calcium carbonate (CaCO₃) and bicarbonate levels are important indicators of water alkalinity and potential scaling. Calcium (Ca), chloride (Cl), hardness, magnesium (Mg), potassium (K), sodium (Na), sulfate (S), nitrate (N), and TDS measurements provide insights into specific ions and compounds present in the water, affecting its taste, corrosiveness, and suitability for different applications such as drinking, agriculture, or industrial use. Alkalinity of water samples in the study area ranged between 1.4 and 5.8 ppm; bicarbonate, 70-300 ppm; Ca, 10-30 ppm; Cl, 17-45 ppm; hardness, 100-340 ppm; Mg, 17-48.6 ppm; K, 0.7-2.3 ppm; Na, 9-40 ppm; S, 6-35 ppm; nitrates, 1.3-4.5 ppm; and TDS, 119-424 ppm. Carbonate was not detected in any of the samples. All measured parameters were within the permissible limits for drinking water as set by the Pakistan Environmental Protection Agency (Pak-EPA et al., 2008), which include Ca ≤75 mg/L, Cl ≤ 250 mg/L, hardness ≤500 mg/L, $Mg \le 150 \text{ mg/L}, \text{ Na} \le 200 \text{ mg/L}, \text{SO}_4 \le 250 \text{ mg/L}, \text{NO}_3 - \text{N} \le 10 \text{ mg/L}$ L, and TDS ≤1,000 mg/L. Although no specific limits are set for alkalinity, bicarbonate, and potassium, the values observed are internationally acceptable ranges. Additionally, microbiological testing showed the absence of E. coli and fecal coliforms, and total coliform levels were within permissible limits, indicating that water is microbiologically safe for consumption. Minimum alkalinity, hardness, and Ca were observed in river water; however, the spring and well (CW-4) showed maximum alkalinity, hardness, and Ca. According to the physicochemical parameters, all samples collected from different sources were safe for drinking.

3.3 Geochemistry of rock samples

The geochemical compatibility of different oxides was examined using X-ray fluorescence spectroscopic analysis. The different oxides

TABLE 1 Physicochemical characteristics of water samples collected from different locations in the Swat District.

Parameter (ppm)	DS- 1	RW	WL	DPC	NS- 2 A	NS- 3 B	AW-	BW-	BW-	CW-	DW- 5	EW-	FW-	GW-	RS- 4
Alkalinity as CaCO ₃	5.6	1.4	2.6	1.6	4.9	4.8	4.6	4	4.4	6	5.2	5.8	5.6	5.4	4
Bicarbonate	280	70	130	80	245	240	230	200	220	300	260	290	280	270	200
Calcium	80	12	20	10	26	28	30	40	40	50	50	55	56	45	20
Carbonate	BD	BD	BD	BD	BD	BD	BD	BD	BD	BD	BD	BD	BD	BD	BD
Chloride	28	20	22	20	24	20	17	25	32	45	29	35	40	30	25
Hardness	300	100	150	100	280	270	260	230	250	340	290	330	310	300	230
Magnesium	24	17	24	18	52	48.6	45	31.6	36	52	40	46.8	41	46	44
Potassium	1.2	0.7	1	0.7	1.1	0.9	1	1.2	1.6	2.1	1.7	1.5	2.3	1.2	1
Sodium	22	12	12	9	15	13	14	19	30	40	23	27	30	21	17
Sulfate	14	15	6	7	22	19	28	24	32	35	25	28	27	18	19
Nitrate	3.6	2.3	3.1	1.3	2.9	2.7	2.5	3.6	3.9	4.5	3.7	4	3.6	3.9	3.9
Total dissolved solids	353	129	177	119	300	285	284	277	321	424	341	385	381	339	263

DS-1, Dadahara Spring; RW, river water; WL, water-logged area; DPC, Dadahara Plain Canal; NS-2-A, Nagoha Spring Pipe; NS-3-B, Nagoha Spring; AW-1, Shamozai Bridge Well (where A represent Group A); BW-2, Dadahara Plane Well (where B represent Group B); BW-3, Aurangzeb Well (where B represent Group B); CW-4, Abbas Mama Well (where C represent Group C); DW-5, Abbas Friend Well (where D represent Group D); EW-6, Iftikhar Well (where E represent Group E); FW-7, Home Well (where F represent Group F); GW-8, Mulasan Baba Well (where G represent Group G); RS-4, Rangela Spring; and BD, below detection.

and elements present in rock samples are presented in Table 2. The highest amount of silicon dioxide was obtained in all rock samples. The maximum SiO₂ was found in DRS-1 (61.193), followed by RRS-4 (49.144), NRS-3 (16.688), and DPRS-2 (12.184). DRS-1 samples contained aluminum oxide (20.62), calcium oxide (8.54), iron (III) oxide (4.93), potassium oxide (3.62), titanium oxide (0.79), strontium oxide (0.067), manganese oxide (0.057), vanadium pentoxide (0.045), chromium oxide (0.025), rubidium oxide (0.017), copper oxide (0.016), zinc oxide (0.015), iridium oxide (0.011), and yttrium oxide (0.003), and nickel oxide and sulfur oxide were not observed. The oxides of vanadium, zirconium, chromium, rubidium, zinc, iridium, yttrium, and sulfur were not found in DPRS-2. Moreover, rubidium oxide, yttrium oxide, nickel oxide, and sulfur oxide were not observed in RRS-4. Oxides of zirconium, iridium, yttrium, and nickel were not detected in NRS-3.

3.4 Well cross-sections and their respective logs

This research investigates the relationship between the variations in depth of the water table in response to its variable distance from the Swat River in the representative wells within the study area. The study area is divided into seven distinct groups, ranging from Group A to Group G, each encompassing five representative wells (Figure 3). The primary objective is to understand how the water level in these wells varies as we move away from the river. The lithological composition of the wells includes gravel, soil, and bedrock, which serve as potential reservoirs/aquifers for groundwater accumulation.

3.5 Machine learning

3.5.1 Model performance analysis

3.5.1.1 Linear regression

RMSE = 22.43, MAE = 17.01, and $R^2 = 0.66$.

Linear regression shows high root mean square error (RMSE) and mean absolute error (MAE), indicating higher prediction errors. R^2 value reveals a moderate correlation, but it is not highly significant.

3.5.1.2 Decision tree

RMSE = 10.49, MAE = 3.88, and $R^2 = 0.93$.

The decision tree model performs well with low values of RMSE and MAE, which indicate smaller prediction errors made by the model during training. An R^2 value of 0.93 indicates a very strongly correlation with the actual values.

3.5.1.3 Support vector machine

RMSE = 22.86, MAE = 15.03, and $R^2 = 0.65$.

Among the models, SVM has the highest RMSE, indicating poor performance; it also has a high MAE, while its R^2 value is low, thus suggesting that this model does not fit the data well.

3.5.1.4 Multi-layer perceptron

RMSE = 15.55, MAE = 10.31, and $R^2 = 0.84$.

Compared to other models, MLP performs moderately, maintaining RMSE and MAE values balanced for prediction purposes. The achieved R^2 value demonstrates a good fit though not as strong as that of the decision tree and random forest models.

TABLE 2 a) Different oxides observed in rock samples from the Swat District. b) Different elements observed in rock samples from the Swat District.

Silicon dioxide (SiO2) 61.193 12.184 16.688 Aluminum oxide (Al2O3) 20.625 7.25 12.487 Calcium oxide (CaO) 8.544 78.04 62.566 Iron (III) oxide (Fe2O3) 4.926 1.474 5.242	49.144 15.783 7.511 23.6 0.07 3.227 0.028
Calcium oxide (CaO) 8.544 78.04 62.566 Iron (III) oxide (Fe ₂ O ₃) 4.926 1.474 5.242	7.511 23.6 0.07 3.227
Iron (III) oxide (Fe ₂ O ₃) 4.926 1.474 5.242	23.6 0.07 3.227
	0.07 3.227
D	3.227
Potassium oxide (K ₂ O) 3.62 0.337 1.419	
Titanium dioxide (TiO ₂) 0.796 0.464 0.802	0.028
Strontium oxide (SrO) 0.067 0.187 0.319	
Manganese oxide (MnO) 0.057 0.029 0.073	0.338
Vanadium pentoxide (V_2O_5) 0.045 0 0.031	0.178
Zirconium dioxide (ZrO ₂) 0.041 0 0	0.011
Chromium oxide (Cr ₂ O ₃) 0.025 0 0.029	0.063
Rubidium oxide (Rb2O) 0.017 0 0.012	0
Copper oxide (CuO) 0.016 0.028 0.026	0.017
Zinc oxide (ZnO) 0.015 0 0.017	0.024
Iridium oxide (Ir ₂ O ₃) 0.011 0 0	0
Yttrium oxide (Y ₂ O ₃) 0.003 0 0	0.006
Nickel oxide (NiO) 0 0.006 0	0
Sulfur trioxide (SO ₃) 0 0 0.289	0
Silicon (Si) 50.88 7.41 9.32	37.4
Aluminum (Al) 16.09 4.46 8.66	13.1
Calcium (Ca) 14.62 84.7 71.6	9.66
Iron (Fe) 9.441 1.89 6.89	35.1
Potassium (K) 6.821 0.48 1.73	0
Titanium (Ti) 1.263 0.67 0.88	3.71
Sulfur (S) 0.233 0 0.16	0
Strontium (Sr) 0.171 0.29 0.53	0.06
Manganese (Mn) 0.118 0.04 0.11	0.55
Zirconium (Zr) 0.095 0 0	0.02
Vanadium (V) 0.06 0.02 0.025	0.19
Chromium (Cr) 0.05 0 0.031	0.085
Rubidium (Rb) 0.048 0 0.022	0
Zinc (Zn) 0.037 0 0.026	0.053
Copper (Cu) 0.035 0.039 0.037	0.032
Iridium (Ir) 0.027 0 0	0
Yttrium (Y) 0.007 0 0.008	0

3.5.1.5 Ridge regression

RMSE = 22.43, MAE = 17.01, R^2 = 0.66.

In terms of results, ridge regression is similar to linear regression, exhibiting relatively high prediction errors and a moderate correlation coefficient.

3.5.1.6 Random forest

RMSE = 8.49, MAE = 40.3, and $R^2 = 95$.

The smallest RMSE and MAE values indicate that random forest outperforms all other models by making the most precise predictions. An excellent fit, reflected by an R^2 value of 0.95, shows that this model accounts for 95% of the variance in the data.

In addition to predicting chemical concentration trends, the models were used to identify spatial zones with high groundwater potential based on their predictive scores, lithological context, and recharge proximity. Model performance was validated using RMSE, MAE, and R^2 values. Among all, random forest performed best (RMSE = 8.49 and R^2 = 0.95), followed by decision tree (R^2 = 0.93). Cross-validation techniques ensured robustness and minimized overfitting. Visual plots further confirmed model reliability. The machine learning-based classification enabled the demarcation of feasible GWPZs, aligning with the objective of well location optimization mentioned in the introduction.

All model configurations of each machine learning model showed that the PCC values ranged from 0.82 to 0.98. This range illustrates that there was a strong to very strong positive linear correlation between the observed and predicted values. The highest correlation (PCC = 0.98) demonstrates great model fit and is particularly important when trends need to be captured accurately. What stood out were the MBE values, which ranged from -5.88 to 1.62, illustrating that some models slightly overestimate, while others underestimate the values; however, the biases are generally acceptable. The MBE value of -5.88 for one model shows a tendency to underestimate, suggesting that the model may need further calibration.

The MBE values also mark the boundaries at which models can be considered robust. RAE values ranging from 0.13 to 0.55 indicate that the model predictions are reliable, with lower values indicating better performance in minimizing relative error compared to a naive benchmark model (i.e., mean predictor). The NSE values ranging from 0.65 to 0.95 corroborate the models' reliability. An NSE value greater than 0.5 denotes superior model performance compared to the mean value extracted from the observed data. Values nearing 1 indicate high skill in prediction. It is clear that the model with NSE = 0.95 performs excellently as it captures both the variability and magnitude of the data.

3.5.1.7 Graphical representation

These images illustrate the comparison between predicted and actual values for each model. Decision tree and random forest models closely align with the actual data points, visually confirming their superior performance. In contrast, linear regression, ridge regression, and SVM show greater deviations from the actual values, implying poorer performance. The MLP model produces predictions that are very close to the ground truth though some fluctuations are present.

Metric	Linear regression	Decision tree	Support vector machine	Multi-layer perception	Ridge regression	Random forest
RMSE	22.43	10.49	22.86	15.55	22.43	8.49
MAE	17.01	3.88	15.03	10.31	17.01	4.03
R-square	0.66	0.93	0.65	0.84	0.66	0.95
STDEV	33.40	38.76	31.07	37.50	33.36	37.09
RSR	0.67	0.27	0.73	0.41	0.67	0.22
PCC	0.82	0.96	0.82	0.92	0.82	0.98
MBE	1.25	-1.65	-5.88	1.62	1.25	-1.54
RAE	0.55	0.13	0.49	0.33	0.55	0.13
NSE	0.66	0.93	0.65	0.84	0.66	0.95

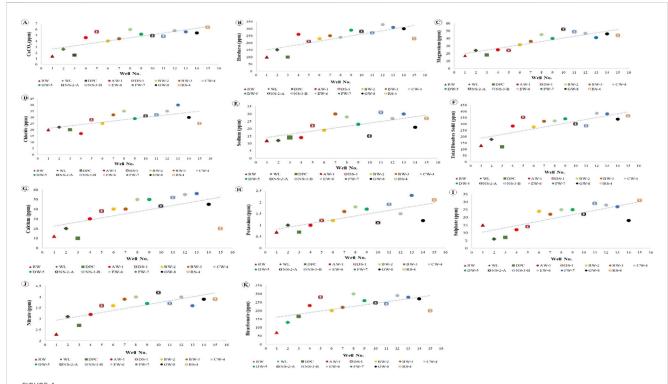


FIGURE 4
Graphs representing the concentration of (A) calcium carbonate, (B) hardness, (C) magnesium, (D) chloride, (E) sodium, and (F) total dissolved solids detected in the water samples against their respective wells and springs, representing an increase in the concentration of (A) calcium carbonate, (B) hardness, (C) magnesium, (D) chloride, (E) sodium, and (F) total dissolved solids. Graphs representing the concentration of (G) calcium, (H) potassium, (I) sulfate, (J) nitrate, and (K) bicarbonate detected in the water samples against their respective wells and springs, representing an increase in the concentration of (G) calcium, (H) potassium, (I) sulfate, (J) nitrate, and (K) bicarbonate in the water samples collected from representative wells.

4 Interpretation of results: recharge source and groundwater potential mapping

This section interprets the analytical and model-based results presented in Section 3 (Results), with a focus on identifying groundwater recharge mechanisms and delineating GWPZs using machine learning predictions.

4.1 Geochemistry of water samples

4.1.1 Calcium carbonate

Interpretation of the analytical data reveals that the concentration of CaCO₃ is variable in the investigated water samples collected from different locations. Furthermore, the amount of calcium carbonate is very high in Dadahara Spring, Group C well (CW-4), and Rangela Spring, representing the

association of these water samples with carbonate-bearing rocks (Figure 4A). The percolated water has passed through carbonate-bearing rocks, i.e., marble, which has enhanced the concentration of dissolved CaCO₃ ions in the analyzed samples. The dashed line indicates the increasing concentrations of CaCO₃ with increasing distance of the wells/location of collected water samples from the Swat River. Increasing distance from the main recharge source (i.e., Swat River) indicates that the percolation and infiltration of surface water (from streams and rainfall) through carbonate-bearing rocks cause chemical weathering/dissolution, resulting in higher CaCO₃ concentrations in water (Figure 4A).

4.1.2 Hardness

Geochemical data interpretation reveals that hardness is variable in the investigated water samples collected from different locations in the study area. Moreover, hardness is very high in Group E well (EW-6), Group F well (FW-7), and Group G well (GW-8), representing the association of these water samples with calciumand magnesium-bearing rocks (Figure 4B). The percolated water has passed through these rocks and enhanced the concentration of dissolved calcium and magnesium ions in the analyzed samples. The dashed line indicates the rising trend of hardness with increasing distance of the wells/location of the collected water samples from the Swat River. Increasing distance from the main recharge source (i.e., Swat River) indicates that the percolation and infiltration of surface water (streams and rainfall) through these rocks cause chemical weathering/dissolution, leading to an increase in hardness in the water.

4.1.3 Magnesium

Interpretation of the geochemical data reveals that the concentration of magnesium is variable in the examined water samples collected from different locations. Additionally, the amount of magnesium is very high in Nagoha Spring, Nagoha Spring Pipe, and Group E well (EW-6), representing the association of these water samples with magnesium-bearing rocks (Figure 4C). The percolated water has passed through the magnesium-bearing rocks, i.e., dolomitic marble [Ca(MgCO₃)₂] and serpentine-bearing rocks, which has enhanced the concentration of dissolved Mg ions in the examined samples. The dashed line indicates the increasing concentrations of Mg with increasing distance of the wells/location of collected water samples from the Swat River. Increasing distance from the main recharge source (i.e., the Swat River) indicates that the percolation and infiltration of surface water (streams and rainfall) through the magnesium-bearing rocks cause chemical weathering/dissolution, leading to an increase in the magnesium concentration in the water.

4.1.4 Chloride

The interpretation of analytical data indicates variations in the concentration of chloride among the investigated water samples collected from different locations. The analysis of chloride (Cl¹-) concentration across the examined water locations reveals a consistent and notable increase in their levels with increasing distance (Figure 4D). This trend indicates that various geological and hydrological factors contribute to the observed chloride variations, particularly in areas such as Group C (CW-4) and Group F (FW-7) where the concentrations are prominently

elevated. The increasing concentrations of chloride are likely influenced by factors such as the dissolution of chloride-bearing minerals or anthropogenic inputs. The proximity of CW-4 and FW-7 to potential sources of chloride, such as chloride-bearing rocks, urban areas, or agricultural activities could contribute to the higher chloride levels observed in these locations. Additionally, the pattern of increasing chloride concentrations with increasing distance from the Swat River suggests that the percolation of surface water through the rocks plays a role in transporting chloride ions into the subsurface water sources, which results in an increase in the concentration of chloride in the water.

4.1.5 Sodium

Interpretation of the analytical data reveals that the concentration of sodium is variable in the examined water samples collected from different locations. Furthermore, the amount of sodium is very high in Group B well (BW-3), Group F well FW-7, and Nagoha Spring Pipe, representing the association of these water samples with sodium-bearing rocks (Figure 4E). The percolated water has passed through the sodium-bearing rocks, which has enhanced the concentration of dissolved Na ions in the studied samples. The dashed line indicates the ascending concentrations of sodium with increasing distance of the wells/ location of collected water samples from the Swat River. Increasing distance from the main recharge source (i.e., Swat River) indicates that the percolation and infiltration of surface water (streams and rainfall) through sodium-bearing rocks cause chemical weathering/ dissolution, leading to an increase in the sodium concentration in the water.

4.1.6 Total dissolved solid

Total dissolved solids (TDS) are a measure of the combined content of all inorganic and organic substances dissolved in water. It includes minerals, salts, metals, cations, anions, and sometimes even small amounts of organic matter.

Interpretation of the analytical data reveals that the concentration of TDS is variable in the inspected water samples collected from different locations in the studied area. Furthermore, the amount of TDS is very high in Dadahara Spring, Group E well (EW-6), and Group F well (FW-7). A cross plot of TDS vs. analyzed samples indicates that the concentrations of TDS increase with increasing distance of the wells/location of collected water samples from the Swat River (Figure 4F). Increasing distance from the main recharge source (i.e., Swat River) indicates that the percolation and infiltration of surface water (streams and rainfall) pass through rocks susceptible to dissolution or chemical weathering, leading to an increase in TDS concentrations in the water.

4.1.7 Calcium

Cross plot of Ca *versus* their corresponding sample locations illustrates that the concentration of calcium varies randomly in the examined water samples collected from the studied area. In particular areas such as Group C well (CW-4), Group D well (DW-5), Nagoha Spring, Group E well (EW-6), and Group F well (FW-7) stand out with notably high calcium concentrations, implying a close connection to calcium-bearing rocks (Figure 4G). The concentration of calcium (Ca²⁺) across the analyzed water

sample reveals a consistent trend of increasing levels with ascending distance from the Swat River. The observed pattern indicates that the percolation of water through calcium-rich rocks, such as marble, or other calcium-bearing rocks like calcic-rich schists, serves as a source of calcium content in the water samples. The increasing concentration of Ca in different water samples is illustrated by a dashed line in the acquired cross plot, which shows that water samples collected from mountainous area possess higher amount of calcium. This increase in the concentration of Ca suggests that the percolated water has interacted with surface/sub-surface rocks, dissolved Ca ions from rocks, and then added them to the groundwater.

4.1.8 Potassium

Analytical data interpretation reveals that the concentration of potassium is variable in the investigated water samples collected from different locations. Again, the amount of potassium is very high in Nagoha Spring Pipe, Group F well (FW-7), and Rangela Spring, representing the association of these water samples with potassium-bearing rocks (Figure 4H). The percolated water has passed through the potassium-bearing rocks, which has enhanced the concentration of dissolved potassium ions in the analyzed samples. The dashed line in the cross plots indicates a linear trend, representing the increasing concentrations of potassium with increasing distance of the wells/location of collected water samples from the Swat River (Figure 4H). Increasing distance from the main recharge source (i.e., Swat River) indicates that the percolation and infiltration of surface water (streams and rainfall) through the potassium-bearing rocks cause chemical weathering/ dissolution, leading to an increase in the potassium concentration in the water.

4.1.9 Sulfate

Geochemical data interpretation of water samples reveals that the concentration of sulfate is variable in the examined samples collected from different locations. It has been observed that the concentration of sulfate is very high in samples collected from Nagoha Spring Pipe, Group E well (EW-6), and Rangela Spring, representing the association of these water samples with sulfatebearing rocks (Figure 4I). The percolated water has passed through the sulfate-bearing rocks, which has enhanced the concentration of dissolved sulfate ions in the examined samples. The dashed line in the cross plot of sulfate versus the sample's location indicates the increasing concentrations of sulfate with increasing distance of the wells/location of collected water samples from the Swat River (Figure 4I). Increasing distance from the main recharge source (i.e., Swat River) indicates that the percolation and infiltration of surface water (streams and rainfall) through the sulfate-bearing rocks cause chemical weathering/dissolution, leading to an increase in the sulfate concentration in the water.

4.1.10 Nitrate

Interpretation of the analytical data reveals that the concentration of nitrate is variable in the investigated water samples collected from different locations. It has been observed that the concentration of nitrate is very high in Group C well (CW-4), Nagoha Spring, and Group E well (EW-6), representing the association of these water samples with nitrate-bearing rocks/soil

(Figure 4J). It demonstrates that the percolated and infiltrated rainwater has passed through the nitrate-bearing rocks/soil zones, which has enhanced the concentration of dissolved nitrate ions in the examined samples. A cross plot of the acquired nitrate concentration vs. their sampling location illustrates the ascending concentrations of nitrate with increasing distance of the wells/location of collected water samples from the Swat River. Increasing distance from the main recharge source (i.e., Swat River) indicates that the percolation and infiltration of surface water (streams and rainfall) through these rocks/soil horizons cause chemical weathering/dissolution, leading to an increase in nitrate ions in groundwater.

4.1.11 Bicarbonate

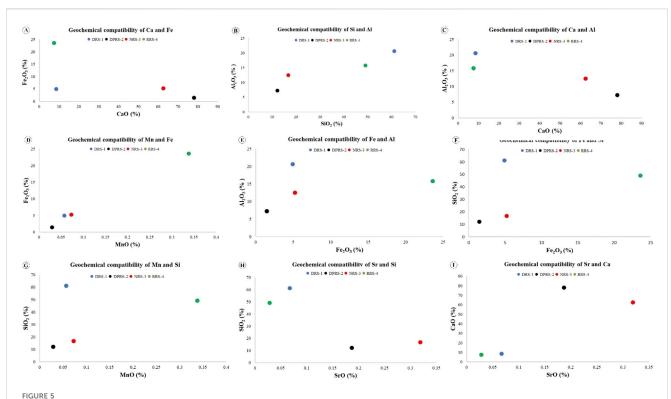
Interpretation of the analytical data demonstrates variability in bicarbonate concentration observed among the investigated water samples collected from various locations of the investigated area. The interpreted data underscores a consistent trend of increasing bicarbonate (HCO3-) concentrations across the water samples collected from different locations. Notably, the concentration of bicarbonate is found to progressively increase (Figure 4K). This pattern is particularly pronounced in areas such as Dadahara Spring (DS-1), Group C well (CW-4), and Group E well (EW-6), where the presence of bicarbonate-rich minerals or rock is evident, like marble, which contains calcium carbonate (CaCO₃) minerals that can release bicarbonate ions (HCO3-) into the water as the rock dissolves over time. The observed trend suggests that subsurface water sources contribute to the elevated bicarbonate levels. As water percolates through the surrounding rocks, it interacts with carbonate minerals, dissolving and carrying bicarbonate ions into the groundwater reservoirs. The dashed line shows an increasing concentration of bicarbonate with increasing distance of the wells/ location of collected water samples from the Swat River. The progressive increase in distance from the Swat River suggests that the percolation and infiltration of surface water (streams and rainfall) through rocks containing carbonates result in chemical weathering and dissolution. This process leads to an increase in bicarbonate levels in the water.

4.2 Geochemistry of rock samples

Geochemical studies using XRF on rock samples are generally conducted to determine their elemental composition. XRF is an analytical technique that provides information on the presence and concentration of various elements within a bulk rock sample. By subjecting the rock sample to XRF analysis, the composition, and the concentrations of elements can be identified, such as major elements (e.g., silicon, aluminum, iron, calcium, magnesium, sodium, and potassium) and trace elements (e.g., zinc, copper, nickel, and chromium) observed in this study.

Cross plots between the above-mentioned elements were established to understand the geochemical compatibility of different oxides and their corresponding relative trends.

Upon analyzing the scatter plots, it was observed that some rock samples exhibited a positive correlation between different oxides, suggesting a potential chemical compatibility between these elements. These samples formed a trend line that inclined



Cross plot representing the mineralogical composition of the analyzed rock samples. (A) CaO vs. Fe_2O_3 , (B) SiO_2 vs. Al_2O_3 , (C) CaO vs. Al_2O_3 , and (D) MnO vs. Fe_2O_3 , representing the geochemical variability of (A) calcium carbonate and iron oxide, (B) silica and aluminum oxides, (C) calcium and aluminum oxides, and (D) manganese and iron oxides. (E) Fe_2O_3 vs. Al_2O_3 , (F) Fe_2O_3 vs. SiO_2 , (G) MnO vs. SiO_2 , (H) SrO vs. SiO_2 , and (I) SrO vs. CaO_3 , representing the geochemical variability of (E) iron and aluminum oxides, (F) iron and silica oxides, (G) manganese and silicon oxides, (H) strontium and silica oxides, and (I) strontium and calcium oxides in the investigated rock sample.

upward or downward, indicating an increase or a decrease in the concentration of oxides. There were also rock samples that displayed a negative or no clear relationship between the observed oxides. These samples appeared as scattered points across the plot, indicating a lack of significant association or compatibility with respect to the plotted oxides.

Groups of rock samples with similar oxide values were also observed, indicating the presence of distinct mineral assemblages in the investigated rock samples collected from the study area. These clusters provided valuable insights into the geochemical variations and rock composition in the analyzed samples. The plotted data allowed for a visual exploration of the geochemical compatibility between different oxides. The scatter plots provided a comprehensive overview of the relationship between these elements, aiding in the interpretation and understanding of the geochemical characteristics of the studied rock samples.

4.2.1 Geochemical compatibility of calcium and iron oxides

Variable calcium oxide values, i.e., 8.54%, 78.06%, 62.56%, and 7.51%, and iron oxide values (4.93%, 1.47%, 5.24%, and 23.6%) were detected in the investigated rock samples. In order to understand the relative trend and the geochemical compatibility of the elemental composition in the analyzed rock samples, a cross plot between CaO and Fe_2O_3 has been established (Figure 5A). This shows an inverse relationship between CaO and Fe_2O_3 contents, respectively (Figure 5A). The given cross plot demonstrates that the quantity

of CaO increases as the concentration of Fe_2O_3 decreases. As evident, DPRS-2 and NRS-3 rock samples possess the highest CaO concentration (78.06% and 62.56%, respectively) and the lowest Fe_2O_3 concentration (1.47% and 5.24%, respectively). On the other hand, rock samples collected from Dadahara Spring (DRS-1) and Rangela Spring (RRS-4) exhibit relatively low CaO content (8.54% and 7.51%) and significantly higher Fe_2O_3 concentration (4.93% and 23.6%). A cross plot of CaO *versus* Fe_2O_3 shows an inverse trend, demonstrating that the concentration of Fe_2O_3 decreases with the increasing concentration of CaO. Furthermore, it indicates that CaO and Fe_2O_3 are not geochemically compatible. Samples collected from springs located in carbonate-bearing rocks indicate higher concentrations of CaO (e.g., Dadahara Plain and Nagoha Spring) and lower concentrations of Fe_2O_3 .

4.2.2 Geochemical compatibility of silica and aluminum oxides

Detected SiO_2 values (i.e., 61.19%, 12.18%, 16.69%, and 49.14%) and $\mathrm{Al}_2\mathrm{O}_3$ values (i.e., 20.62%, 7.25%, 12.49%, and 15.78%) in the representative rock samples exhibit measurable variability. In order to better understand the relative trend of elemental composition in different rock samples, a cross plot of SiO_2 versus $\mathrm{Al}_2\mathrm{O}_3$ has been established (Figure 5B). The given figure illustrates a direct relationship between the concentrations of silica oxide and aluminum oxide. The linear trend indicates that the concentration of $\mathrm{Al}_2\mathrm{O}_3$ gradually increases with the increasing concentration of SiO_2 . The interpreted data presented in the

figure show that as the amount of $\mathrm{Al_2O_3}$ increases, the amount of $\mathrm{SiO_2}$ also increases (Figure 5B). Interpretation of geochemical data demonstrates that the rock samples collected from Dadahara Plain and Nagoha Spring correspond to silica-deficient rocks, i.e., most probably, marble. Similarly, the concentration of $\mathrm{SiO_2}$ is much higher in the rock samples representing Dadahara and Rangela springs, resembling the chemical composition of acidic igneous/ metamorphosed pelitic rocks.

4.2.3 Geochemical compatibility of calcium and aluminum oxides

Variable concentrations of CaO (8.54%, 78.06%, 62.56%, and 7.51%) and Al₂O₃ (20.62%, 7.25%, 12.48%, and 15.78%) were detected during geochemical investigations. To understand the geochemical relationship between CaO and Al₂O₃ distribution in the examined rock samples, a cross plot of CaO versus Al₂O₃ has been established (Figure 5C). The interpreted data shows an inverse relationship between CaO and Al₂O₃ contents (Figure 5C). The figure shows an extremely contrary association between CaO and Al₂O₃ contents among these rock samples. Dadahara and Rangela spring rock samples exhibit higher concentrations of Al₂O₃ and lower levels of CaO. On the other hand, the rock samples collected from the vicinity of Dadahara Plain and Nagoha Spring display higher percentages of CaO and lower amounts of Al₂O₃. This observation indicates a distinct contrast in the composition of these rocks, possibly reflecting different mineralogical compositions or geological origins. The elevated concentration of CaO represents calcium-rich rock, i.e., marble, while the higher amount of Al₂O₃ demonstrates metamorphosed pelitic rocks.

4.2.4 Geochemical compatibility of manganese and iron oxides

Minor oxides, i.e., MnO values detected in the investigated rock samples are 0.05%, 0.02%, 0.07%, and 0.33%, whereas the acquired Fe₂O₃ values in these samples are 4.92%, 1.47%, 5.24%, and 23.6%. In order to understand a probable relationship between MnO and Fe₂O₃ distribution in the representative rock samples, a cross plot of MnO vs. Fe₂O₃ has been established (Figure 5D). The given cross plot exhibits a direct relationship and linear trend between MnO and Fe₂O₃, respectively (Figure 5D). The cross plot shows variations in the manganese and iron content among different rock samples. The concentration of MnO increases with the increasing concentration of Fe2O3 in the investigated rock samples. A high percentage of Fe₂O₃ and MnO in the RRS-4 sample illustrates its derivation from a ferromagnesian mineral-rich metamorphosed rock, while the lower concentration of Fe₂O₃ and MnO in DRS-1, DPRS-2, and NRS-3 indicate a lack of ferromagnesian minerals in the investigated rock samples. Lower concentrations of Fe and Mn are mostly associated with acidic igneous rocks or calcareous rocks.

4.2.5 Geochemical compatibility of iron and aluminum oxides

Extremely variable concentrations of Fe_2O_3 (4.92%, 1.47%, 5.24%, and 23.6%) and Al_2O_3 (20.62%, 7.25%, 12.48%, and 15.78%) were detected during the geochemical investigation of the representative rock samples. In order to understand the probable geochemical relationship between Fe_2O_3 and Al_2O_3 in various rock samples, a cross plot between Fe_2O_3 and Al_2O_3 has been

established, which indicates a direct relationship between the concentrations of Fe_2O_3 and Al_2O_3 except the DPRS-2 rock sample. DPRS-2 samples exhibit an inverse relationship to the overall trend between Fe_2O_3 and Al_2O_3 . Interpretation of the detected data demonstrates that the amount of Fe_2O_3 increases with the increasing concentrations of Al_2O_3 (Figure 5E). To conclude, a direct geochemical relationship has been found between Fe_2O_3 and Al_2O_3 in the DRS-1, NRS-3, and RRS-4 rock samples. High percentages of Al_2O_3 in DPRS-2 illustrate metamorphosed pelitic rock, while the higher concentration of Fe_2O_3 in RRS-4 exhibits the ferromagnesian character of the investigated rock sample.

4.2.6 Geochemical compatibility of iron and silica oxides

Fe₂O₃ values determined in representative rock samples are 4.93%, 1.47%, 5.24%, and 23.61%, whereas SiO₂ values are 61.19%, 12.18%, 16.69%, and 49.14%. In order to understand the geochemical relationship between Fe₂O₃ and SiO₂ distribution in the investigated rock samples, a cross plot between Fe₂O₃ and SiO₂ has been established (Figure 5F). The cross plot of Fe₂O₃ vs. SiO₂ illustrates a direct relationship between the concentrations of iron oxide and silicon oxide. There is a linear trend (the amount of silica increases with increasing concentration of silica), which represents a direct relation between Fe₂O₃ and SiO₂ in the DPRS-2, NRS-3, and RRS-4 rock samples. The percentages of Fe₂O₃ and SiO₂ are much higher in RRS-4 and lower in DPRS-2, exhibiting two different lithological units, i.e., SiO2-rich and SiO2-deficient, respectively. DRS-1 illustrates contrasting geochemical behavior, e.g., a lower concentration of Fe₂O₃ and a very high amount of SiO₂, indicating a metamorphosed intermediate/acidic igneous rock.

4.2.7 Geochemical compatibility of manganese and silicon oxides

Major and minor oxides with variable concentrations were detected in the investigated rock samples, which include SiO₂ (61.19%, 12.18%, 16.68%, and 49.14%) and MnO (0.05%, 0.02%, 0.07%, and 0.33%), respectively. These major and minor oxides were plotted in order to determine geochemical compatibility between SiO₂ and MnO in the investigated rock samples. The acquired cross plot demonstrates a direct relationship between the increasing concentrations of manganese oxide and the ascending amount of silicon oxide. DPRS-2 and NRS-3 exhibit lower concentration of SiO₂, which is an indication of silica-deficient rock, i.e., marble. Similarly, the concentration of SiO₂ is high in the DRS-1 and RRS-4 rock samples, which is indicative of silica-rich metamorphosed rocks. The data presented in the figure show that as the amount of manganese increases, the amount of silica also increases (Figure 5G). Except for DRS-1, there is a direct relationship between SiO2 and MnO in the investigated rock samples, which illustrates that these minerals are geochemically compatible with each other.

4.2.8 Geochemical compatibility of strontium and silicon oxides

Variable concentrations of SrO determined in the examined rock samples are 0.06%, 0.18%, 0.31%, and 0.02%, whereas similar variations in the SiO_2 contents were also observed, i.e., 61.19%,

12.18%, 16.68%, and 49.14%, respectively. The detected major (SiO₂) and minor (SrO) oxides were then used to determine their geochemical compatibility in the inspected rock samples. In order to understand the relative trend of the abovementioned elemental composition in different rock samples, a cross plot between SrO and SiO₂ has been established (Figure 5H). The cross plot of these major and minor oxides indicates an inverse relationship between the concentrations of strontium oxide and silicon oxide. The concentration of SiO2 is high in the DRS-1 and RRS-4 samples, while the amount of SrO is very low in these samples. Similarly, the percentage of SiO₂ oxide is very low in DPRS-2 and NRS-3, whereas the concentration of SrO is high in these samples. Based on the abovementioned observations in the given cross plot, SiO2 is not geochemically compatible with SrO (Figure 5H). It is clearly shown in the graph that the amount of SrO decreases with the increasing concentration of SiO₂ and vice versa. Furthermore, it demonstrates that calcium-rich rock, i.e., marble, possesses a high amount of Sr, while silica-rich rocks are deficient in Sr.

4.2.9 Geochemical compatibility of strontium and calcium oxides

Major and minor oxides detected in the investigated rock samples collected from the study area include variable concentrations of SrO (0.06%, 0.18%, 0.31%, and 0.02%) and CaO (8.54%, 78.06%, 62.56%, and 7.51%), respectively. Normally, we cannot classify rock types on the basis of trace elements/oxides, but it can be used for the determination of geochemical compatibility. Minor oxide (SrO) was plotted against major oxide (CaO), and a relatively direct relationship was observed between the concentrations of strontium oxide and calcium oxide. The cross plot exhibits that the concentrations of SrO and CaO are lower in DRS-1 and RRS-4, while the amounts of SrO and CaO are high in the DPRS-2 and NRS-3 samples. There is a direct relationship between these oxides, i.e., the percentage of SrO increases with increasing CaO contents, which illustrates a linear trend. Based on the abovementioned values of the examined rock samples, SrO is geochemically compatible with CaO (Figure 51). Furthermore, the concentrations of CaO and SrO are high in DPRS-2 and NRS-3, representing calcareous-rich rock, i.e., marble.

5 Discussion

Data collected during detailed field activity, i.e., distance from the Swat River, water depth, depth of the well, and lithological variation in the well, were plotted in cross-sections, and a direct relationship was observed between water depth and distance from the Swat River. Increasing water depth in wells represents its increasing distance from the main recharge source, i.e., Swat River.

Atomic absorption spectroscopic studies of the collected water samples from representative wells of each group, nearby springs, water-logged areas, and canals demonstrate that the probable recharge source for groundwater in the lower Swat area is the Swat River, as well as its contributory channels and rainwater. Acceptable similarities were observed in the geochemical composition of the rock samples, spring water samples, and representative wells in their immediate neighborhood.

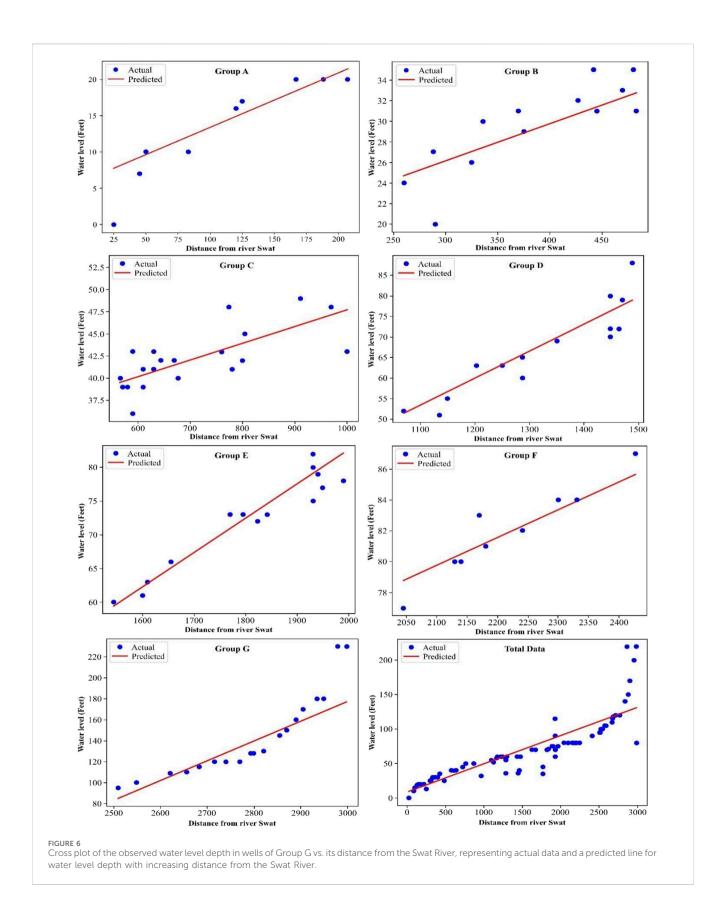
Similarly, X-ray fluorescence analysis of the spring's host rocks was compared with the dissolved mineral constituents of the analyzed water samples, and it was noted that the concentration of rock-forming minerals increases in water with increasing distance from the Swat River. This increase in dissolved minerals illustrates the interaction of groundwater with the bedrock during its migration from the source to the reservoir. Analytical data interpretation reveals that the recharge source for groundwater in the floodplain regime is the Swat River, while infiltration and percolation of rainwater act as probable recharge sources in the mountainous and elevated areas.

Overall, the data from all seven groups consistently demonstrate the impact of distance from the Swat River on the fluctuation of groundwater level in the floodplain area of the Swat River. The progressive decrease in the water level as we move away from the river supports the understanding that proximity to the river is a crucial factor affecting groundwater resources in the study area. Two main aquifers were encountered in this study, i.e., gravel deposited by the Swat River in its floodplain and fractured bedrock. The primary recharge sources for these aquifers include the main trunk and contributory channels of the Swat River, irrigation channels derived from the Swat River, and surface precipitation. More than 80% of the producing wells have been drilled in the gravel layer, while bedrock contributes only 20% as an aquifer. The study area is covered with high-grade metamorphic rocks. Normally, metamorphic rocks do not possess porosity and permeability for the accumulation of groundwater. In this case, intense fractures and inclined geometries of the bedrock provide the best possible pathways for the primary migration of rainwater into the main aquifer.

Group G comprises several representative wells located within a range of 2,501–3,000 m from the Swat River. These wells have water table/level depths ranging from 80 feet to 220 feet. The obtained graph from field data presents the relationship between distance from the Swat River and water table/level depth for Group G (Figure 6). The upward-sloping predicted line indicates that water table/level depths tend to increase with an increase in the distance from the river. The linear regression model's predicted line serves as a valuable tool for predicting water table/level depths in wells at different distances from the Swat River.

The cross plot compares the observed depth of the water table/level in wells of Group G with their respective distances from the Swat River. The plot includes both actually acquired data and a predicted line, which represents a linear trend of water table/level depth with the increasing distance from the Swat River (Figure 6). The predicted line is obtained from a machine learning program (linear regression model), which allows us to predict the actual depth of the water table/level in the potential zone of floodplain region of the Swat River at variable distances from the river (Figure 7).

Water table/level depths were plotted against their respective distances from the Swat River, and a general trend of increasing water table/level depth with increasing distance from the river in the floodplain regime was observed. The acquired data were then plotted and processed using the linear regression model of the machine learning program. We obtained a predicted line for the drilling of wells in suitable locations with the defined depth of the water table/ level and its corresponding distance from the river in the floodplain



area. The use of linear regression is very helpful in the accurate demarcation of potential groundwater zones in the investigated area. It has been concluded from this study that the obtained predicted

line demonstrates a linear trend, indicating that as the distance from the river increases, the water table/level depth in the wells also increases (Figure 7).

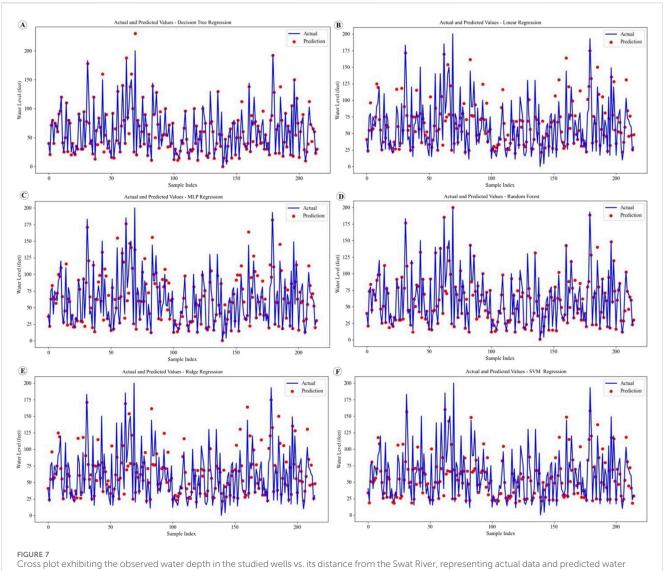


FIGURE 7
Cross plot exhibiting the observed water depth in the studied wells vs. its distance from the Swat River, representing actual data and predicted water depth with increasing distance from the Swat River using the (A) decision tree regression model, (B) linear regression model, (C) MLP regression model, (D) random forest model, (E) ridge regression model, and (F) SVM regression model.

The observed recharge mechanisms (river infiltration in floodplain zones and rainwater percolation in elevated zones) are consistent with findings by Xu and Beekman (2003) in southern Africa and Panda et al. (2020) in India. Similarly, our high model accuracy ($R^2 = 0.95$ for RF) parallels recent success in hybrid ML applications in groundwater prediction (Naghibi et al., 2017b). The results validate the reliability of coupling geochemical data with AI models for spatial groundwater forecasting, as also reported by Rahmati et al. (2016).

However, unlike prior studies that rely solely on remote sensing or modeling, our field-based, chemically validated approach enhances local relevance and reduces uncertainty. This multi-source validation provides a significant methodological advancement.

5.1 Future perspectives

The findings of this study lay the foundation for future groundwater exploration in data-scarce mountainous regions.

Integration of remote sensing and real-time hydrological data with AI-driven models could significantly enhance prediction accuracy. Moreover, the methodology developed in this study can be adapted for similar terrains in other parts of Pakistan and globally, aiding in the sustainable management of water resources under changing climatic conditions.

6 Conclusion

The severe exploitation of groundwater resources is compromising not only the quality but also the quantity of groundwater. In this study, acceptable similarities were observed in the geochemical composition of the rock samples, spring water samples, and representative wells in their immediate neighborhood. Moreover, the concentration of rock-forming minerals increases in water with increasing distance from the Swat River. This increase in dissolved minerals illustrates the interaction of groundwater with

the bedrock during its migration from the source to the reservoir. Analytical data interpretation reveals that the recharge source for groundwater in the floodplain regime is the Swat River, while infiltration and percolation of rainwater act as probable recharge sources in the mountainous and elevated areas. The linear regression was observed between the water table and the distance from the Swat River, demonstrating that water depth in wells increases with increasing distance from the main recharge source. Different parameters (analytical data and field data) were plotted in Python and used to demarcate the predicted zones of potential groundwater in model wells using linear regression algorithms from machine learning techniques. The multi-model ML approach allowed for the cross-verification of predictions, while the use of geochemical compatibility analysis ensured field-based reliability. This combined methodology enhances the scientific validity and practical utility of the results, setting it apart from conventional single-model approaches.

Data availability statement

The original contributions presented in the study are included in the article/supplementary material; further inquiries can be directed to the corresponding authors.

Author contributions

IA: Writing – original draft, Resources, Supervision, Conceptualization. IU: Methodology, Writing – original draft, Investigation. MA: Writing – original draft, Visualization, Software. IG: Writing – review and editing. MK: Writing – review and editing, Validation. KK: Writing – review and editing,

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Conflict of interest

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