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Modeling groundwater quality using three novel hybrid support vector regression models

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ABSTRACT

During recent decades, the excessive use of water has led to the scarcity of the available surface and groundwater resources. Quantitative and qualitative surveys of groundwater resources indicate that accurate and efficient optimization methods can help to overcome the numerous challenges in assessment of groundwater quality. For this purpose, three optimization meta-heuristic algorithms, including imperialist competitive (ICA), election (EA), and grey wolf (GWO), as well as the support vector regression method (SVR), were used to simulate the groundwater quality of the Salmas Plain. To achieve this goal, the data of the groundwater quality for the Salmas plain were utilized in a statistical period of 10 years (2002-2011). The results were evaluated according to Wilcox, Schuler, and Piper standards. The results indicated higher accuracy of the GWO-SVR method compared to the other two methods with values of R^2=0.981, RMSE=0.020 and NSE=0.975. In general, a comparison of the results obtained from the hybrid methods and different diagrams showed that the samples had low hardness and corrosion. Also, the results indicated the high capability and accuracy of the GWO-SVR method in estimating and simulating the groundwater quality.

1. Introduction

The use of groundwater is one of the basic solutions for providing drinking and agricultural water in arid and semi-arid regions, including Iran. In recent years, the levels and quality of groundwater have declined due to the growing consumption of these resources as well as low levels of natural nutrients. The sodium absorption ratio (SAR) of groundwater is a very important parameter in soil management and stability. Electric conductivity (EC) is also considered as a major parameter in monitoring the quality of drinking and agricultural water. This parameter is directly related to the amount of water salinity, sodium absorption, and drinking water quality [1]. The total dissolved solids (TDS) is also a very effective parameter that indicates the palatability of drinking water. In a way, the increased salinity and reduced quality of groundwater are some of the most important worldwide environmental challenges. Given the importance of the quality of water resources, water quality parameters are components that must be carefully predicted and simulated. In the simulation of complex nonlinear systems in water resource management topics conducted by various researchers, evolutionary algorithms and artificial neural networks have provided favorable results. Artificial neural networks and evolutionary algorithms with compatibility and unpredictable changes are good alternatives to physical and regression models to estimate the behavior of water resources. Evolutionary algorithms and artificial neural networks have shown satisfactory results in modeling non-linear complex systems in water resources management issues, which have been reported in various areas by researchers. Due to their compatibility and impressive progresses, they are an appropriate alternative to physical and regression models for estimating the behavior of water

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resources systems. Various studies have been conducted regarding groundwater level modeling and estimating. Table 1 shows the most practical studies on the management and estimation of groundwater quality parameters using meta-altruistic algorithms and artificial neural network (ANNs) methods.

Table 1. Most practical studies on the management and estimation of groundwater quality parameters

Year							
2012	2013	2015	2016	2017	2018	2019	2020
Adhikary et al. [4]	Adiat et al. [5]	Jalalkamali [3]	Al-Rekabi et al. [1] Mokarram [4] Wagh et al. [10]	Kisi et al. [11] Khan and Jhariya [8]	Pramada et al. [14] Khudair et al. [2]	Kisi et al. [9]	Gaikwad et al. [15] Shyamala et al. [16]

Zareh-Abianeh (2011) used artificial neural networks to predict groundwater nitrate in the Hamadan Plain. The results showed a good agreement between the values obtained from the implementation of the artificial neural network and the observed values [17]. Rafati et al. (2013) examined the trend of fluoride changes and monitored the groundwater in Hamadan province. The results showed that the trend of anion changes was between 0 and 1.78 mg/l, and its rate in 49% of the stations was less than the standard proposed by the Environmental Protection Agency [18]. Moasheri et al. (2013) used geostatistical techniques, a neural network, and a genetic algorithm to predict the amounts of sodium, calcium, and magnesium in the groundwater of the Kashan Plain, which reported the results of their proposed model at 90.9% [19]. Emami et al. (2017) evaluated an imperialist competitive and genetic algorithm for estimating the groundwater quality parameters in the Bostanabad Plain. The validation of the simulation with the ICA model showed that the mean square error (MSE) in the testing sample for SAR and Cl were 0.0134 and 0.0098, respectively. Also, the R^2 of validity for SAR and Cl were 0.93 and 0.952, respectively [20]. Jalalkamali and Jalalkamali (2018) applied the geographic information systems (GIS) and ANN methods to predict the groundwater quality in the Kerman Plain. The results showed that the ANFIS-GA method performed well compared to the ANFIS model [21]. Asefi and Zamani-Ahmadmahmoodi (2018) used principal component analysis (PCA) to determine the degree of significance of the qualitative parameters of the water resources in the Karkheh River in southwestern Iran. The PCA factors indicated that the parameters influencing the changes in the water quality were generally related to weathering and land washing in response to floods, organic contamination from household wastewater, waste from sand washing, and runoff from chemical fertilizers [22]. Bhat et al. (2018) evaluated the physico-chemical parameters and water quality of the Yamuna River in India on a seasonal basis. The assessment of physico-chemical parameters indicated that the selected stations were greatly impacted by industrial effluents and domestic sewage; thus, the river water needed to be treated before consuming to avoid water-related diseases that could have harmful effects on humans and aquatic biota [23]. Movagharnejad et al. (2017) designed a multi-layer perceptron artificial neural network model to predict the calcium, sodium, chloride, and sulfate ion concentrations of the Karaj River. The results indicated that the ANN model was successfully applied to predict calcium ion concentration [24]. Jafari et al. (2019) used four soft computing methods to estimate the TDS values of groundwater in the Tabriz plain: multilayer perceptron (MLP), adaptive neuro-fuzzy inference system (ANFIS), support vector machine (SVM), and gene expression programming (GEP). The results showed that the MLP, ANFIS, SVM, and GEP models performed well in estimating the TDS changes [25]. Maroufpoor et al. (2020) used a neuro-fuzzy system integrated with fuzzy c-means data clustering (FCM) and grid partition (GP) methods to model groundwater quality [26]. Barzegari Banadkooki et al. (2020) predicted the groundwater level (GWL) of precipitation and temperature data based on different time delays. The results showed the MLP-WA model performed well compared to other models [27]. According to the literature, the Salmas Plain is one of the most important plains in North-West of Iran and supplies water to various sections of its neighboring areas; thus, estimating and modeling the groundwater quality in this plain is crucial. Therefore, the purpose of this study was to apply the GWO-SVR, EA-SVR, and ICA-SVR hybrid models and compare their results with each other; also, the Wilcox, Schuler, and Piper diagrams were used in estimating and optimizing the water quality parameters.

2. Materials and methods

2.1. Case study

The Salmas plain is located in northwestern Iran in the province of West Azerbaijan. It is located between the latitude of 37˚ 6' to 44˚ 20' N and 45˚ 20' E. The total area of the Salmas Plain is 4268 km^2, and the average elevation is 1340 meters above the sea level. Its main feeding river is the Zolachai, which originates from the west to the east of the Turkish border heights, and after passing the Salmas plain, finally flows into the Urmia Lake. Figure 1 shows the location of the study area on the map [28].

The required statistics and data on the study wells from 2005-2015 were used to model the groundwater quality by each of the methods, and the required analyses were performed. The studied parameters included EC, TDS, pH, Ca^{2+}, Mg^{2+}, Na^{+}, K^{+}, HCO_3^-, CO_3^-, Cl^-, and SO_4^{2-}.

2.2. The used algorithms

2.2.1. Gray wolf optimizer algorithm (GWO)

The flowchart of the GWO algorithm is shown in Figure 2.

2.2.2. Election algorithm (EA)

A path through the EA's components is shown as a flowchart in Figure 3 [29].

2.2.3. Imperialist competitive algorithm (ICA)

The flowchart of the ICA algorithm is shown in Figure 4. [30]:

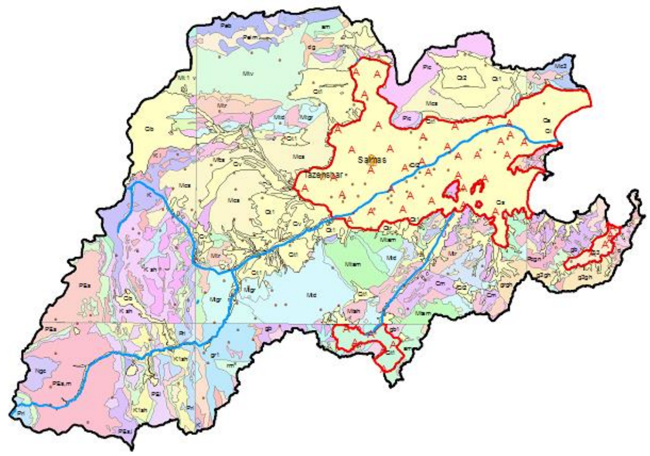

Fig. 1. Location of the Salmas plain on the map

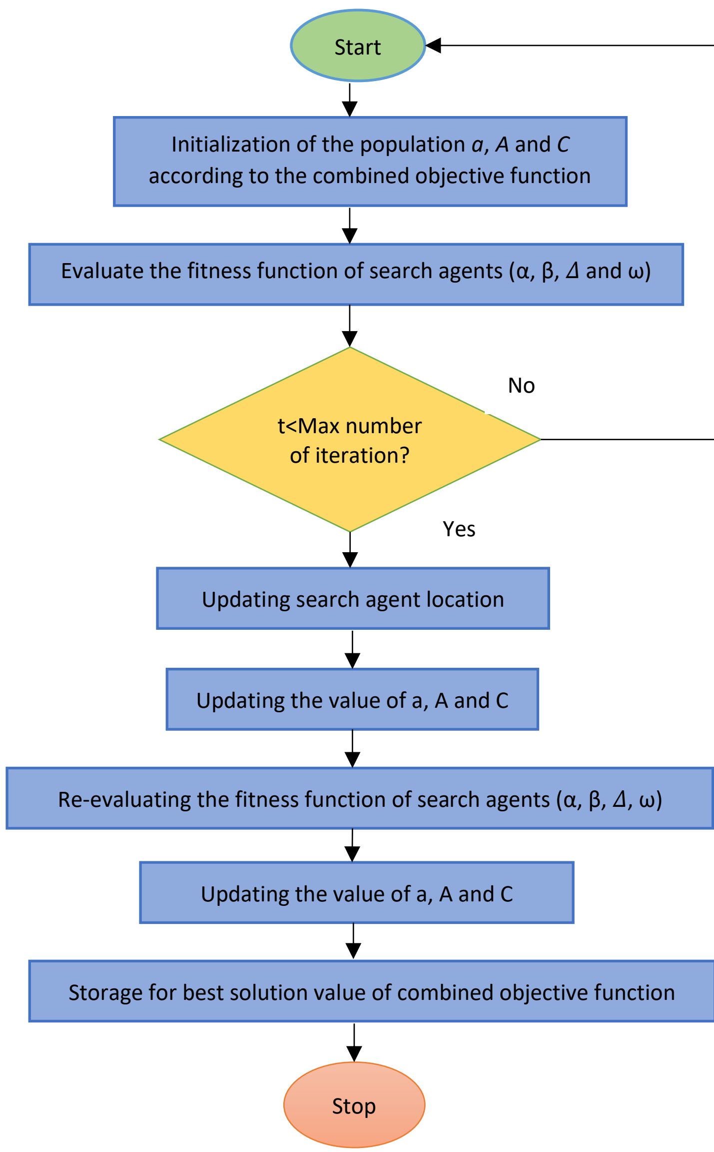

Fig. 2. Flowchart of the GWO algorithm [29]

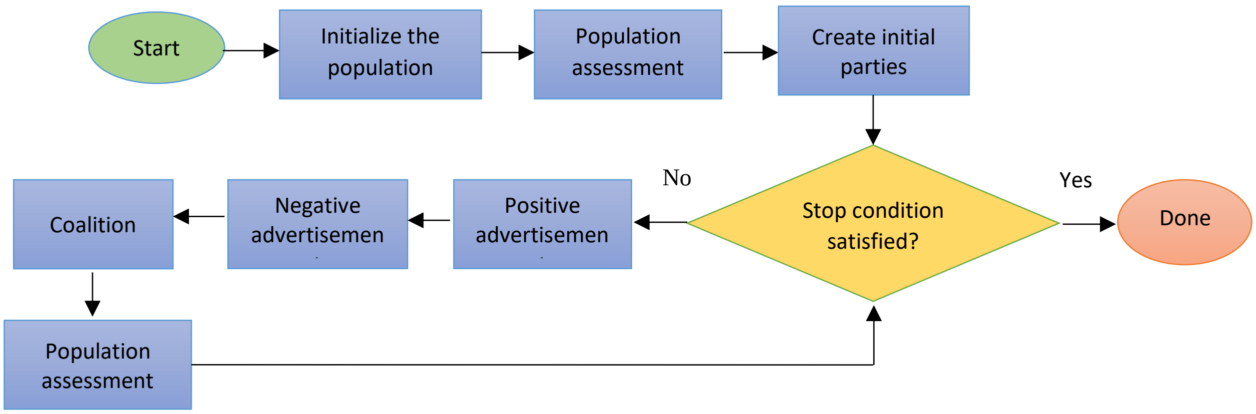

Fig. 3. Flowchart of the EA algorithm [30]

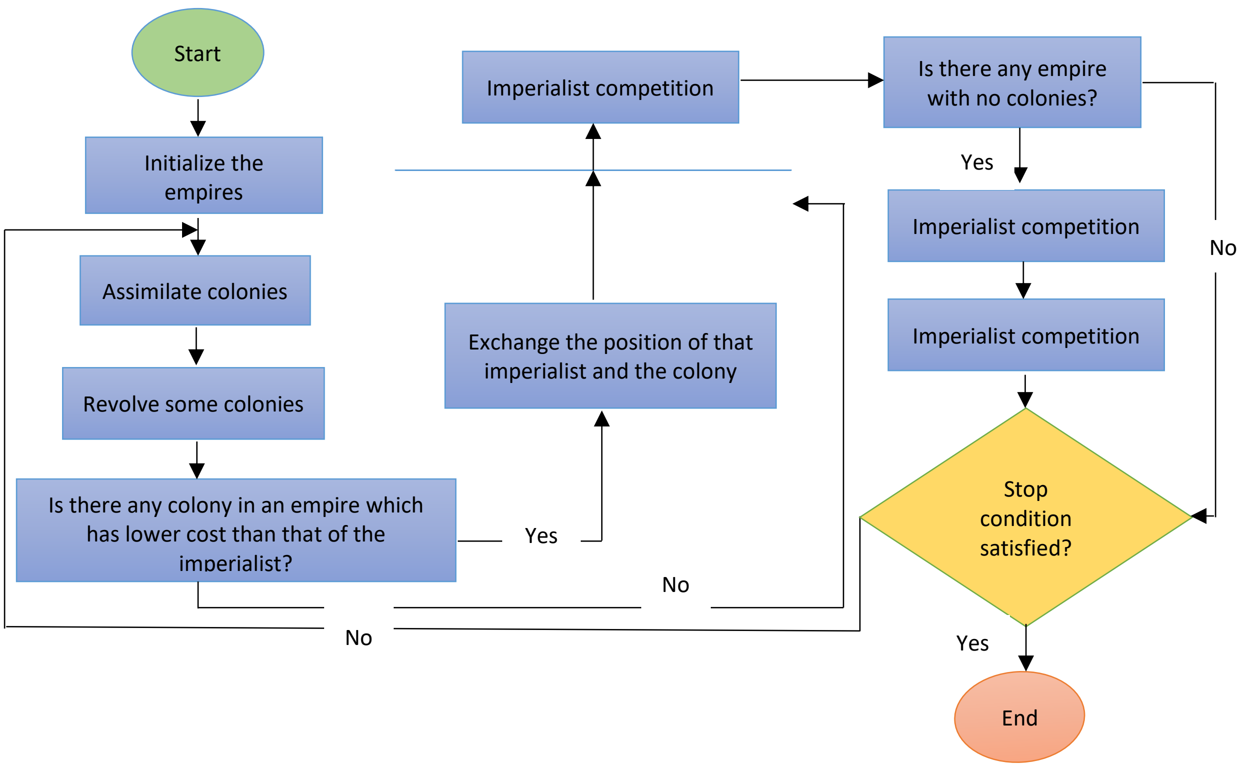

Fig. 4. Flowchart of the ICA algorithm [31]

2.2.4. Support vector regression

Support vector regression (SVR) is an SVM-based regression method. The SVM is a supervised machine learning method equipped with learning algorithms [32]. The main principle behind SVR is the same as the SVM: it is a discriminative classifier, which takes training data as input and computes an optimal hyperplane that maximizes the margin to efficiently separate data points. For the dataset $D=\{X_i, y_i\}_{i=1}^{N}$, N is the number of data objects, $X_i=\{x_{i1}, x_{i2}, ..., x_{im}\}$ is a m-dimensional data-defined object, and y_i is the label assigned to X_i. In the SVR algorithm, each data object $X_i \in D$ is considered as a point in m-dimensional space. The goal is to create a prediction model based on some training data to separate data objects by finding a hyperplane that differentiates the data objects into some separate groups. This hyperplane is calculated based on a few data points, known as support vectors. In other words, SVR aims to maximize the minimum distance of data points from the hyperplane. In SVR, the goal is to solve the following equations to obtain an optimal hyperplane:

$$f(x) = w\varphi(x) + b \quad (1)$$

in which w is a normal vector, b is a scaler, and φ is the kernel function.

$$\text{minimize } \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}(\xi_i + \xi^*{}_i \quad (2)$$

$$\text{subject to} \begin{cases} y_i - < w, x_i > -b & \leq \varepsilon + \xi_i \\ < w, x_i > -b - y_i & \leq \varepsilon + \xi^*{}_i \\ \xi_i, \xi^*{}_i & \geq 0 \end{cases} \quad (3)$$

where ζ_i and ζ_i^* show the slack variables that determine the upper and lower excess deviations, $\frac{1}{2}\|w\|^2$ is the regularization term, C is the error penalty factor used to regulate the difference between the empirical risk and the regularization term, and ε is the loss function that identifies the accuracy of the training data point. A generic form of Eq. (4) can be defined by using the Lagrange multiplier technique and optimality constraints, as follows:

$$w = \sum_{i=1}^{n}(\alpha_i - \alpha^*{}_i)$$

$$f(x) = \sum_{i=1}^{n}(\alpha_i - \alpha^*{}_i)K(x, x_i) + b \quad (4)$$

$$k(x, x_i) = \varphi(x_i) \times \varphi(x_j) \quad (5)$$

where $K(x, x_i)$ is the kernel function, and it is the product of the two inner vectors x_i and x_j in the feature space $\varphi(x_i)$ and $\varphi(x_j)$, respectively. Three well-known kernel functions are sigmoid, polynomial basis function, and radial basis function (RBF). In this paper, the RBF kernel function is used in SVR due to its high performance and easy configuration compared to other kernel functions. The RBF kernel is defined as

$$k(x, x_i) = \exp(-\|x_i - x\|/2\sigma^2 \quad (6)$$

The proper setting of C, σ, and ε plays an important role in the prediction performance of the SVR.

2.2.5. Wilcox, schuler and piper diagrams

The Wilcox classification method and its diagram are the most practical means for categorizing water in agriculture sector in hydro-chemical studies. In the Wilcox diagram, the horizontal axis represents the water salinity (µm/cm) while the sodium absorption ratio (SAR) is plotted on the vertical axis. In the Schuler diagram, a separate axis is considered for each of the cations (Na, K, Mg, and Ca), Cl, So_4, Hco_3, TDS and Total hardness (TH). By connecting the corresponding points for any parameter on these axes, the suitability of water for drinking purpose can be determined. In the Piper diagram, it is possible to compare a large amount of analyzed data. The available options are also more limited and accumulated in this diagram. The size of the circles in the Piper diagram is used to show the amount of total solute. This diagram shows the chemical properties of water in terms of its relative concentration.

2.2.6. Evaluation criteria

The efficiency of the proposed methods was evaluated using the correlation coefficient (R^2), root mean square error (*RMSE*), and the Nash–Sutcliffe efficiency index (*NSE*) [33]:

$$R^2 = \left[\frac{\sum_{i=1}^{n}(e_i - \bar{e})\ (p_i - \bar{p})}{\sum_{i=1}^{n}\sqrt{(e_i - \bar{e})^2}\ \sqrt{(p_i - \bar{p})^2}}\right]^2 \quad (7)$$

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(e_i - p_i)^2} \quad (8)$$

$$\text{NSE} = 1 - \frac{\sum_{i=1}^{n}(e_i - p_i)^2}{\sum_{i=1}^{n}(e_i - \bar{p})^2} \quad (9)$$

where p_i is the predicted C_{d_i}, e_i is the observed C_{d_i}, and $\bar{p}$ and $\bar{e}$ are the average predicted and observed C_d values, respectively. The ideal values for R^2 and RMSE are 1 and 1-10%, respectively. The Nash-Sutcliffe criterion (NSE) values vary from 1 to - ∞, so that the range of 0.75-1, 0.36-0.75, and less than 0.36 indicate the very good, satisfactory, and weak performance of the model, respectively. The data used in the models was normalized by equation 10.

$$Z_n = \frac{Z - Z_{min}}{Z_{max} - Z_{min}} \quad (10)$$

in which Z represents the raw data, Z_n is the normalized data, Z_{min} is the minimum data, and Z_{max} is the maximum data.

3. Results and discussion

In order to analyze the groundwater quality of the Salmas plain, GWO-SVR, EA-SVR, and ICA-SVR models along with the Wilcox, Schuler, and Piper diagrams are utilized. The results of the proposed methods for the training and testing stage are based on the performance criteria presented in Tables 2 and 3.

Table 2. Performance of proposed hybrid methods in the training stage

Method	R^2	RMSE	NSE
EA-SVR	0.952	0.06	0.852
GWO-SVR	0.981	0.02	0.975
ICA-SVR	0.912	0.11	0.722

Table 3. Performance of proposed hybrid methods in the test stage

Method	R^2	RMSE	NSE
EA-SVR	0.922	0.08	0.790
GWO-SVR	0.966	0.03	0.950
ICA-SVR	0.870	0.14	0.702

After comparing and selecting the superior model, the groundwater quality parameters were estimated using GWO-SVR, EA-SVR, and ICA-SVR hybrid models (Figures 5 to 7). Initially, all the available data were standardized; after introducing the input structures and finding the optimal values of the SVR parameters and applying them, 80% of the data was used for training and 20% for testing the model.

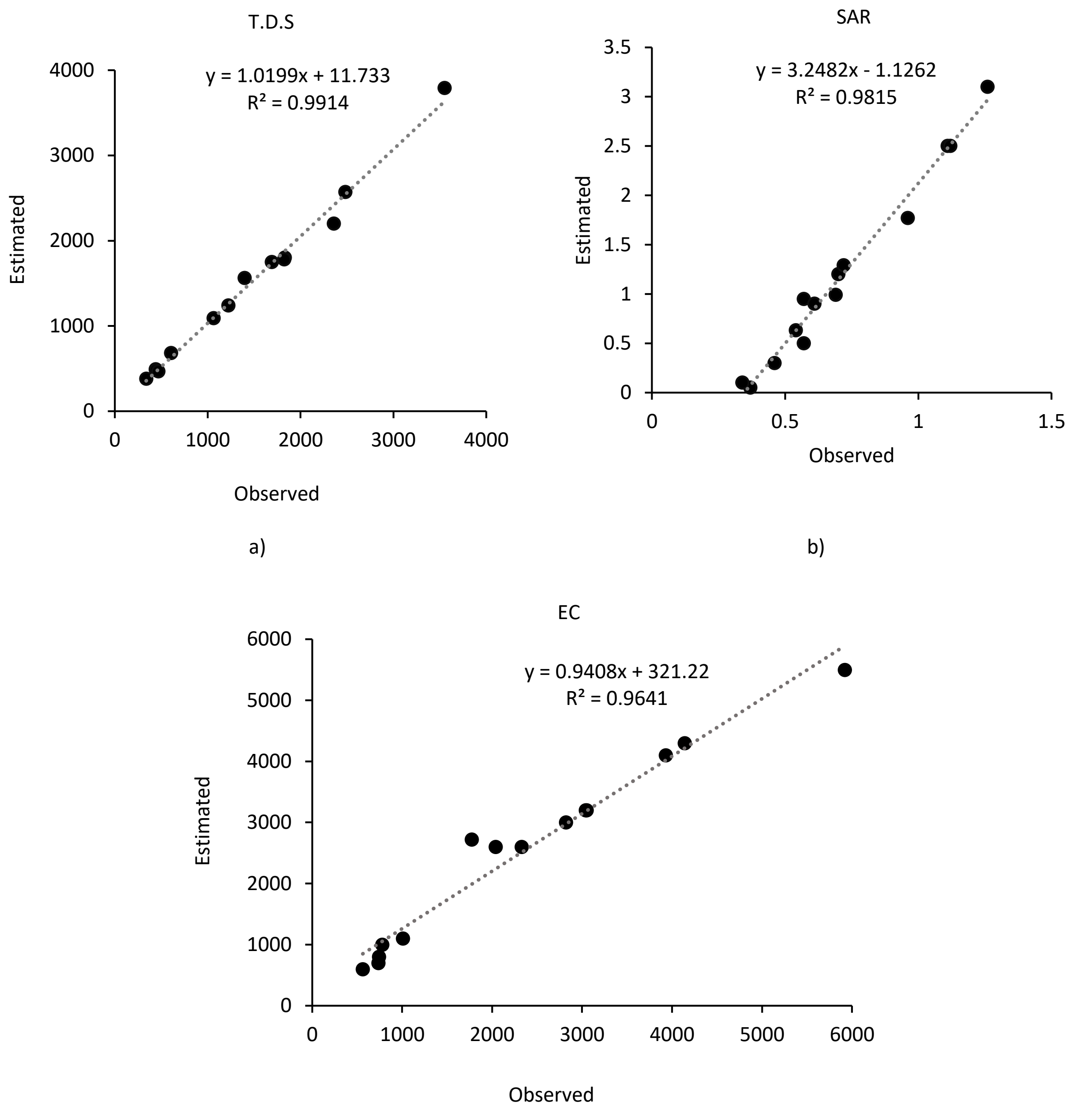

Fig. 5. a to c: Scatterplot of observed and estimated values of GWO-SVR model on the test dataset

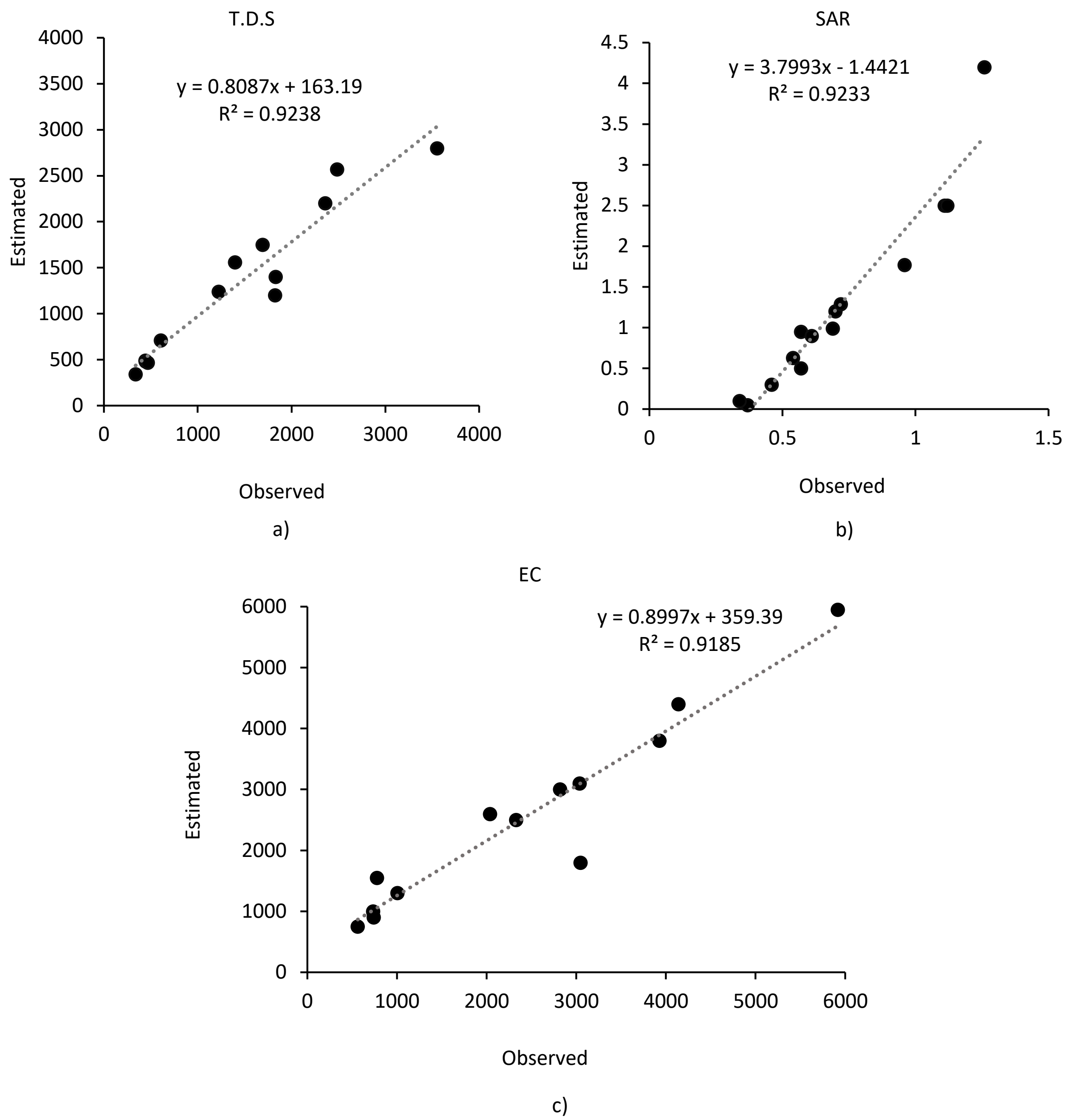

Fig. 6. a to c: Scatterplot of observed and estimated values of EA-SVR model on the test dataset

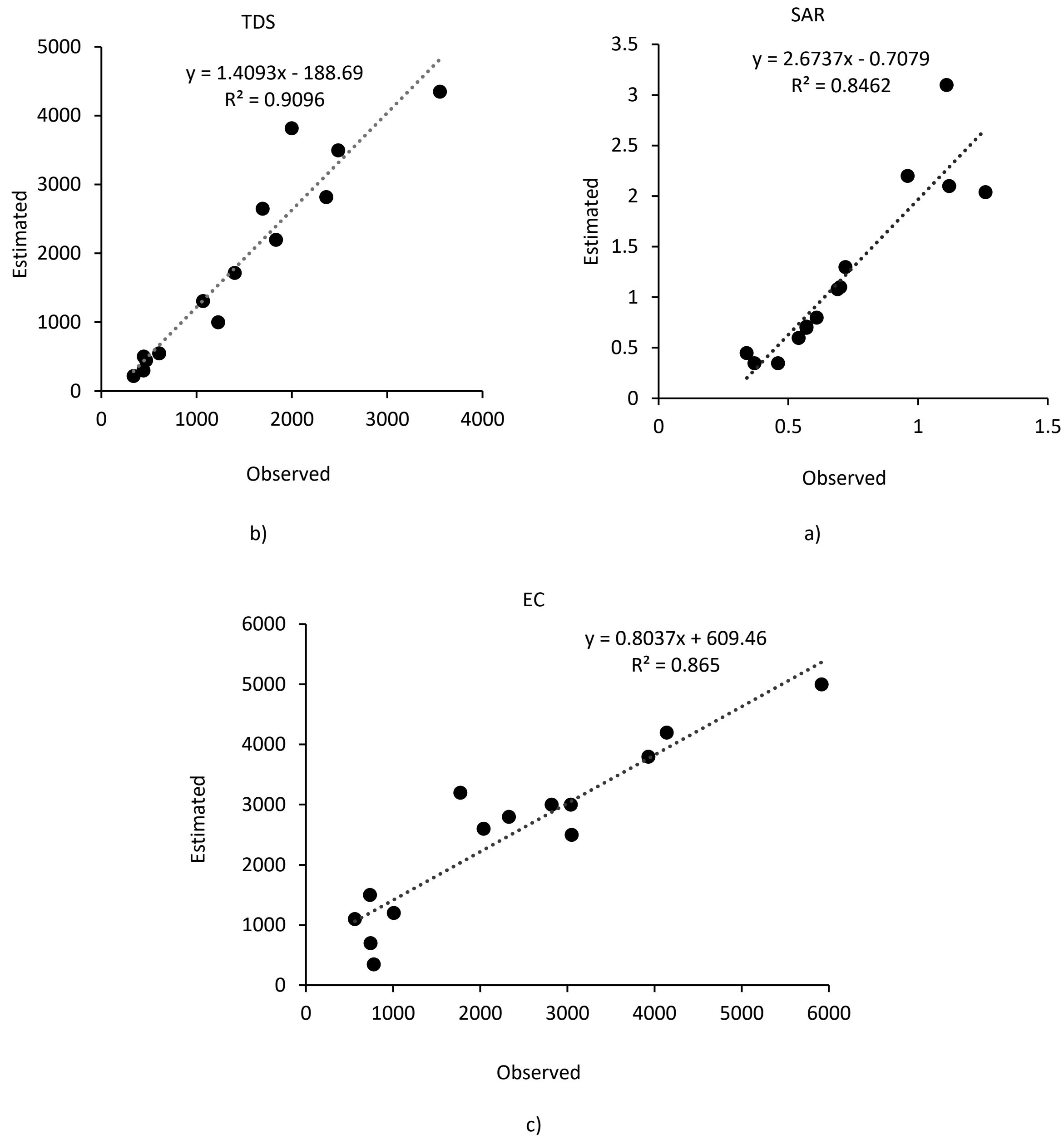

Fig. 7. a to c: Scatterplot of observed and estimated values of ICA-SVR model on test dataset

The results of this study showed that the proposed GWO-SVR model is able to estimate the groundwater quality variables in the Salmas Plain with high efficiency. The results of this study are consistent with the results of Isazadeh et al. (2016), Mirzavand et al. (2015), Zare-abyaneh et al. (2011), and Nourani et al. (2016). They also showed that intelligent methods are highly efficient in modeling groundwater quality parameters. The amount of EC increased by 300 µs/cm during the statistical years, indicating a decrease in water quality. This increase in EC during the summer season was due to a rise in temperature. Consequently, it increased the water temperature, which was one of the factors in increasing both the EC and evapotranspiration, and a decline in groundwater level. Also, the results showed that the magnitude of EC in the Salmas Plain groundwater varied from 500 and 3100 µs/cm, hence, EC can be used as a proper water quality indicator for different water consumption sectors. The analysis of the groundwater samples showed that the amount of sodium in the water varied from 15-60, which indicates that the quality of the water is good and acceptable for agricultural sector. For further investigation, Figures 8 to 10 show the Wilcox, Schuler, and Piper diagrams for the hydro-chemical analysis of the Salmas plain groundwater.

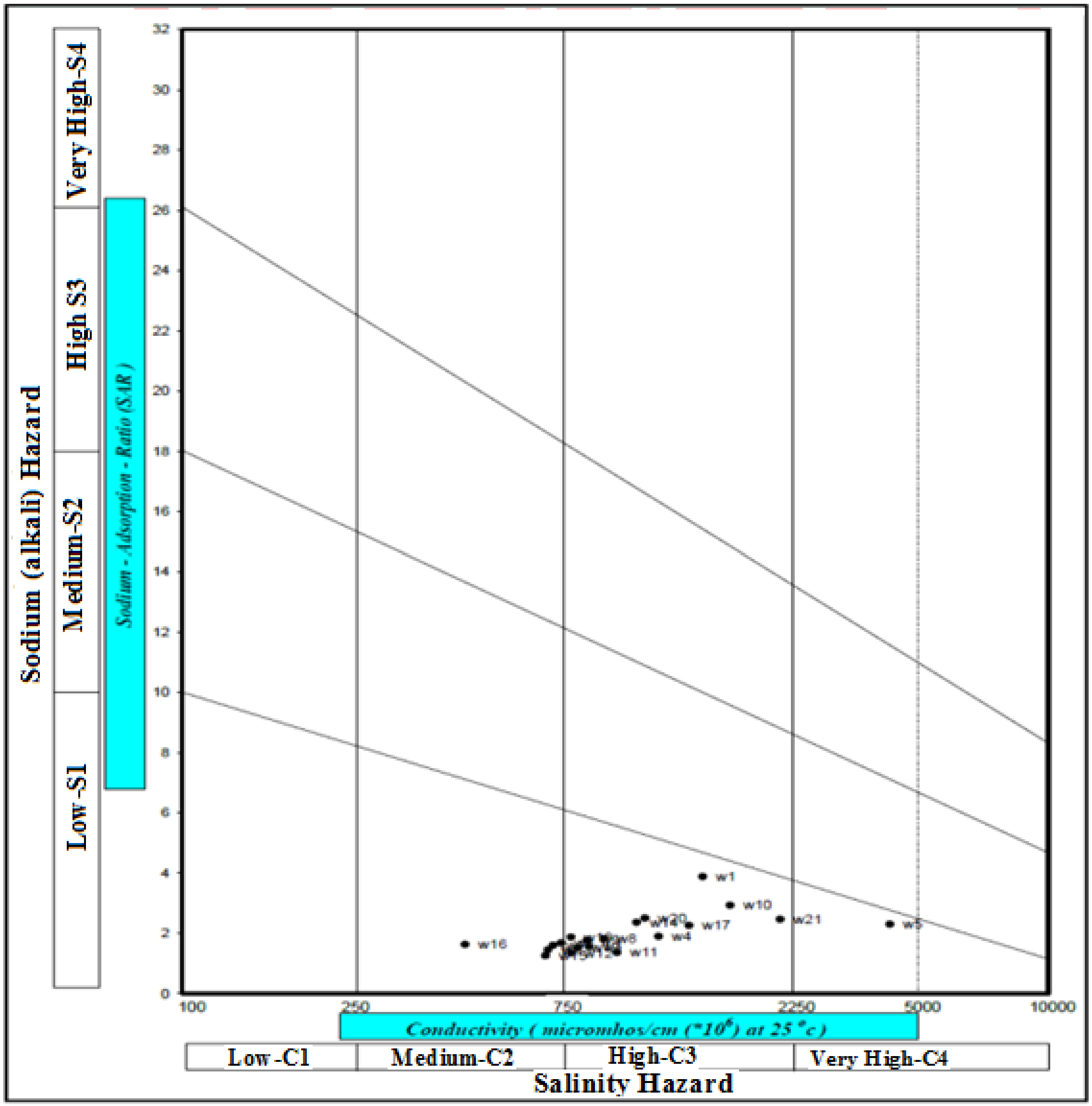

Fig. 8. Wilcox diagram of the Salmas Plain groundwater

According to the Wilcox diagram, the groundwater of the Salmas plain is divided into five classes: C2-S1, C3-S1, C4-S1, C4-S3 and C4-S4. As shown in Figure 9, most of the groundwater samples of the Salmas plain are in zone B. In this zone, the anions CO_3^- and HCO_3^- and the cations Ca_2^+ and Mg_2^+ are predominant and represent freshwater with moderate hardness. Several samples, especially those taken from the southeastern part of the plain, are located in zone E, in which no anions or cations are predominant. The S9, S10, and S13 samples are located in zone C of the diagram, which are located between the layers of the gypsum interlayers, indicating that the water is saline. According to the Piper diagram, the groundwater of the Salmas Plain is mostly of good quality and is part of the fresh and very hard water. The predominant type of the groundwater is calcium-magnesium bicarbonate. According to the Schuler diagram, a significant part of the groundwater of the Salmas plain is flawless in terms of potable water, and only the northern parts of the plain are unsuitable. In general, the results of the diagrams show that the groundwater of the Salmas Plain is acceptable for drinking purposes. Also, according to the Wilcox diagram, the groundwater is in the medium to good range.

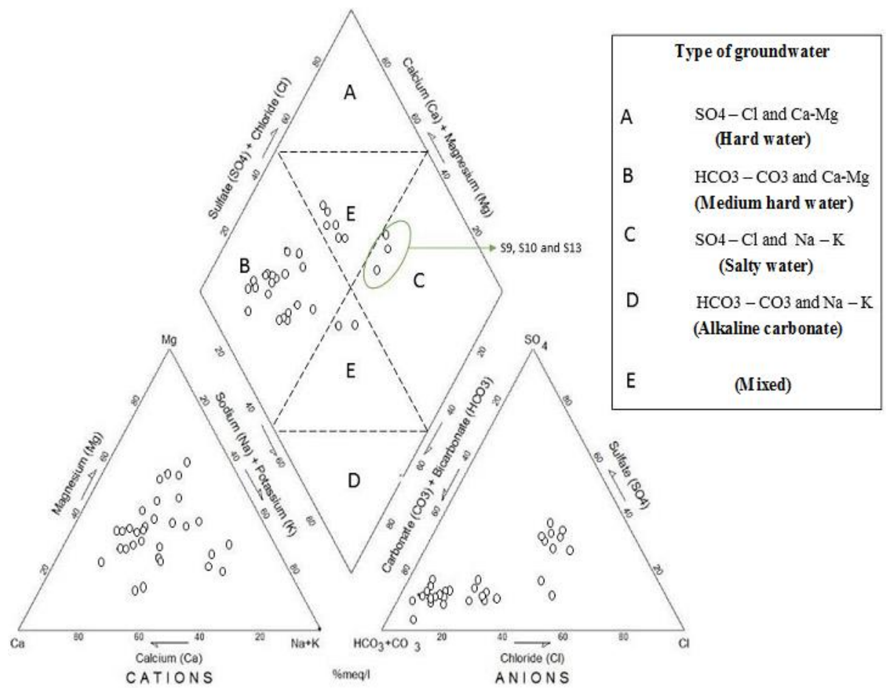

Fig. 9. Piper diagram of the Salmas plain groundwater

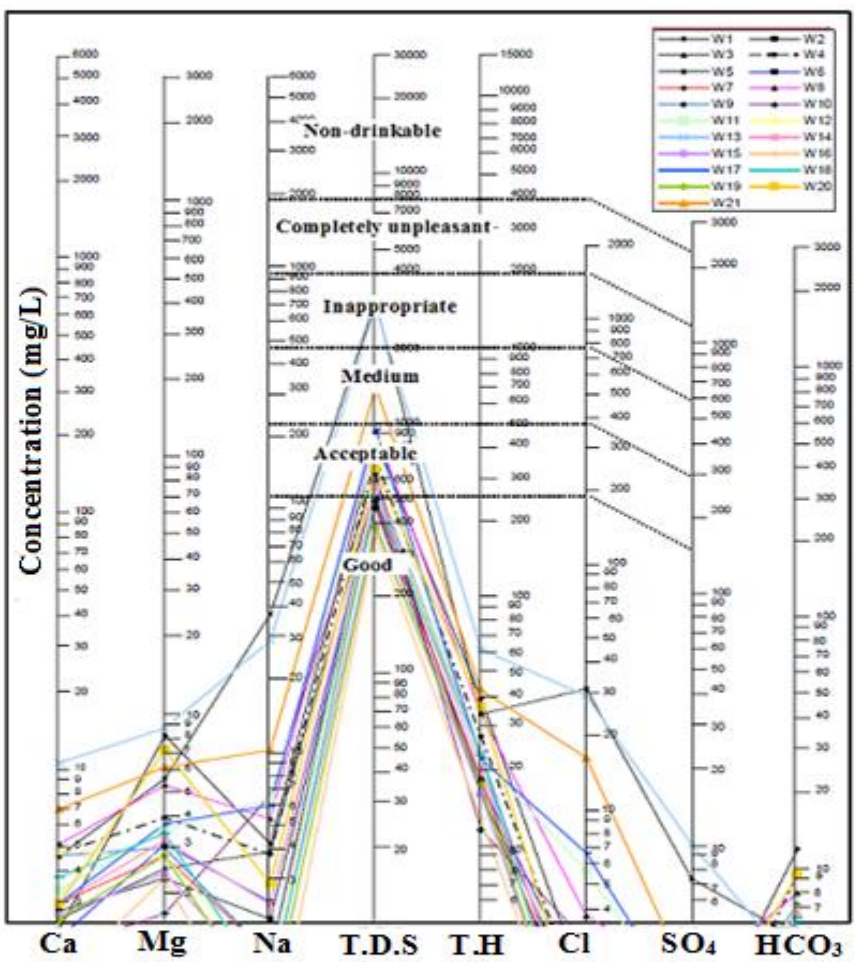

Fig. 10. Schuler diagram of the Salmas plain groundwater

4. Conclusions

In this study, three hybrid models, namely GWO-SVR, EA-SVR, and ICA-SVR, were proposed to obtain the groundwater quality parameters of the Salmas plain. The results obtained from these models matched well with the observed data, which showed the high performance of these methods. The high correlation coefficient (R^2) obtained from the GWO-SVR model in comparison to the other two models indicated the capability and the accuracy of the GWO-SVR model for estimating the groundwater quality parameters. The results of the hydro-chemical analysis of the Salmas plain groundwater by the Wilcox, Schuler, and Piper diagrams also indicated that the groundwater is acceptable and good for drinking and agricultural purposes.

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