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Parametric and non-parametric kriging techniques for delineating water quality in the major cities of Pakistan

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ABSTRACT

Geostatistics is the knowledge of manifestations that vary in space and time. The analysis of spatial data is currently of great interest in statistical modeling. Various parametric and non-parametric kriging techniques are widely used for modeling and prediction of spatially reference data. In this article, we have applied and compared the parametric and non-parametric kriging techniques to model groundwater quality parameters. The data used in this study consists of 366 water samples collected from major cities of Pakistan by the Pakistan Council of Research in Water Resources (PCRWR) survey. The water quality parameters are grouped by spatial variation using cluster analysis and principal component analysis. In order to generate prediction maps and evaluate the probability of groundwater quality parameters, parametric and non-parametric kriging techniques are used. Non-parametric kriging techniques showed better performance than parametric kriging techniques when the normality assumption of kriging is violated.

Keywords: Parametric kriging; Non-parametric kriging; Groundwater quality; Geographic Information System; Pakistan

1. Introduction

Water is playing an important role for nourishing life and development on earth. Groundwater play a key role in nourishing agricultural, human and industrial activities [1]. Water quality decreases day by day due to the access of anthropogenic activities alike wastewater expulsion and nutrient access [2]. The use of contaminated water cause many health problems in the developing countries [3]. Pakistan is listed as water stressed state and threat of water scarcity in nearby future [4]. It was observed that 30% of all the diseases and 40% of all deaths were because of contaminated water [5]. Various contaminants and other metals were found in the drinking water of major cities of Pakistan [6–10].

The presence of significant quantities of physiochemical pollutants and their impact on health were used to evaluate the quality of drinking water [11]. The Environmental Protection Agency (EPA) had investigated the presence of more than 200 organic chemicals in drinking water [12]. It was found that seawater intrusion has contaminated some of the coastal groundwater aquifers [13]. The World Health Organization had warned that dangerous hydrogen (PH) levels could lead to numerous skin and eye illnesses. Water polluted with arsenic can lead to cancer of the lungs, bladder, and membrane. Additionally, skin pigmentation and thickness may result from it [14]. Bone disorders and stomach troubles are caused by drinking water with a high total dissolved solids (TDS) level [15].

Geographic Information System (GIS) and multivariate statistical techniques are applied for the assessment

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of water quality parameters. Adhikary et al. [16] applied non-parametric kriging methods to assess the spatial variation in water quality parameters in New Delhi, India. In order to determine the spatial distribution of groundwater depth and quality parameters in the Ardabil plain in northwest of Iran, Talaee [17] applied parametric kriging method (ordinary kriging). The groundwater quality was assessed by using parametric and non-parametric kriging techniques in Iran and it was found that the non-parametric kriging methods perform better than parametric when assumptions of parametric kriging are not fulfilled [18]. Principal component analysis (PCA) and cluster analysis (CA) were used for identification of the highly correlated and significant water quality parameters [19]. In literature various parametric and non-parametric kriging techniques were used for the evaluation and extrapolation of spatial variation of water quality parameters and it was reported that non-parametric kriging techniques provide better prediction in the case of non-normal data [20,21]. In this study, we have made a comparison between parametric and non-parametric kriging techniques. Non-parametric kriging techniques showed better performance than parametric kriging techniques when the normality assumption of kriging is violated.

The main objective of this study is to assess, model and predict the water quality by applying parametric and non-parametric kriging techniques. For this purpose, we have considered a case of groundwater quality parameters for which the assumption of normality does not hold. Several geo-statistical non-parametric methods as indicator kriging, probability kriging and CDF kriging are used for the purpose of prediction at ungauged locations. Rest of the paper unfolds as follows: in Section 2, material and methods are provided. While Section 3 provides the results and discussion. Finally, the paper is concluded in Section 4.

2. Material and methods

Pakistan is a country in South Asia that borders with Iran to the west, China to the northeast, India to the east and Afghanistan to the northwest (Fig. 1). According to the 2017 census, Pakistan has a total area of 881,913 km^2 and a population of 220 million. In Pakistan, the rivers, groundwater, and rainfall are the main sources of water. The Indus, Sutlej, Chenab, Beas, Jhelum, Sindh, and Kabul are the major rivers. The majority of the territory has a dry climate, although a small portion of the north has a humid climate. The rainiest area in Pakistan is Murree (Rawalpindi), with an average of 1,484 mm of rainfall annually. The majority of the area in Pakistan has less than 250 mm of rainfall annually. Pakistan has four different seasons: a cool, dry winter (December to February); a dry spring (March to May); a rainy summer (June to September); and an autumn (October to November). The water resources of Pakistan are dependent on monsoon precipitation, which occurs from July through September during the summer. According to its topography, Pakistan can be split into six primary regions: the Indus

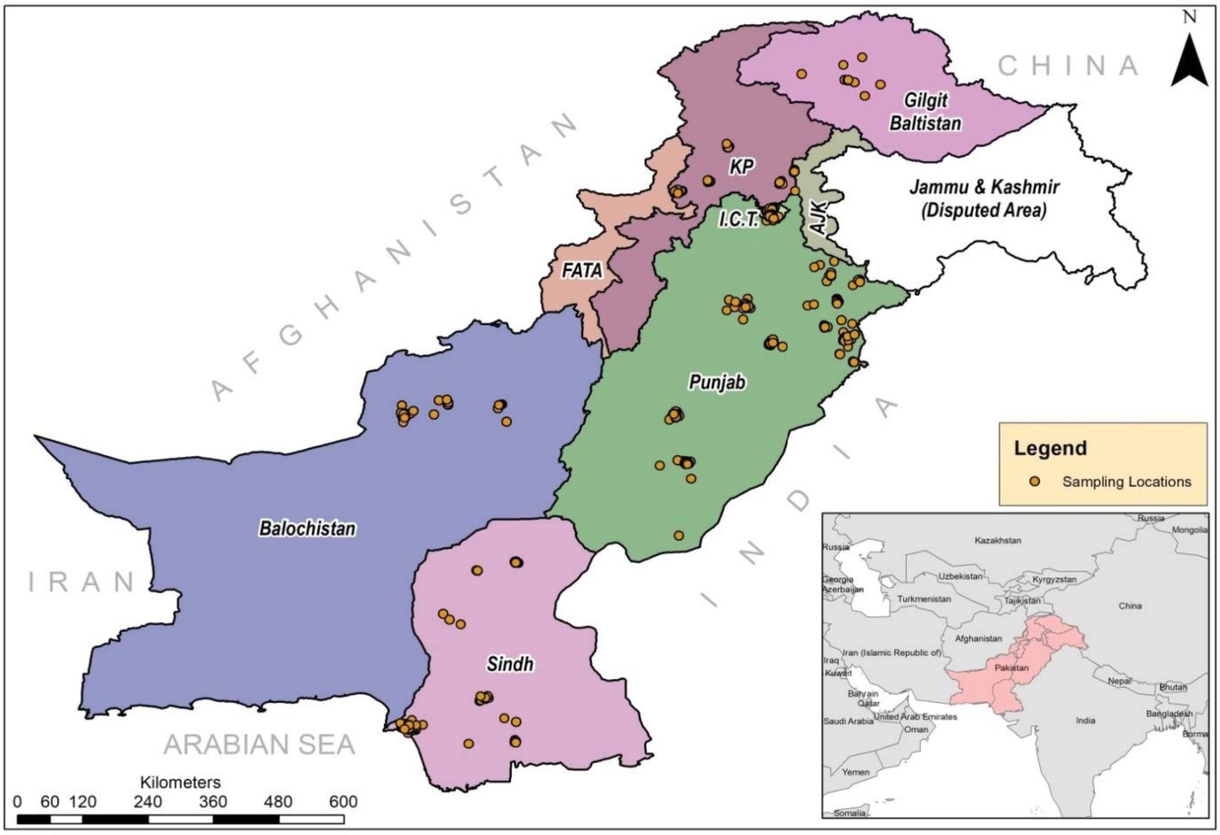

Fig. 1. Study site and sampling locations of major cities of Pakistan.

river plain, the desert regions, the northern highlands, the western mountains, the Baluchistan plateau, the Pothohar plateau, and salt range [22].

2.1. Groundwater samples

Pakistan Council of Research in Water Resources (PCRWR) had conducted a water quality monitoring survey in 2015–16 in 25 main cities of Pakistan including Lahore, Faisalabad, Multan, Gujranwala, Karachi, Peshawar, Rawalpindi, Islamabad, Quetta, Sargodha, Kasur, Sialkot, Bahawalpur, Mardan, Hyderabad, Badin, Loralai, Sukkur, Gujrat, Sheikhupura, Abbottabad, Ziarat, Mingora, Gilgit and Muzaffarabad [23]. Water quality parameters were measured from 366 water samples in the major cities of Pakistan. Samples were taken from a few chosen wells, hand pumps, taps, streams, and water supply systems. The distance between the two monitoring stations was kept between 1 and 16 km. The permanent public locations were preferred, and 0.5 and 1.5 L clean, sterile plastic bottles were used to collect the water samples. Bottles were carefully washed before samples were taken. As a preservative, nitric and boric acids were added to the sampling bottles for trace elements. While being transported to the laboratory, the samples were kept refrigerated and in the dark. The physiochemical parameters are very essential and important to test the water for drinking, domestic, agricultural or industrial purpose. Thus, the role of these parameters is important in determining quality of water. Eleven physiochemical parameters are evaluated in groundwater samples, including (electric conductivity, power of hydrogen, bicarbonate, calcium, magnesium, hardness, sodium, potassium, sulfate, total dissolved solid, and arsenic).

2.2. Variogram and variogram models

Variogram is used to measure the spatial dependency among the spatial neighboring locations. It has three parameters; sill, range and nuggets (Fig. 2) which are used in further prediction techniques.

$$\gamma(h)=\frac{1}{2N(h)}\sum_{i=1}^{N(h)}\left[Z(x_i+h)-Z(x_i)\right]^2 \tag{1}$$

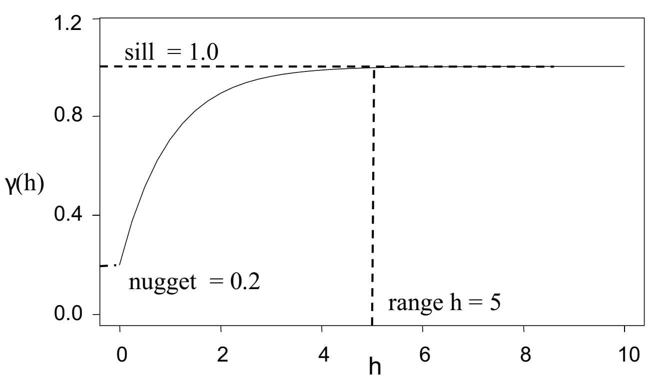

Fig. 2. Description of variogram parameters (sill, range and nuggets).

where $\gamma(h)$ is denotes for spatial correlation and h be the lag distance between the locations. $N(h)$ represents the total number of pairs separated by range h and $Z(x_i)$ indicates the observation at the measured location. Variogram models are fitted because the spatial prediction (kriging) requires the estimates of variogram. The matern model is also called Whittle–Matern model after the name of Whittle [24]. It is used to define the spatial covariance between two points.

$$\gamma(h)=\tau^2+\sigma^2\left(1-\frac{(|h|)}{\varnothing}\right)^{v} k_v\left(\frac{|h|}{\varnothing}\right) \tag{2}$$

where $|h|>0$ and τ^2, σ^2, v and $\varnothing \geq 0$ where k_v is bassel functionality of order v. This particular variogram model is an intermediate option among Gaussian and exponential model [25].

The exponential method for spatial correlation is:

$$\gamma(h)=\tau^2+\sigma^2\left\{1-\exp\left(-\frac{(|h|)}{\varnothing}\right)\right\} \tag{3}$$

for $|h|>0$ and τ^2, σ^2 and $\varnothing \geq 0$ where, where $\tau^2+\sigma^2$ is the sill and τ^2 is called the real nugget effect of the model [26]. The mathematical model of the spherical family is described as:

$$\gamma(h)=\begin{cases}\tau^2+\sigma^2\left(\dfrac{3|h|}{2\varnothing}+\dfrac{|h|^3}{2\varnothing^3}\right) & 0<|h|\leq\alpha\\ \tau^2+\sigma^2|h|>0 & \end{cases} \tag{4}$$

for τ^2, σ^2 and $\varnothing \geq 0$. Spherical model gradually increases from the nugget effect τ^2 to sill quantity $\tau^2+\sigma^2$ when the spatial lag quantity $h \geq \varnothing$ [26].

2.3. Spatial prediction techniques

We have applied the parametric spatial techniques for the prediction spatial data. The ultimate goal of these techniques is to model and test the significance of the environmental data and prediction of ungauged locations. The primary gateway for spatial statistical development is kriging [27]. There are mainly two types of kriging, that is, parametric and non-parametric kriging. Parametric kriging requires the normality of data along with (spatial dependence and spatial continuity). If these assumptions are violated then it is recommended to use non-parametric kriging techniques [21]. Several geo-statistical non-parametric methods as indicator kriging, probability kriging and CDF kriging are used for the purpose of prediction at ungauged locations. It is important to highlight the importance of correct choice of kriging method to obtain efficient prediction.

Ordinary kriging is the extensively applied kriging technique. It is a method based on the assumption of unknown mean and widely used in practice [28]. Ordinary kriging algorithm is given in Eq. (5):

$$Z(x_o)=\sum_{i=1}^{m}w_i\cdot z(x_i),\ \sum_{i=1}^{m}w_i=1$$
$$w_{ij}=\begin{cases}1 & \text{if } i,j \text{ are adjacent neighbors}\\ 0 & \text{otherwise}\end{cases} \tag{5}$$

where $Z(x_o)$ denotes for expected measure of unmonitored locations x_o and m is the number of adjacent points and w_i is the weight assigned to the calculated value $z(x_i)$.

Co-kriging is an expansion of the ordinary kriging. It is a very versatile technique for spatial prediction, which facilitates the user to analyze cross-correlation graphs and autocorrelation [29].

$$\gamma_{uv}(x_j,x)=\sum_{i=1}^{v}\sum_{i=1}^{n_l}w_{il}\gamma_{lv}(z_i,z_j)+u_v \tag{6}$$

where w_{il} denotes the weight function and $\gamma_{lv}(z_i,z_j)$ is the covariance among the variables l and v at locations z_i and z_j.

A binary variable is used in indicator kriging instead of the initial observations. The indicator variable separates the original data based on specific threshold values into binary data [30].

$$I(x_i;z_k)=\begin{cases}1 & \text{if } z(x_i)\geq z_k\\ 0 & \text{otherwise}\end{cases}\quad k=1,2,\ldots,K \tag{7}$$

The number of the threshold is denoted by K and z_k is the preferred threshold. Where w_i denotes the weight coefficient.

Probability kriging is a non-parametric kriging method which is depends upon co-kriging [30]. The standardized ranks are used in calculating the probability kriging which is defined as:

$$U(x)\approx\frac{r}{n} \tag{8}$$

where rank of the r'th order statistic is represented by r and n denotes for the total number of values. The probability kriging estimator is defined as:

$$I^{x_o,z_k}=\sum_{i=1}^{n}w_iI(x_i;z_k)+\sum_{i=1}^{n}w_{ui}U(x_i) \tag{9}$$

where w_i and w_{ui} are the weight functions associated with $I(x_i,z_k)$ and $U(x_i)$, respectively.

2.4. Evaluation of kriging methods

Cross validation was used to evaluate the predictive performance. Three non-parametric kriging methods were considered in this study and were compared for mean error, mean squared error (MSE) and root mean square error (RMSE). Cross validation can be calculated as follow [31]:

$$\text{ME}=\frac{1}{n}\sum_{i=1}^{n}\left[z(x_i)-z^*(x_i)\right] \tag{10}$$

$$\text{MSE}=\frac{1}{n}\sum_{i=1}^{n}\left[z(x_i)-z^*(x_i)\right]^2 \tag{11}$$

$$\text{RMSE}=\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left[z(x_i)-z^*(x_i)\right]^2} \tag{12}$$

where $z(x_i)$ is the observed value at location x_i, $z^*(x_i)$ is the predicted measure at the same location x_i and n is the number of pairs of measured and predicted values. The mean error (ME) value near to zero is an indicator of better model. A model with minimum value of MSE and RMSE is considered the best-fit model among the others.

3. Results and discussions

The descriptive results of hydro chemical parameters are given in (Table 1). ArcGIS 10.7 and R language software's are used for spatial statistical analysis and descriptive measures of water quality parameters. Shapiro–Wilk normality test is used to check the normality of the water quality parameters (Table 1). It is shown in the Table 1 that, except pH, all the water quality parameters are non-normal based on Shapiro–Wilk normality test. Skewness and kurtosis also confirm these results.

3.1. Principal component analysis and cluster analysis

The PCA is applied to highlight the most significant water quality parameters. Form Table 2, it has been demonstrated that the seven water quality parameters have larger loadings and account for 70.96% of the variation overall. Three axes were produced by the analysis, and they account for 83.96% of the total variation (Table 2). Only 12.01% of the entire variation is explained by the second axis, which contains positive loadings for the water quality parameters Ca, Mg, SO_4, and TDS. The third axis, which has a positive loading for HCO_3, accounts for 10.99% of the overall variation.

Cluster analysis is used to classify objects into similar groups. The dendrogram highlights that the first

Table 1
Normality tests for water quality parameters EC, HCO_3, Ca, Mg, HARD, Na, K, SO_4, pH, TDS, and As

Parameters	Shapiro–Wilk normality test	*P*-value	Skewness	Kurtosis
EC	0.26265	<0.000	8.40	80.90
pH	0.99435	0.1951	0.01	0.36
HCO_3	0.82757	<0.000	2.20	7.94
Ca	0.6428	<0.000	4.43	30.11
Mg	0.43285	<0.000	6.21	47.95
HARD	0.50116	<0.000	5.86	45.10
Na	0.28338	<0.000	7.52	65.43
K	0.33507	<0.000	4.63	22.76
SO_4	0.37043	<0.000	5.48	34.03
TDS	0.30842	<0.000	7.41	64.29
As	0.55021	<0.000	2.72	7.18

cluster have seven water quality parameters as in PCA and the other water quality parameters are placed in different clusters shown in colors (Fig. 3). The K and As are placed in a different class according to the dendrogram, which demonstrates that they have a lower correlation with the other parameters. It is to be noted that the cluster analysis results support the classification of the principal component analysis.

3.2. Geostatistical analysis

In this section, variogram parameters of the selected water quality parameters are estimated on the basis of kriging. Ordinary least square, weighted least square, maximum likelihood and restricted maximum likelihood estimation techniques are used with the well-known variogram models to estimate the variogram parameters.

Table 3 shows that the matern model with REML estimation technique is best fitted to electrical conductivity (EC) concentration based on coefficient of determination (R^2 = 0.92). The water quality parameter EC has the sill value of 2.02×10^8 with a range of 2.50×10^2 and nugget 4.82×10^6. The best fitted model for the corresponding water quality parameters are listed in Table 3.

Table 2
Principal component analysis of water quality parameters

Variable	Factor 1	Factor 2	Factor 3
TDS	0.972	0.027	–0.154
EC	0.960	–0.069	–0.162
HARD	0.958	–0.034	–0.117
Mg	0.947	0.060	–0.044
Na	0.946	–0.104	–0.132
SO_4	0.934	0.569	–0.095
Ca	0.838	0.188	–0.200
HCO_3	0.683	–0.112	0.506
K	0.044	–0.083	0.199
pH	–0.351	–0.544	–0.266
As	–0.030	–0.056	–0.440
Explained variation (%)	70.960	12.010	10.990
Cumulative explained variation (%)	70.960	82.970	83.960

3.3. Comparison of kriging methods

To assess the predictive performance of theoretical models, cross-validation statistics are calculated for the water quality parameters. For the significant water quality parameters EC, Ca, Mg, HARD, Na, SO_4, and TDS, ME, MSE, and RMSE are calculated (Table 4). It can be observed that the HARD, EC and TDS parameters are all have minimum value of RMSE and ME for indicator kriging. Probability kriging performed better in the cases of Mg, Na and SO_4. The results show that the indicator kriging and probability kriging performed better than ordinary kriging and co-kriging.

3.4. Spatial prediction of water quality parameters

Based on the results of Table 4, the indicator and probability kriging are further used to generate the water quality prediction maps. The prediction map of parameter EC shows that the EC parameter has values higher towards south and southwestern area (Fig. 4a). It is observed from the Fig. 4b that Ca concentration exceeds its permissible limits in the south-west area. It is clearly depicted from the prediction maps (Fig. 4), that the values of water quality parameters are higher in the southwest region of the study area. The higher values of these parameters may cause cancer, dehydration, laxative effects, and many other skin diseases.

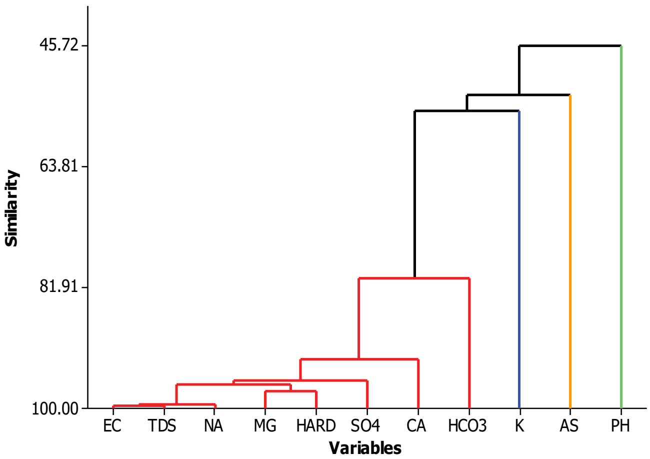

Fig. 3. Dendrogram for clustering the correlated water quality parameters.

Table 3
Variogram model and estimation technique for the water quality parameters

Groundwater parameter	Best-fitted model	Estimation method	Sill (σ^2)	Range (ϕ)	Nugget (τ^2)	R^2
EC	Matern	REML	2.02×10^8	2.50×10^2	4.82×10^6	0.92
Ca	Spherical	REML	4.37×10^2	0.123	1.55×10^3	0.83
Mg	Matern	WLS	3.59×10^3	1.40×10^4	2.87×10^3	0.90
HARD	Exponential	REML	2.95×10^5	19.26	7.79×10^4	0.76
Na	Matern	WLS	3.80×10^5	3.86×10^4	1.33×10^5	0.87
SO_4	Spherical	REML	2.01×10^4	0.48	5.86×10^4	0.83
TDS	Matern	WLS	4.25×10^6	4.16	9.25×10^4	0.91

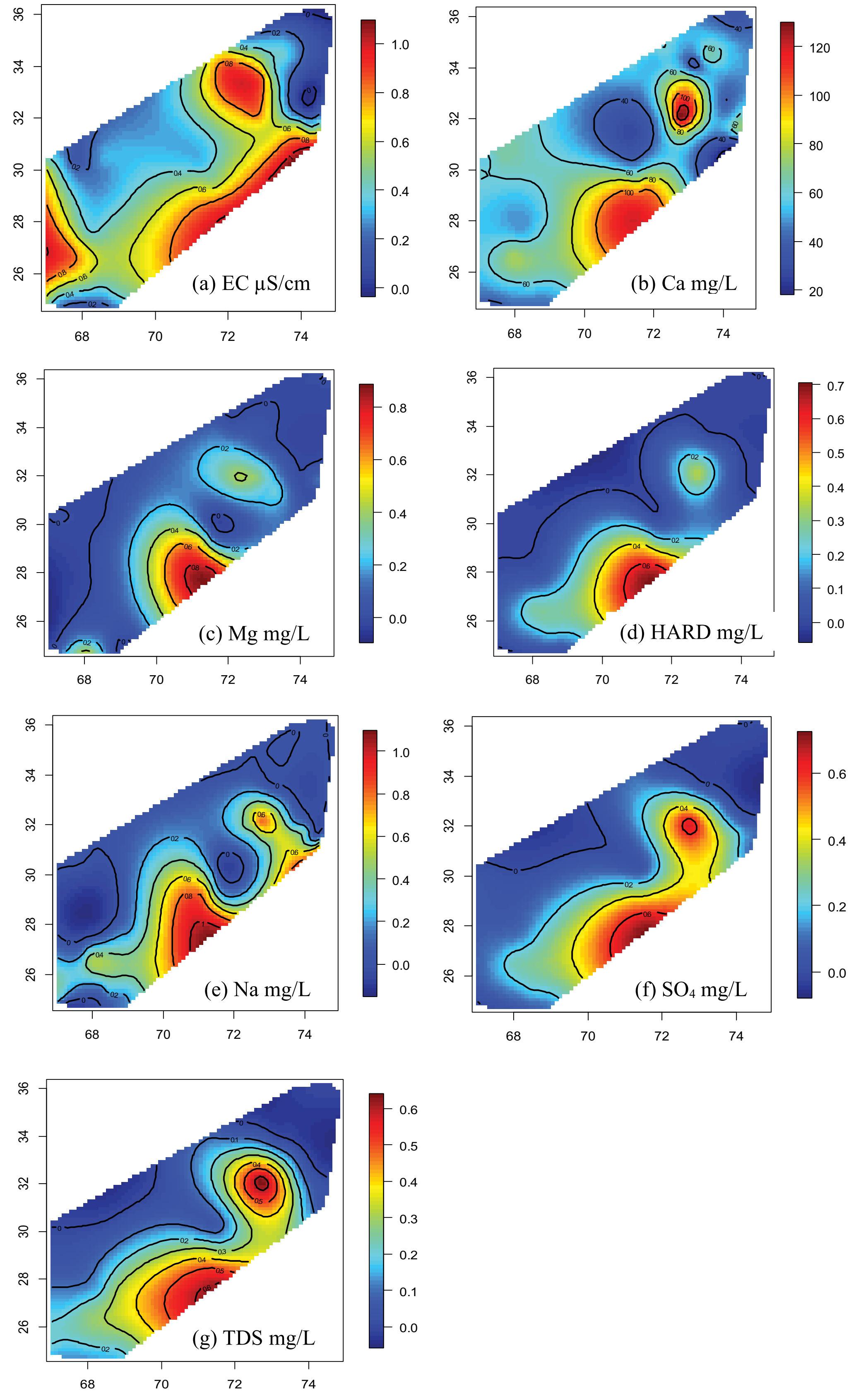

Fig. 4. Prediction maps for seven water quality parameters of major cities of Pakistan.

Table 4
Comparison between parametric and non-parametric kriging techniques

Water quality parameters	Ordinary kriging		Co-kriging		Indicator kriging		Probability kriging	
	ME	RMSE	ME	RMSE	ME	RMSE	ME	RMSE
EC	5.34	15.28	3.76	14.69	**1.81**	**11.13**	1.98	12.34
Ca	3.24	10.73	**2.33**	**8.66**	3.31	9.58	2.56	9.33
Mg	0.98	4.31	0.45	2.52	0.30	1.25	**0.18**	**0.92**
HARD	2.09	7.05	0.78	4.82	**0.02**	**3.61**	0.22	4.02
Na	4.90	7.24	1.45	5.38	0.44	3.92	**0.35**	**2.62**
SO_4	8.35	7.51	4.09	4.88	1.06	2.39	**0.45**	**1.83**
TDS	0.78	10.58	0.05	6.36	**0.01**	**3.08**	0.03	5.67

In general, the flow of groundwater is from east to west in Pakistan. The quality of groundwater is reduced from east to west as shown in the prediction maps given in Fig. 4. Out of 366 water samples, only 113 (31%) are suitable for drinking whereas 69% of samples are highly contaminated and not suitable for drinking purposes. It is also observed from this study that 47% in KPK, 65% in Punjab, and for both Sindh and Baluchistan (81%) of water samples are unsafe and not suitable for drinking. Groundwater contamination is caused by rapid population growth and industrialization.

4. Conclusion

This study investigated the spatial distribution of groundwater quality parameters in the major cities of Pakistan. Various parametric and non-parametric kriging techniques are used widely for modelling and prediction of spatially reference data. All the water quality parameters except pH are non-normal. The results show that the non-parametric kriging techniques (i.e., indicator kriging and probability kriging) have performed better than the parametric kriging (i.e., ordinary kriging and co-kriging). These two better performing non-parametric kriging techniques are used further for generating the prediction maps for water quality parameters. The quality of groundwater deteriorates from east to west. It is found that out of 366 water samples, only 113 (31%) are suitable for drinking whereas 69% of samples are highly contaminated and not suitable for drinking purposes. This study highlights that the groundwater contamination is caused by rapid population growth and industrialization.

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