Spatial estimation of SAR and CL in ground water using cokriging and kriging methods

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ABSTRACT
Today in water and soil sciences, many attentions have been arisen on Geostatistical methods to estimate spatial parameter using some data (kriging) or using auxiliary variables (cokriging). The quality of ground water for agriculture is very important, however its measurement is time consuming and expensive. Therefore, finding solution to estimate such parameters from easily measurable parameters is essential. In this study, two estimation models (spatial and regression models) were used to estimate SAR and CL in Tehran region using Geostatistic theory and spatial parameter concept. In this regard, ArcGIS software was used to estimate these parameters. Multi-parameter estimate of cokriging was applied using water salinity as an auxiliary variable. In addition, different estimation methods, cokriging, kriging and regression models, were compared and evaluated by RMSE statistic index. The results of this study showed that cokriging method with high correlations coefficient and with Gaussian Semivariogram is more precise than kriging and the selected regression models in estimating SAR and CL.

Introduction
Groundwater is the main source of irrigation in arid and semi-arid regions in the world. Crop production in arid zones consumes large quantities of water. While the production of 1 kg of grain in a temperate zone takes less than 0.5 m3 of water, 1.5–2.5 m3 is normal in a arid zone (Smedema and Shiati 2002). Groundwater is, however, the main and more reliable resource of irrigation. Both over-exploitation from aquifers to address the irrigation needs, and drought events have caused severe decrease of water Table level in many areas. Where groundwater is used for irrigation, aquifers are also being depleted at an alarming rate. In Iran, the current groundwater abstraction exceeds the safe yields by some 15–20% and water Tables in some irrigated areas are falling at 0.5–1.0 m/year (Shiati 1999). The situation is equally alarming in some parts of the Indo-Gangetic plains in India, the North China Plain and in the south-west of the USA (Smedema and Shiati 2002). In Iran that is located in arid to semi-arid region of the world, about 95% of fresh water is allocated for agriculture, out of which 80% is supplied through groundwater. So, it is clearly concluded that groundwater is the vital component for sustainable agriculture. In recent years, many fertile and agricultural plains suffered from 0.5 to 15 m water Table level drop, in which many wells are now out of use.

Monitoring the groundwater level using observation wells is the major source of information on the effects of hydrologic stresses on groundwater systems. Water level data collected over periods of days to months are useful for such purposes; however, data collected over years to decades are required to address the long term effects of aquifer development and to compile a hydrologic record that defines water level fluctuations (Alley and Taylor 2001). Understanding the behavior of the groundwater body and its long term trends are essential for making any management decision in a given watershed (Regahunath et al. 2005). Therefore, having a deep knowledge and insight on the groundwater system seems necessary for optimum exploitation of water.

The recently large variations of groundwater levels over years in many parts of Iran, suggest a precise and detailed study to be undertaken to elucidate the behavior of groundwater level fluctuations. A very useful tool for analyzing such processes is geostatistics (Ahmadi and Sedghamiz 2007; Rouhani and Wackernagel 1990). Regahunath et al. (2005) and Kumar et al. (2005) have emphasized the use of Geostatistics for better management and conservation of water resources and sustainable development of any area. Theodossiou and Latinopoulos (2006) worked on spatial analysis on groundwater level of 31 wells using kriging. They used the kriging method aiming at the evaluation and optimization of the groundwater level observation networks and the improvement of the quality rather than the quantity of the obtained data. Ahmadi and Sedghamiz (2007) used the kriging method to evaluate the spatial and temporal variations of groundwater level of 39 observation wells. They showed that groundwater level variations have strong spatial and temporal structure.

Groundwater can affect water quality in many regions because of its salinity. Irrigation by saline water causes salt accumulation and reduces water infiltration in clay soils and decrease soil productivity. Soils may be saline, alkaline or saline-alkaline on which incorrect management of applied water may intensely decrease plant yield. In many managements is necessary to know the spatial and temporal behaviors of groundwater.

Water quality measured according to Sodium Adsorption Ratio (SAR) and CL amounts and their diffusion and their effect upon agricultural soils and plants. Available sodium in irrigation causes soil dispersion and soil destruction and decrease plant yield. So it is important to measure CL and Na in irrigation water for suitable management and yield maximization.
Considering hard measurement of SAR in laboratory and simple measurement of electrical conductivity (EC), then estimation of SAR according to EC is very important. Kriging is a technique of making optimal, unbiased estimates of regionalized variables at unsampled locations using the structural properties of the semi variogram and the initial set of data values (David; 1977). In this study, both the kriging and cokriging methods were applied to investigate their precision in mapping SAR and CL in ground water. So it may be possible to gain a clear picture of aquifer behavior across the study area, which leads to an efficient management and conservation of the current groundwater resources. Detailed description of the methods and required data will be presented in the next sections.

Material and methods

Study area

The study area is Tehran-Karaj plain which is located in the middle of Tehran province, northern Iran; between 35° 6′–35° 56′ north and 50° 42′–51° 41′ east, with an elevation about 1,250 m above sea level and includes an area about 4830 square kilometers (Fig. 1). Groundwater resources in this region consist of 18175 wells (4021 deep wells, 11434 semi deep wells, and 2720 shallow wells), 608 springs, and 619 usual gully systems. This research was accomplished in Tehran-Karaj region with an area equal to 1663.5 square kilometers (Tehran Regional Water Organization 1998).

Data availability

In this research, samples provided from 120 wells which their spatial distribution was showed in Figure2. Geographical altitude and longitude was measured with Global positioning system (GPS). In the next step, any sample in plastic containers was carried to laboratory and chemical analysis was performed on these samples. Measured chemical parameters included SAR, Cl and EC. In order to evaluate salinity distribution in this region, ArcGIS program and cokriging and kriging methods were selected due to high performance of these techniques to estimate salinity. Regressional model fitted using SPSS program. Shape of case study and point spatial distribution are showed in Figure1.

In order to extend and to generalize point information by attention to measured points need to models which predict spatial and temporal behaviors in places which were not measured. Regressional models in classic statistics science were not suitable for estimation of points which were not measured because of these models considered the point absolute effect. But In Geostatistical models the prediction is based on land topography structures. Geostatistical estimation is a process that determines some parameters with unknown value but with given coordinate using measured values of the same parameter.

Theoretical basis

The theoretical basis of geostatistics has been fully described by several authors (Webster and Oliver 2001; Goovaerts 1997; Kitanidis 1997; Isaaks and Srivastava 1989). The main tool in Geostatistics is semi-variogram, which expresses the spatial dependence between neighboring observations. The Semi-variogram, $\gamma(h)$, can be defined as one-half the variance of the differences between the attribute values at all points separated by a distance $h$, as follows:

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

Where $Z(x)$ indicates the magnitude of variable, and $N(h)$ is the total number of pairs of attributes that are separated by a distance $h$. However, for simplicity, for the remaining of the text, the term variogram will be used instead of semi-variogram.

Prior to the geostatistical estimation, we require a model that enables us to compute a variogram value for any possible sampling interval. The most commonly used models are Spherical, Exponential, Gaussian, and Pure nugget effect (Isaaks and Srivastava 1989).

The adequacy and validity of the developed variogram model was tested satisfactorily by a technique called cross-validation. The idea of cross-validation consists of removing a datum at a time from the data set and re-estimating this value from remaining data using different variogram models. Interpolated and actual values are compared, and the model that yields the most accurate predictions is retained (Isaaks and Srivastava 1989; Goovaerts 1997; Leuangthong et al. 2004). Crossing plot of the estimate vs. the true value shows the correlation coefficient (R2). The most appropriate variogram was chosen based on the highest correlation coefficient by a trial
and error procedure (Ahmadi and Sedghamiz 2007). Leuangthong et al. (2004) reported that the variograms obtained through cross-validation satisfy the minimum acceptance criteria for geostatistical analysis.

Fig 4. fitted empirical and computational semi-variogram for SAR

Kriging technique is an exact interpolation estimator used to find the best linear unbiased estimate. The best linear unbiased estimator must have minimum variance of estimation error. Detailed discussions of kriging methods and their descriptions can be found in Goovaerts (1997). The general equation of kriging estimator is:

\[
\hat{Z}(x_p) = \sum_{i=1}^{n} \lambda_i Z(x_i) \tag{2}
\]

\[
\sum_{i=1}^{n} \lambda_i = 1
\]

In order to achieve unbiased estimations in kriging, the following set of equations should be solved simultaneously.

where \(Z^*(x_p)\) is the kriged value at location \(X_p\), \(Z(x_i)\) is the known value at location \(X_i\), \(\lambda_i\) is the weight associated with the data, \(\mu\) is the Lagrange multiplier, and \(\gamma(X_i, X_j)\) is the value of Variogram corresponding to a vector with origin in \(X_i\) and extremity in \(X_j\). The general form of Cokriging equations are:

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \gamma(X_i, X_j) Z(X_j) - \mu = \gamma(X_i, X) \tag{3}
\]

\[
\sum_{i=1}^{n} \lambda_i = 1
\]

Where \(u\) and \(v\) are the primary and covariate (secondary) variables, respectively.

In the cokriging method, \(u\) and \(v\) are cross-correlated and the covariate contributes to the estimation of the primary variable.

Generally, measuring the covariate is simpler than measuring the primary variable. For cokriging analysis, the cross semi-variogram (or cross-variogram) should be determined in prior. Provided that there are points where both \(u\) and \(v\) have been measured, the semi cross-variogram is estimated by:

\[
\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [Z_u(x_i) - Z_u(x_i + h)] [Z_v(x_i) - Z_v(x_i + h)] \tag{4}
\]

For investigation the relationship between CL and SAR with EC in classic statistics, we used correlation analysis with Pearson method to select the best model between CL and SAR (EC and SAR considered as independent variable) and between EC and CL (EC and CL considered as independent variable). Various models (linear, quadratic, cubic, exponential, logistic, logarithm models) fitted by using SPSS program. After selection of the best model between CL and SAR by using EC, obtained equations were tested by real data which were not used in calibration process (these data are 20 percents). In order to evaluate cokriging and kriging methods, (RMSE) of the models were calculated using this equation:

\[
\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} [Z(x_i) - Z(x_i)]^2/n}
\]

Where \(Z(x_i)\) is estimated value at \(X_i\) and \(n\) is the number of measured point.

In this research, in any step one measured point was deleted and this deleted point was estimated using the remained points and this work repeated for all the measured points. Finally for any measured point exists one estimated point. In order to evaluate selected regression equation for CL and SAR estimation uses these parameters.
Result and discussion

Some statistical parameter such as average, standard deviation, minimum, maximum, variation coefficient, skewness, kurtosis and variation distance are in Table 1.

For data analysis, histogram of any investigated variables obtained (Fig.3). Considering histograms, due to high skewness of two variables (CL and SAR), all the data should be normalized. After normalization, the histograms were obtained and showed in Fig.3 (right part of Fig3).

Based on Table 4, cubic, quadratic and linear models have high correlation coefficient. Because of simple justification of linear model, this model selected for estimation of SAR from EC parameter.

\[ \text{SAR} = 0.005 \text{EC} - 1.287 \quad (7) \]

Where: EC (mmohs/cm), SAR: (meq/lit)

Figure 8 illustrates the observed values in comparison to predicted values of SAR for linear model estimation.

According to Table 4, cubic, quadratic models have high correlation coefficient. Because of simple justification of quadratic model, this model selected for estimation of CL from EC parameter.

\[ \text{CL} = 1.11 \times 10^{-6} \text{EC}^2 + 0.001 \text{EC} + 0.024 \quad (8) \]

Where: EC (mmohs/cm), CL (meq/lit)

Figure 9 illustrates the observed values in comparison to predicted values of CL for quadratic model estimation.

Evaluation of Geostatistical and classic statistics

In order to check the accuracy of the geostatistical and classic statistics methods, we estimated the SAR and CL of the known points by geostatistical (Kriging and Cokriging) and classic statistics methods. Root Mean Square Error (RMSE) was used to evaluate the precision.

Based on Table 5, classic statistics method has shown low performance in comparison with geostatistical methods (RMSE=18.46, 101.49 for estimation of SAR and CL, respectively). Geostatistical methods consider the quantity and spatial position of a parameter whereas classic statistics methods consider the quantity of a parameter only.

In geostatistical method, while the calculated RMSE values for SAR and CL in kriging was 3.15 and 3.89; the calculated RMSE in cokriging were 3.07 and 3.82, respectively. Moreover, t test (α=0.05) revealed that there was no significant difference between the estimated values of the two methods against the real measurements of SAR and CL. It is obvious that cokriging has resulted in more accurate estimation of SAR and CL than kriging, though; there is a slight difference between the kriging and cokriging estimations of Li. However, the calculated RMSE values are acceptable for kriging and cokriging. It again emphasized the unbiasedness of the kriging and cokriging estimations (Leuangthong et al. 2004; Sepaskhah et al. 2005; Ahmadi and Niazi Ardekani 2006; Ahmadi and Sedghamiz 2007).

Conclusion

In this research, groundwater chemical parameters were estimated using water salinity data. Results of two Geostatistical methods (cokriging and kriging) have nearly the same precision for estimation of SAR and CL and these models have high performance in comparison with classic statistics.

In order to evaluate semi-variograms, initially semi-variograms of any variable was depicted by GS+. Suitable model on empirical semi-variograms were selected. Based on Table 5, classic statistics method has shown low performance in comparison with geostatistical methods.

The some chemical parameters affected by environmental factors. Cokriging model can use these factors for estimation of main variable. Correlation coefficients between SAR and EC, CL and EC are 77% and 75%, respectively. Accordingly, cokriging model used of EC parameter as auxiliary variable parameter for estimation of main variables SAR and CL. The results showed the cokriging method has high performance for estimation of variables.

Classic statistics

Fitted models for SAR and EC data showed meaningful and positive correlation in the level of 1% (Table 3).
References

Table 1. value of obtained statistical parameter

<table>
<thead>
<tr>
<th>variable</th>
<th>mean</th>
<th>minimum</th>
<th>maximum</th>
<th>Coefficient variation</th>
<th>Std deviation</th>
<th>skewness</th>
<th>kurtosis</th>
<th>Range</th>
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</thead>
<tbody>
<tr>
<td>SAR</td>
<td>3.32</td>
<td>0.288</td>
<td>23.99</td>
<td>0.99</td>
<td>3.31</td>
<td>2.52</td>
<td>10.57</td>
<td>23.7</td>
</tr>
<tr>
<td>CL</td>
<td>5.45</td>
<td>0.12</td>
<td>37.44</td>
<td>1.89</td>
<td>4.3</td>
<td>2.77</td>
<td>7.44</td>
<td>37.22</td>
</tr>
</tbody>
</table>

Table 2. Properties of the fitted variograms for each variable based on cross validation in CL and SAR

<table>
<thead>
<tr>
<th>variable</th>
<th>model</th>
<th>Nugget</th>
<th>Sill</th>
<th>Range effective</th>
<th>C0/(C0+C)</th>
<th>R2</th>
<th>RSS</th>
</tr>
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<tbody>
<tr>
<td>SAR</td>
<td>Spherical</td>
<td>4.8</td>
<td>26.75</td>
<td>163300</td>
<td>0.179</td>
<td>0.931</td>
<td>0.132</td>
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<tr>
<td>CL</td>
<td>Gaussian</td>
<td>3.4</td>
<td>307.7</td>
<td>30596</td>
<td>0.043</td>
<td>0.934</td>
<td>0.341</td>
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### Table 3. Fitted models and related parameters for estimation SAR using EC

<table>
<thead>
<tr>
<th>Model</th>
<th>Sig</th>
<th>$R^2$</th>
<th>constant</th>
<th>b1</th>
<th>b2</th>
<th>b3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>0.000</td>
<td>0.907</td>
<td>-1.287</td>
<td>0.005</td>
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<td>Logarithmic</td>
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<td>0.672</td>
<td>-28.89</td>
<td>4.871</td>
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<td>Universe</td>
<td>0.000</td>
<td>0.311</td>
<td>6.208</td>
<td>-2021.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Polynomial-2</td>
<td>0.000</td>
<td>0.912</td>
<td>-6.79</td>
<td>0.003</td>
<td>3.25-07</td>
<td>-1.29-10</td>
</tr>
<tr>
<td>Polynomial-3</td>
<td>0.000</td>
<td>0.912</td>
<td>-0.404</td>
<td>0.003</td>
<td>1.04-06</td>
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<td>Power</td>
<td>0.000</td>
<td>0.769</td>
<td>0</td>
<td>1.372</td>
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<td>0.641</td>
<td>0.605</td>
<td>0.001</td>
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<td></td>
</tr>
<tr>
<td>Logistic</td>
<td>0.000</td>
<td>0.641</td>
<td>1.653</td>
<td>0.999</td>
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### Table 4. Fitted models and related parameters for estimation CL using EC

<table>
<thead>
<tr>
<th>Model</th>
<th>Sig</th>
<th>$R^2$</th>
<th>constant</th>
<th>b1</th>
<th>b2</th>
<th>b3</th>
</tr>
</thead>
<tbody>
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<td>0.525</td>
<td>0.001</td>
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</tr>
<tr>
<td>Logistic</td>
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<td>0.701</td>
<td>1.906</td>
<td>0.999</td>
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</table>

### Table 5. The measured RMSE in performance evaluation of statistical and geostatistical methods in estimation of SAR and CL parameters

<table>
<thead>
<tr>
<th>Estimation method</th>
<th>Classic statistics</th>
<th>Kriging</th>
<th>Cokriging</th>
<th>SAR</th>
<th>CL</th>
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<tbody>
<tr>
<td>SAR</td>
<td>18.46</td>
<td>3.15</td>
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<td>CL</td>
<td>101.49</td>
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<td>3.82</td>
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