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Metaheuristic kriging: A new spatial estimation method

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Abstract

Kriging is one of the most widely used spatial estimation method. In kriging estimation, weights assigned to the neighboring data are determined by minimizing the estimation error variance (EEV). Due to the minimization of the EEV the variability of the estimation result is lower than the original data. This paper presents the metaheuristic kriging (MK) as a new estimation method which has similar structure with kriging. But unlike kriging MK does not minimize the estimation error variance, instead converges to the EEV minimum which provides MK to increase the variability of the estimation. The MK uses the metaheuristic differential evolution algorithm in minimization of the EEV which gives names the MK. As a case study, Ordinary kriging (OK) and MK are applied to the Jura data set to estimate the spatial distribution of the Nickel (Ni) content. Results of the estimations are compared. Results shows that metaheuristic kriging over performed to the ordinary kriging in terms of variability of the estimation. The MK can be used any place where kriging is applied due to the variability of the estimation is higher than OK. The parameters used in MK are case specific so parameter tuning have to be made in the estimations to reach the desired outcomes. This study only exposes the univariate spatial estimation.

Keywords: Kriging, Metaheuristic Kriging, Differential Evolution, Spatial Estimation, Optimization.

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1. Introduction

Estimation of the spatial distribution problem is encountered in many areas such as mining, environmental science, agriculture, public health, meteorology, civil engineering, hydrogeology, fisheries [2, 3, 4, 5, 7, 10]. Due to the limited time and economic reasons data collected in the mentioned fields are limited. So the estimation of the spatial distribution of the target variable have to be made by using only the available data which makes the estimation of the spatial distribution at every location important.

In estimation of the spatial distribution inverse distance weighting, nearest neighborhood, bilinear, kriging interpolation and geostatistical simulation methods are used. Among them kriging and geostatistical simulation are most widely used and most sophisticated methods. Kriging produces the best estimate of the spatial distribution by minimizing the estimation error variance and estimation results are unbiased form the view point of the mean. Local estimates are the best estimates due to the minimization of the estimation error variance. But this method has some shortcoming like results are less variable and spatial continuity is different than original variable. To overcome this problem geostatistical simulation can be used. In geostatistical simulation results shows similar variability and similar spatial continuity to original variable. But this method has shortcoming; estimation error variance is the twice of the kriging estimation variance which makes estimations less reliable and restricts the use of the method only in characterization of the uncertainty of the spatial distribution rather than mapping of the spatial distribution. For the estimation of the spatial distribution of the random variable a method that both minimizes the estimation error variance as much as possible like the kriging and mimics the spatial continuity of the original variable like geostatistical simulation is required. For this purpose, covariance matching constrained kriging (CMCK) is proposed by the Aldworth and Cressie [1]. But CMCK does not always guaranties to produce an estimation result.

In this study, Metaheuristic Kriging (MK) is introduced as a new estimation method. The method uses the EEV in estimation like kriging. But, unlike kriging method does not minimize the EEV. Instead method converges to the minimum of the estimation error variance using the optimization method Differential Evolution (DE) which is the member of the metaheuristic optimization. This convergence forces the estimations to become more variable than kriging estimations which is desired property. As an example MK is applied in Jura data set where the Ni concentration selected as target variable. Experimental variograms of the Ni are calculated and model fitted to these variograms. Spatial distribution of the Ni concentrated mapped for both Ordinary Kriging (OK) and MK. Estimation results of the both method are compared with raw data.

2. Methodology

2.1. Kriging. Kriging aims to estimate the value of the random variable, Z, at given support $z(x_1, x_2, ..., x_n)$ at the points $(x_1, x_2, ..., x_n)$. Data can be in one, two or three dimension but in most applications generally in two or three dimensions. Estimation of the Z at location x_0 by;

(2.1) $\hat{Z}(X_0) = \sum_{i=1}^{N} \lambda_i z(x_i)$

where λ_i are weights. Lambdas are determined by the minimization of the cost function which is most widely named as estimation error variance. EEV can be in terms of variogram and estimation weights as;

(2.2) $2\sum_{i=1}^{N} \lambda_i \gamma(x_i, x_0) - \sum_{i=1}^{N} \sum_{j=1}^{N} \lambda_i \lambda_j \gamma(x_i, x_j)$

where $\gamma(x_i, x_j)$ is the variogram of distance between the x_i and x_j data points and $\gamma(x_i, x_0)$ is the variogram value of the distance between data used in estimation and estimation. Variogram is a measure of the spatial dependence and widely used in spatial estimation. The EEV function (Eq. 2.2) is convex, continues, differentiable and has one global minimum. One may find the minimum of such a function by using partial derivatives. The partial derivative of the estimation error function respect to estimation weights (lambdas) yields the system of equations which is known as the kriging equation;

$$\Delta\lambda = b \tag{2.3}$$

where, Δ matrix of the all possible combinations of the variogram values between the data used in estimation; b is all possible combinations of the variogram values between data and estimation location.
Solution of this equation for λ ;

$$\lambda = \Delta^{-1} b \tag{2.4}$$

Where lambdas are used in estimation of the random variable Z.

2.2. Metaheuristic Kriging. Metaheuristic optimization methods which often nature inspired are general family of the algorithms that aims to find the near minimum of the complex optimization problems. Ant colony, artificial bee colony, particle swarm and differential evolution optimization algorithms are just few examples of the metaheuristic optimization algorithms. By nature, metaheuristic optimization techniques are non-deterministic which means that in every minimization problem different results are expected but these results are approximate to the real solution. Differential evolution (DE) algorithm is widely used in metaheuristic optimization which is first proposed by the Price and Storn in 1995 as a technical report [8]. Algorithm finds the near optimal solution of the cost function by iteratively perturbing the candidate solution. DE is well known algorithm and the details of the algorithm is not exposed here, readers are referred the seminal work by the Price et al. [6]. Algorithm have four basic steps which are initialization, mutation, crossover and selection. First the population (P_x) which contains the candidate solutions ($x_{i,g}$) is created as

$$\begin{aligned} P_{x,g} &= (X_{i,g}), \quad i = 0, 1, .., N_p - 1, \quad g = 0, 1, ..., g_{max}, \\ & \qquad x_{i,g} = (x_{j,i,g}), j = 0, 1, ...D - 1 \end{aligned} \tag{2.5}$$

where g indicates the generation number.
Once the initialization step is completed, DE mutates the candidate solution and produces trial $P_{v,g}$ and mutated vectors $V_{i,g}$ using the mutation scale factor (SF)

$$\begin{aligned} P_{v,g} &= (v_{i,g}), \quad i = 1, 2, .., N_p, \quad g = 1, 2, ..., g_{max}, \\ & \qquad v_{i,g} = (v_{j,i,g}), j = 1, 2, ...D \end{aligned} \tag{2.6}$$

In order to finish the search strategy after the mutation uniform crossover is performed which basically copies the values form candidate solutions one to other and creates the trial vector $u_{i,g}$ using the crossover parameter value (CR):

$$\begin{aligned} P_{v,g} &= (u_{i,g}), \quad i = 1, 2, .., N_p, \quad g = 1, 2, ..., g_{max}, \\ & \qquad u_{i,g} = (u_{j,i,g}), j = 1, 2, ...D \end{aligned} \tag{2.7}$$

Finally, selection step is performed by comparing trial vector with target vector. If the target vector produces better result than the trial vector trial vector is rejected, otherwise trial vector is replaced with target vector in next generation. The DE algorithm is easy to use, robust and have few control parameters like CR, SF, P and GEN [9]. The determination of these parameters are case specific. But with increasing number of P and GEN solution converges to the optimality. MK shares the same root with kriging but ignores the minimization of the estimation error variance assumption. Instead, finds the near optimal solution of the Eq. 2.2 using the differential evolution algorithm. The parameters of the P and GEN are selected at lower values than ordinary DE optimization problem which avoids the DE algorithm to find the optimal solution. This non-optimal solution gives flexibility to increase the variability of the estimation which is root of the MK. The MK estimation steps are very similar to the OK estimation. The steps are as follows;

(1) Experimental variogram calculation and model variogram fitting
(2) Eliminating anisotropy structure in data (if exists)
(3) Selecting neighboring data for estimation location
(4) Calculating estimation weights for neighboring data by using differential optimization algorithm by converging the minimum of the estimation error variance
(5) Determining estimation results by weights.
(6) Repeating steps 1 to 5 for each estimation location
(7) Comparing the estimation results with raw data, if the results needs improvement, modify the P and GEN parameters in differential evolution algorithm.

Due to the similar structure with kriging, the parameters of the estimations are mainly can be selected similar to the kriging practices. The first three steps of the metaheuristic kriging estimation are identical to the ordinary kriging estimation. So, the variogram modelling, anisotropic correction and conditioning data selection steps are as the same as the OK. This makes MK easy to implement and compare with OK rationally. Only the difference from the OK is that determination of the weights are made based on the differential evolution algorithm. IN MK, like every metaheuristic optimization algorithms selection of the algorithm specific parameters are subjective and changes respect to specific application. While the convergence to the DE algorithm is good to the real solution the setting the DD and DF parameter to the high values makes MK results similar to OK results. So, variability of the estimation results has to be checked and parameters of the DD and DF have to be changed in order to capture the required variability. This property makes the MK an iterative method.

3. Case Study

3.1. Data. In this study comparative study of the metaheuristic kriging with ordinary kriging is made. For demonstration purpose Jura data set is used. Data set collected by the Swiss Federal Institute of Technology form the topsoil in Swiss Jura. Ni concentration of the topsoil samples are measured at 259 sampling sites which is heavy metal and can be reason of serious concerns when is in excessive amount. The map of sample locations is given in Fig. 1.

Histogram and the summary statistics of the Ni concentration is in Fig. 2.

3.2. Variogram Modelling. For the purpose of variogram modelling, experimental variograms are calculated at four main direction having azimuth $0^0, 45^0, 90^0$ and 135^0. Experimental variograms are given in Fig. 3.

As seen from Fig. 3 Ni shows similar spatial variability in the all directions omnidirectional experimental variogram is calculated and model fitted to the experimental variogram. Spherical model used as a variogram model. This variograms are given in Fig. 4

Nugget, sill and range of the variogram model is 10, 57 and 960 m respectively which means that data relation disappears beyond the 960 m.

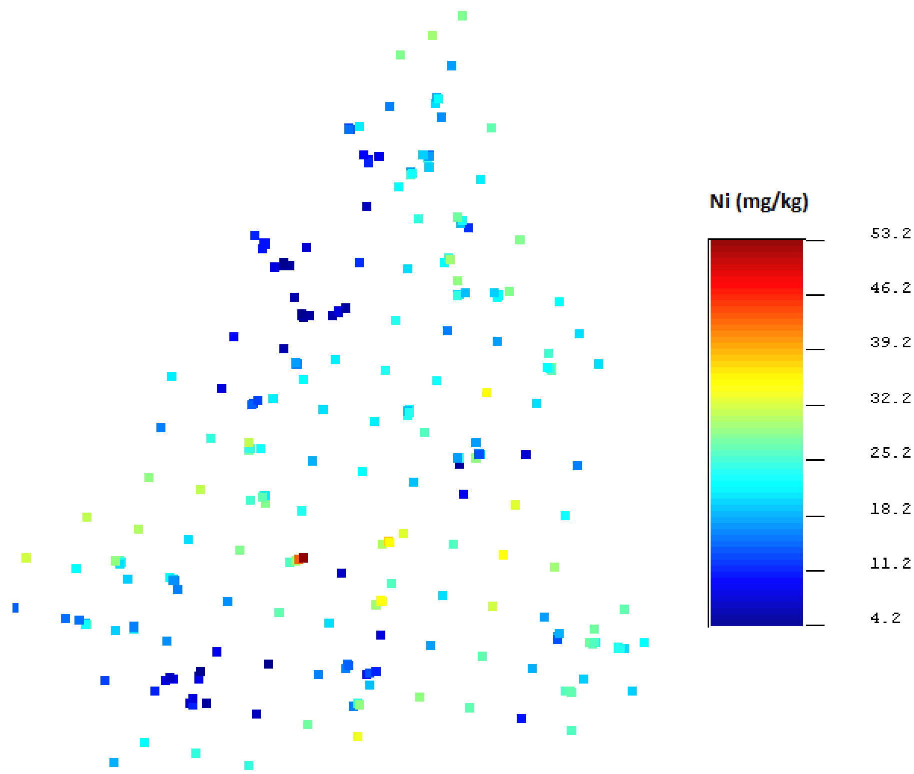

Figure 1. Sampling locations

Table 1. Summary statistics of the estimation results with raw data

	Raw Data	OK	MK
Minimum	4.20	5.28	4.21
Median	20.56	21.89	20.37
Average	19.73	21.17	20.25
Maximum	53.20	41.62	44.78
Variance	67.78	33.93	42.97

3.3. Spatial Estimation. Spatial distribution of the Ni is estimated using Metaheuristic Kriging and Ordinary Kriging. The search neighborhood strategy and variogram model parameters are identical for both methods. For this reason, variogram parameters are used in estimations and search radius is selected as 1000 m which is slightly greater than range of the variogram are used in estimation for both methods. For metaheuristic kriging additional DD and DF parameters are selected as 4 and 10 respectively. Resulting map of the estimates are given in Fig.5 for OK and MK.

Summary statistics of the estimates with raw data are given in both methods in Table 1.

Summary statistics of the estimations shows that both methods are unbiased where mean of the both methods are close to the mean of the raw data. Metaheuristic kriging

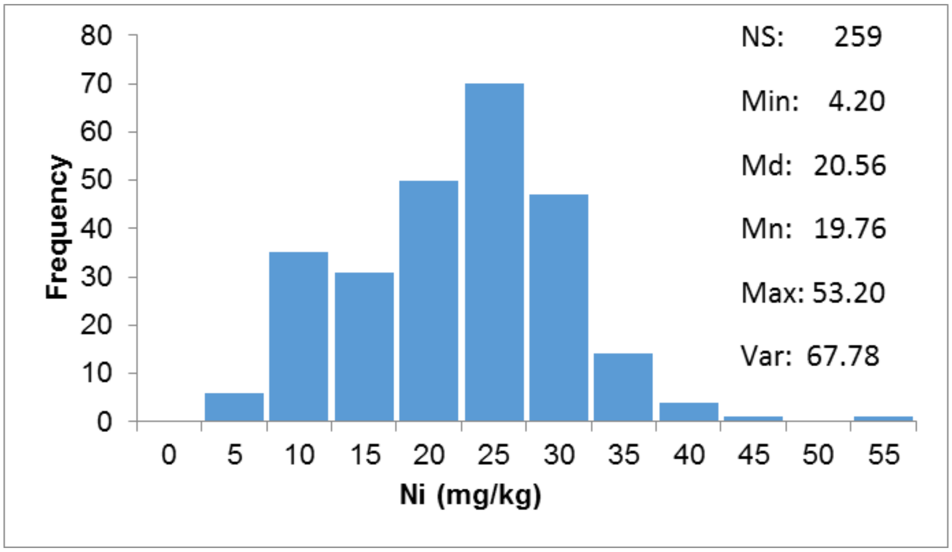

Figure 2. Histogram of the Ni concentration with summary statistics
(NS: Number of samples, Min: Minimum, Md: Median, Mn: Mean, Max: Maximum, Var: Variance)

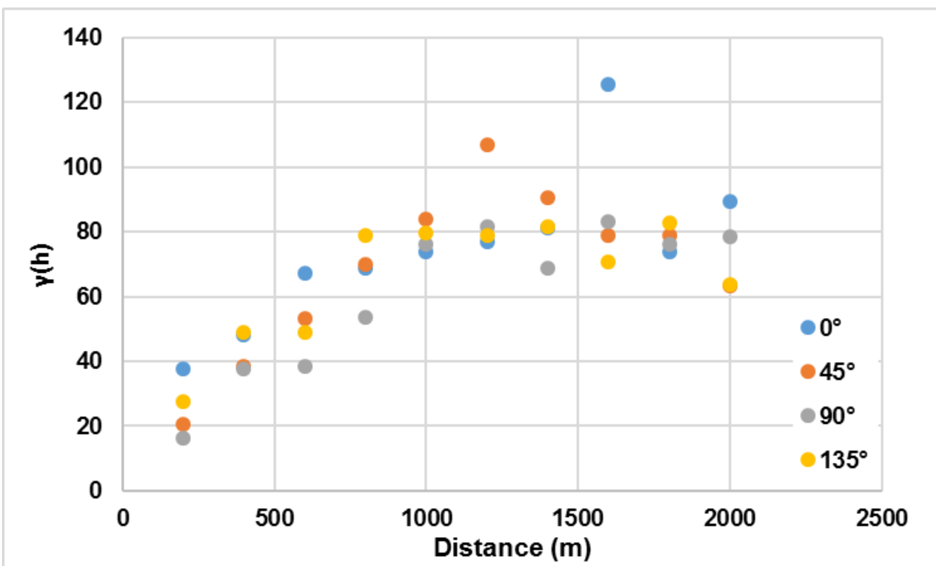

Figure 3. Experimtantal variogram values

resulted are higher ranged in terms of minimum and the maximum when compared to the ordinary kriging. But still smoothing effects applies for the both methods but smoothing effect is less in metaheuristic kriging that ordinary kriging. Metaheuristic kriging over performed the ordinary kriging from the viewpoint of the variability where variance of the metaheuristics kriging is closer to the raw data then ordinary kriging. Variograms of

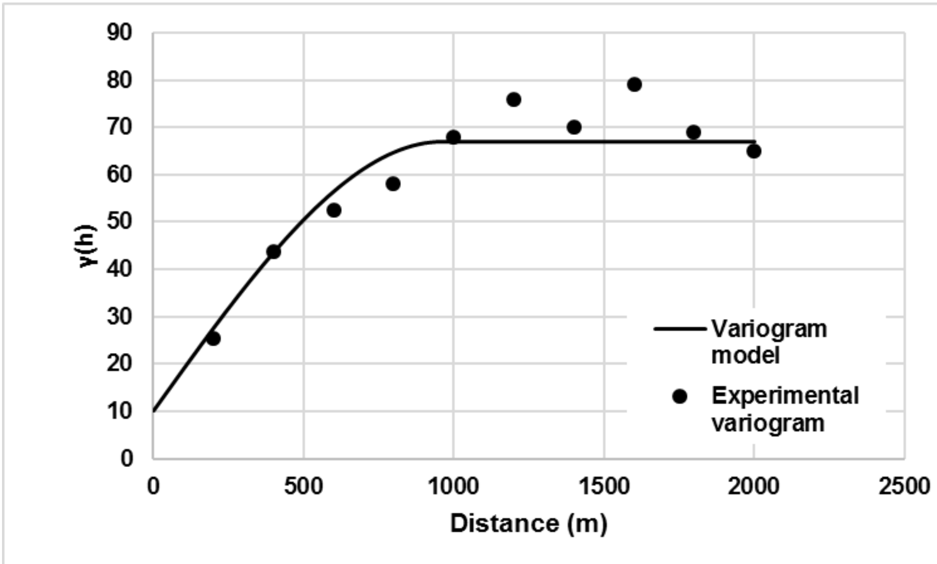

Figure 4. Omni-direction variogram with variogram model

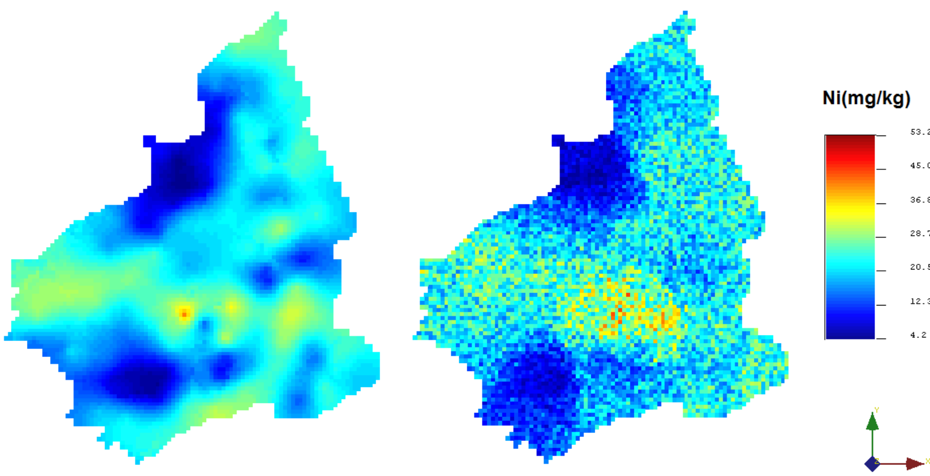

Figure 5. OK (left) and MK (right) estimation map

the estimates are calculated and given in Fig. 6 with raw data variogram.

As seen from the Fig. 6 metaheuristic kriging experimental variograms are closer to the raw data variograms. Which means that metaheuristic kriging better result than ordinary kriging in terms of spatial continuity and variability.

Swath plots can be used to assess the locational unbiasedness of the estimation results. To assess the unbiasedness of the estimates swath plots of the for the X and Y directions are plotted for the raw data, ordinary kriging estimates and metaheuristic kriging and given in Fig. 6.

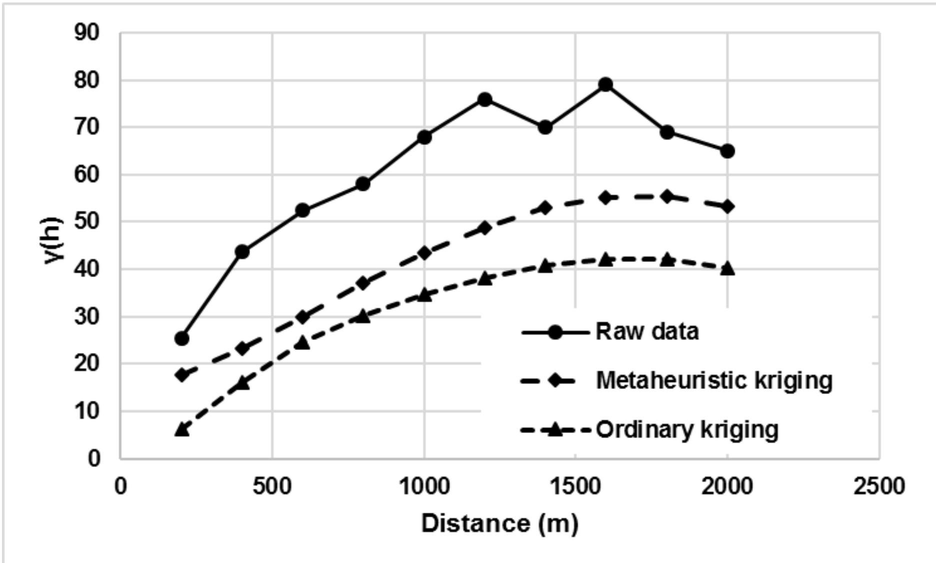

Figure 6. Experimental variograms of raw data, MK and OK

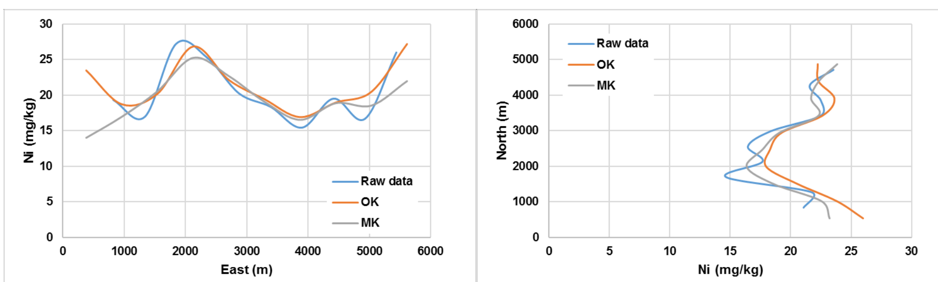

Figure 7. Swath plots of the raw data, MK and OK estimation results

Fig. 7 shows that in East and West directions both methods produced acceptable results from the viewpoint of the directional conditional averages.

4. Discussion

Due to the collected data is limited, in order to estimate the spatial distribution of the random variable geostatistical methods are widely used. Kriging and geostatistical simulations are most popular methods. Kriging produces an estimation result by minimizing the estimation error variance while geostatistical simulation produces multiple realization of the spatial distribution by not minimizing the estimation error variance. The short coming of the kriging and geostatistical simulations are over smoothed and unreliable estimation results which only use in assessment of the risk in estimation respectively. The method having the advantage of the both kriging and geostatistical simulation can be very useful in mapping the spatial distribution of the random variable. CMCK is a method that captures the advantage of the both method. But, one shortcoming of the method is that it does not guaranties to produce an estimation result.

In this study MK is proposed as a new method in estimation of the spatial distribution of the random variable. MK is very similar to kriging but only difference with kriging is the determination of the weights of the data in estimation. Unlike kriging, MK does not minimize the estimation error variance instead slightly approaches the minimum of the estimation error variance. The MK uses the DE optimization algorithm which is a metaheuristic optimization algorithm. MK produces estimation results which is more variable than kriging estimation results which is desired property. Swath plots of the estimations and raw data are also drawn. Results shows that estimation results are acceptable and conditionally unbiased.

As an application Ni distribution of the Jura data set is estimation using OK and MK. Experimental variograms are calculated and variogram model are fitted. Variograms shows that Ni shows isotropic distribution. The variogram model of the omni-directional variogram is spherical with 10, 57 and 960 m with nugget, sill and range respectively. Results of the estimations shows that MK better performed than OK in realization of the variability of the data.

OK is widely used in many areas like mining, environmental science, agriculture, public health, meteorology, civil engineering, hydrogeology, fisheries. While MK shares the same root with OK, it can be used in these areas also where spatial mapping of the variable is required.

In metaheuristics optimization determination of the method specific parameter is subjective. By being the member of the metaheuristic optimization DE also inherit this disadvantage. This makes method iterative to reach the desired outcomes. Also, DE has good property of the converging to the minimum. When DD and DF parameters set to the high values results of the MK approaches to the OK results which decreases the variability of the estimation results.

In this study only single variable is estimated and mapped. But in most case secondary data increases the estimation quality especially in heterotopic cases. Multivariate extension of the MK can be considered for future studies.

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