# ANALYZING AMBIGUITIES IN THE DATA COLLECTION NETWORK DESIGN BY GEOSTATISTICAL ESTIMATION VARIANCE  REDUCTION METHOD

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*Ambiguities in the data collection network design mainly based on the geostatistical estimation variance reduction method have been analyzed using a few numerical examples. The method of locating new measurement points with the help of an estimation variance (also called kriging variance) map has an ambiguity on the number of new data collection points, and hence does not provide an optimal network. The method of optimizing measurement points by reducing estimation variance at the central point of the considered area has an ambiguity that the same network will be valid for an even much larger area, if the center remains unchanged. In the examples considered it was found that the kriging variance calculated for an estimation over the entire area/block increases if the area/block is increased keeping the center of the area unchanged for the same network. However, a few ambiguities were found while considering an area whose center point was also shifted with the origin. The exercise was repeated by arbitrarily adding some new data collection points to the considered network. Further, the method of estimating the mean of the parameter by ordinary kriging was applied to calculate the kriging variance for different networks. Although the ambiguity that the same network representing different areas remains, this method provides a comparatively lesser kriging variance.*

## INTRODUCTION

Variance reduction geometry of measurement points (i.e. relative position of the measurement points) using various geostatistical estimation techniques has been a powerful tool in optimizing or designing an adequate data collection network in earth sciences. The technique utilizes a unique property of geostatistical estimation that the variance of the estimation error depends upon the structure of the selected parameter and <u>does not</u> depend on the measured values at additional selected points. This advantage enables one to select a new measurement point and analyze its effect, in the form of its utility on the estimation, prior to making a measurement. A number of works have been reported, particularly in the field of water resources e.g., Bras and Rodriguez-Iturbe (1976), Hughes and Lettenmaier (1981), Sophocleous et al. (1982), Carrera et al. (1984), Virdee and Kottegoda (1984), Rouhani (1985), Bogardi et al. (1985), Rouhani and Hall (1988), Dillon (1988), Barnes (1989), Aspie and Barnes (1990), Hudak and Loaiciga (1993), Das et al. (1995), and Gao et al. (1996).

Hughes and Lettenmaier (1981) have suggested an algorithm to optimize the location of data collection points by minimizing the variance of the error in estimating the parameter over the entire area of the aquifer. Sophocleous et al. (1982) have applied the technique of Universal Kriging in analyzing the network of wells for water-level measurement in Kansas, USA with respect to cost of the network and the accuracy obtained. Virdee and Kottegoda (1984) have proposed a map of kriging estimation error ($\sigma_k$) and located new measurement points at places where a high value of $\sigma_k$ was calculated. They have applied this method to a network of transmissivity and water-level measurements. This procedure has two drawbacks; (1) it is difficult to decide a limit to compare the $\sigma_k$ values to, and (2) an additional point improves the estimation variance not only at that point but also at the neighboring points forcing the procedure to work in an iterative way only. Carrera et al. (1984) proposed an iterative procedure based on non-linear programming to select the optimal location of measurement points and applied it to optimize monitoring fluoride concentration in the San Pedro River basin, Arizona. Bogardi et al. (1985) used composite programming with a combination of geostatistics and multicriterion decision making in optimizing a network of measuring thickness and porosity of a two layer aquifer system. Rouhani(1985) and Rouhani and Hall (1988) have used the method of estimation variance reduction calculated at the center of a set of discretized blocks in the area. Dillon (1988) has described a number of crucial features considered in monitoring network design methods. Hudak and Loaiciga (1992 and 1993) developed an analytical method integrating practical implementation aspects applied to a multilayered groundwater flow system for contaminant detection. Gao et al. (1996) presented a simple algorithm to rapidly compute the revised kriging estimation variance when new sample locations are added. Moreover, we believe that this algorithm is useful only if a network has to be improved from a sparse one by adding additional measurement points. This algorithm may not be useful for optimizing a dense network either by deleting the measurement points or by shifting them.

It has been clearly established that (a) more measurement points improve/decrease the variance of the estimation error either in the point or block estimation, and (b) to calculate a revised estimation variance due to addition of a new measurement point, only the location of the new point is required *not* the measured values.

However, it is a matter of discussion as to where the estimation should be made. One can therefore select a central point of the area or the whole area as the block for this purpose. One can select several points or blocks (e.g., by discretizing the area) but two problems remain; (a) the number of

points/blocks discretized and (b) the cut-off value of $\sigma_k$ used to decide the maximum number of additional measurement points.

In this paper, certain ambiguities have been analyzed for the cases of point estimation for the central point of the area and block estimation considering the whole area as a block.

A few numerical examples with different parameters and obviously different variability have been used to analyze the variance of the estimation error used to design an adequate data collection network. The first example is transmissivity (T) taken from Virdee and Kottegoda (1984). Five more data sets were prepared by adding new measurement points arbitrarily to this data set on T. The method of calculating kriging variance at the central point of the aquifer area, over the aquifer area, as well as in estimating mean of the data, were applied to compare various kriging variances and analyze the ambiguities. Two more data sets, one on air temperature (Sirayanone, 1988), and the other on electrical transverse resistance of an aquifer (Ahmed, 1987), were also considered to verify these ambiguities.

## THEORY OF GEOSTATISTICAL METHODS

A number of geostatistical methods based on the theory of regionalized variables (Matheron 1963, 1971) are used in almost all fields of earth sciences. The methods used in the above mentioned work are briefly described here.

### Ordinary Kriging (Point estimation)

The estimator:

$$z*(x_0) = \sum_{i=1}^{N} \lambda_i^0 z(x_i) \tag{1}$$

The kriging system:

$$\sum_{j=1}^{N} \lambda_j^0 \gamma_{ij} + \mu = \gamma_{i0} \quad i=,...N \tag{2}$$

$$\sum_{i=1}^{N} \lambda_i^0 = 1 \tag{3}$$

Variance of the estimation error:

$$\sigma_k^2(x_0) = \sum_{i=1}^{N} \lambda_i^0 \gamma_{i0} + \mu \tag{4}$$

where $z$ is the parameter to be monitored with $z(x_i)$, ($i$=1,...N) values already measured at $x_i$, $z*(x_0)$ is the estimated value at the point $x_0$.

$\lambda_i^0$ are kriging weights

$\gamma_{ij}$ are variograms of the parameter $z$

$\mu$ is a Lagrange multiplier

**Ordinary Kriging** (Block Estimation)

The estimator:

$$z*(V) = \sum_{i=1}^{N} \lambda_i^V z(x_i) \tag{5}$$

The kriging system:

$$\sum_{j-1}^{N} \lambda_j^V \gamma_{ij} + \mu = \bar{\gamma}_{iV} \quad i=1,\dots N \tag{6}$$

$$\sum_{i=1}^{N} \lambda_i^V = 1 \tag{7}$$

Variance of the estimation error:

$$\sigma_k^2(V) = \sum_{i=1}^{N} \lambda_i^V \bar{\gamma}_{iV} + \mu - \bar{\gamma}_{VV} \tag{8}$$

where

$$\bar{\gamma}_{iV} = \frac{1}{V} \int_V \gamma(x_i, x_j) dx_j \tag{9}$$

and

$$\bar{\gamma}_{VV} = \frac{1}{VV} \int_V \int_V \gamma(x_i, x_j) dx_i \; dx_j \tag{10}$$

**Kriging of Mean**

The estimator:

$$m* = \sum_{i=1}^{N} \lambda_i^m z(x_i) \tag{11}$$

The kriging system:

$$\sum_{i=1}^{N} \lambda_i^m C_{ij} = \mu_m \quad j=1,\dots N \tag{12}$$

$$\sum_{i=1}^{N} \lambda_i^m = 1 \tag{13}$$

Variance of the estimation error:

$$\sigma_{km}^2 = \mu_m \tag{14}$$

Here $C_{ij}$ is the covariance of the parameter as it is clear from the hypothesis of stationarity of second order that if the mean exists, then the covariance can be calculated. Thus one can work on covariance instead of the variogram. On the contrary, if we work on the variogram, the mean does not necessarily exist.

## NUMERICAL EXAMPLES

Three case studies taking data from earlier work were considered to calculate the variance of the estimation error in different cases described above, and the ambiguities were analyzed. The data sets were chosen from different areas to have a wide range in parameters and their variability.

### Transmissivity of a chalk aquifer

*The study area and the data*

The values of transmissivity (T) from a chalk aquifer in the Kennet valley in the upper Thames river, United Kingdom (Virdee and Kottegoda, 1984), were taken to calculate kriging variances for the three methods described earlier. In the aquifer area, 44 values of T were available ranging from $10\,m^2/day$ to $8000\,m^2/day$. The locations of data points are mainly concentrated in the central eastern part with clear gaps in the southeastern and northwestern parts (Figure 1). Ten more measurement points were arbitrarily selected in areas having this gap (Figure 1). Thus six data sets were prepared by adding two measurement points at a time and calculating the estimation variance, (i) at the center of the area using punctual (point estimation) ordinary kriging, (ii) over the area using block ordinary kriging and (iii) by kriging of the data mean.

*Variography*

A mean variogram was calculated using 44 values of log T. The logarithm of T values was taken because the histogram of T has shown a log-normal distribution. Also a geometric mean of T between two meshes of an aquifer model is preferred to have continuity in the flow (Marsily, 1986). However, most of the computer codes use a harmonic or arithmetic mean. Thus, if log-T were used, the arithmetic mean becomes a geometric mean.
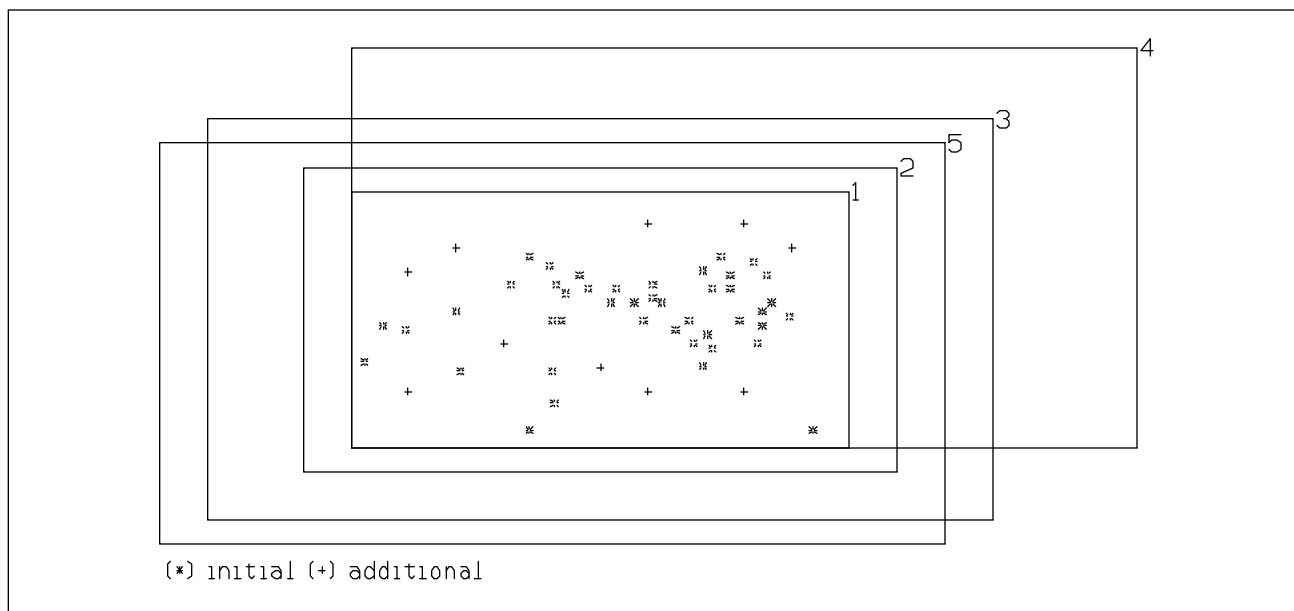


Figure 1. Location of measurement points (example 1) and areas used to calculate $\sigma_k$ values.
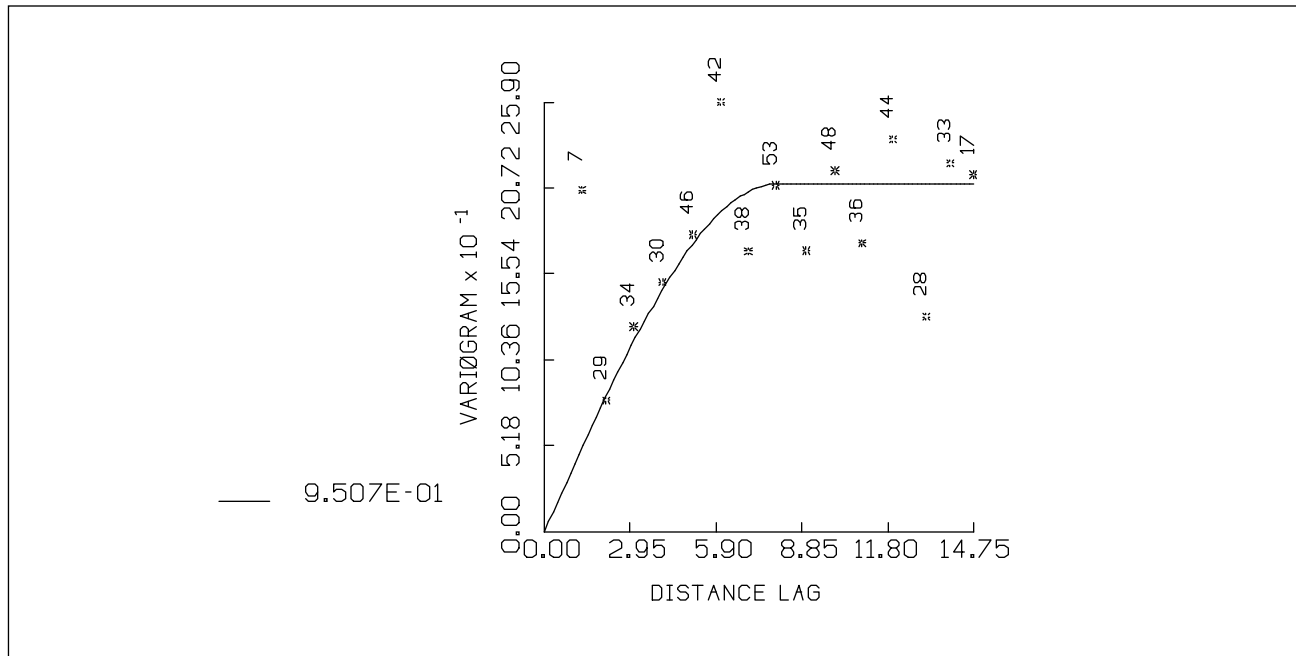
Figure 2.  Experimental and theoretical variogram of log-T (example 1).

The experimental variogram was modeled using a theoretical variogram of spherical type with the following parameters (Figure 2).

Nugget effect ($c_0$)    0.0

Sill (c)              2.1 (log-m$^2$/day)$^2$

Range (a)            8.0 km

Virdee and Kottegoda (1984) fitted an exponential model with following values.

Nugget effect ($c_0$)    0.0

Sill (c )             2.5 (log-m$^2$/day)$^2$

Range (a)            5.0 km

*Calculation and analysis of variance of the estimation error*

Since the two variograms (i.e. obtained by Virdee and Kottegoda (1984) and calculated in this study) are different, both were used in calculating the variance of the estimation error in all cases. Table 1 presents the value of $\sigma_k$ calculated in different cases.

The area of the aquifer was increased to analyze the change in the estimation variance, particularly in the case of block kriging. The initial area of the aquifer was 50 x 25 km which was increased to (i) 60 x 30 km and (ii) 80 x 40 km keeping the center of the area unchanged (see cases 1, 2 and 3 of Figure 1). Furthermore, the center and the origin were also shifted and $\sigma_k(V)$ was calculated (see cases 4 and 5 of Figure 1).

Since the variogram obtained is a bounded variogram with a defined sill value, we calculated the covariance, $C_{ij}$. Thus the estimation variance in the case of estimation of the parameter mean was also calculated for the six data sets. The $\sigma_{km}$ values for different cases are given in Table 1.

Table 1.  Values of $\sigma_k$ in Different Cases for the First Example
$\gamma_1 = 0.0 + 2.1$ Sph (8)  and  $\gamma_2 = 0.0 + 2.5$ Exp (5)

| Area | No. of Obs. Points | $\sigma_k(V)$ | | $\sigma_k(x_0)$ | | $\sigma_{km}$ |
|---|---|---|---|---|---|---|
| | | $\gamma_1$ | $\gamma_2$ | $\gamma_1$ | $\gamma_2$ | |
| **1** | 44 | 0.2494 | 0.3035 | 1.0599 | 1.1060 | 0.210 |
| (50 km x 25 km) | 46 | 0.2270 | 0.2783 | 1.0598 | 1.1056 | 0.187 |
| | 48 | 0.2153 | 0.2697 | 1.0588 | 1.1060 | 0.173 |
| origin (0, 0) | 50 | 0.1978 | 0.2553 | 1.0332 | 1.0849 | 0.150 |
| center (25, 12.5) | 52 | 0.1782 | 0.2352 | 1.0330 | 1.0849 | 0.120 |
| | 54 | 0.1616 | 0.2213 | 0.0330 | 1.0850 | 0.097 |
| **2** | 44 | 0.2813 | 0.3514 | 1.0599 | 1.1060 | -- |
| (60 km x 30 km) | 46 | 0.2636 | 0.3303 | 1.0598 | 1.1056 | -- |
| | 48 | 0.2530 | 0.3221 | 0.0588 | 0.1060 | -- |
| origin (-5, -2.5) | 50 | 0.2381 | 0.3095 | 0.0332 | 1.0849 | -- |
| center (25, 12.5) | 52 | 0.2204 | 0.2922 | 0.0330 | 1.0849 | -- |
| | 54 | 0.2074 | 0.2802 | 0.0330 | 1.0850 | -- |
| **3** | 44 | 0.3053 | 0.4296 | -- | -- | -- |
| (80 km x 40 km) | 46 | 0.2896 | 0.4128 | -- | -- | -- |
| | 48 | 0.2804 | 0.4044 | -- | -- | -- |
| origin (-15, -7.5) | 50 | 0.2667 | 0.3936 | -- | -- | -- |
| center (25, 12,5) | 52 | 0.2510 | 0.3759 | -- | -- | -- |
| | 54 | 0.2409 | 0.3664 | -- | -- | -- |
| **4** | 44 | 0.3065 | 0.4439 | -- | -- | -- |
| (80 km x 40 km) | 46 | 0.2941 | 0.4306 | -- | -- | -- |
| | 48 | 0.2854 | 0.4217 | -- | -- | -- |
| origin (0, 0) | 50 | 0.2718 | 0.4131 | -- | -- | -- |
| center (40, 20) | 52 | 0.2553 | 0.3948 | -- | -- | -- |
| | 54 | 0.2447 | 0.3829 | -- | -- | -- |
| **5** | 44 | 0.3027 | 0.4314 | -- | -- | -- |
| (80 kmx 40 km) | 46 | 0.2863 | 0.4142 | -- | -- | -- |
| | 48 | 0.2772 | 0.4068 | -- | -- | -- |
| origin (-20, -10) | 50 | 0.2634 | 0.3985 | -- | -- | -- |
| center (20, 10) | 52 | 0.2479 | 0.3826 | -- | -- | -- |
| | 54 | 0.2392 | 0.3729 | -- | -- | -- |

## Air Temperature in Colorado, USA

*The study area and the data*

The second example was taken for a data set on temperature in degrees F from the State of Colorado, USA (Sirayanone, 1988) observed on August 1, 1986. There are 21 measured values in an area of 142 x 173 km. The values range between 62.0 °F to 80.4 °F with a mean of 74.29 °F and variance of 17.7 (°F)$^2$. The locations of the observation points are shown in Figure 3. The histogram of the measured values show a near normal distribution.

*Variography and analysis of the kriging variance*

The variogram of the temperature was calculated and modelled using a spherical model (Figure 4). The parameters of the modelled variogram are as follows:
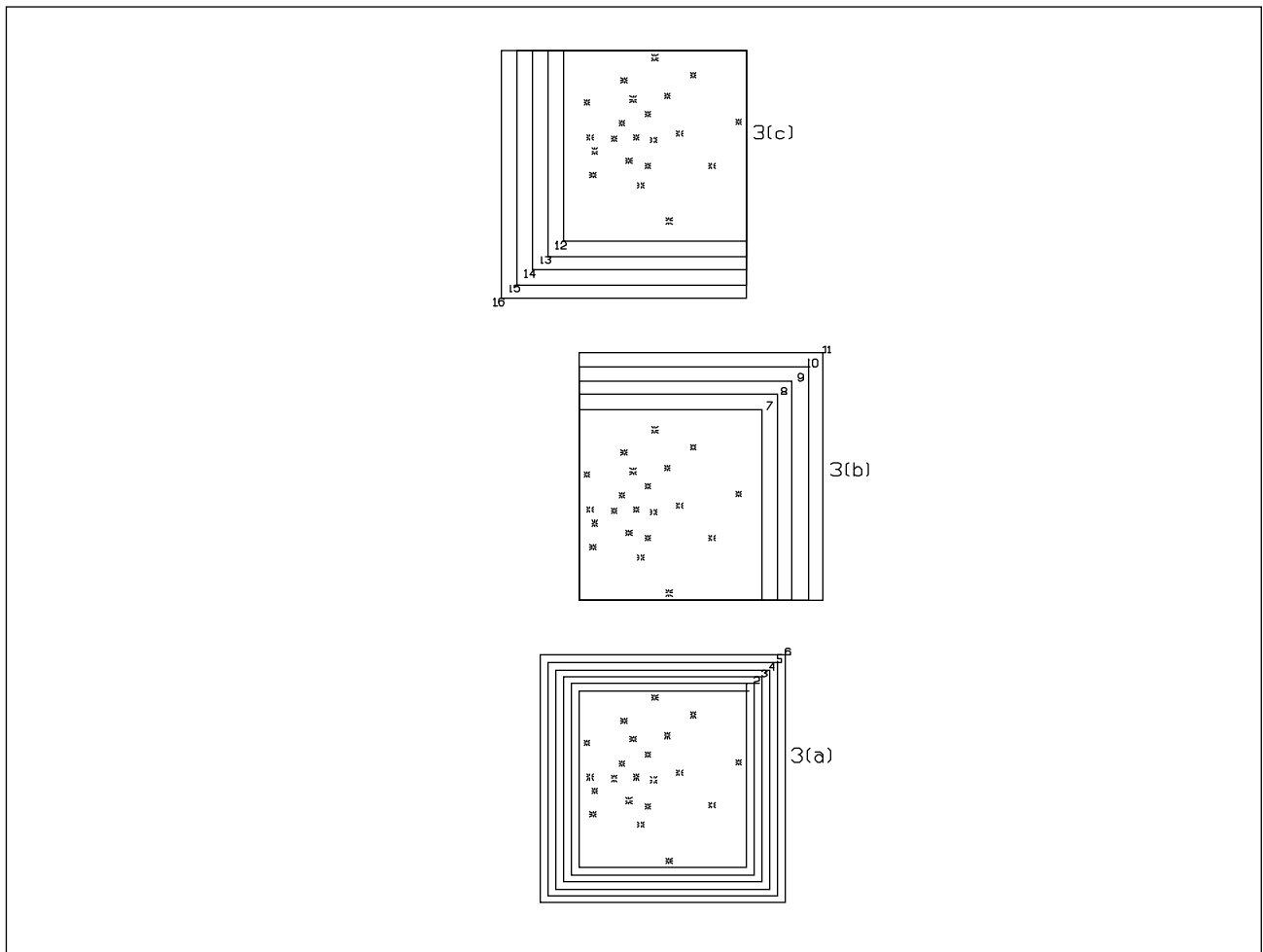
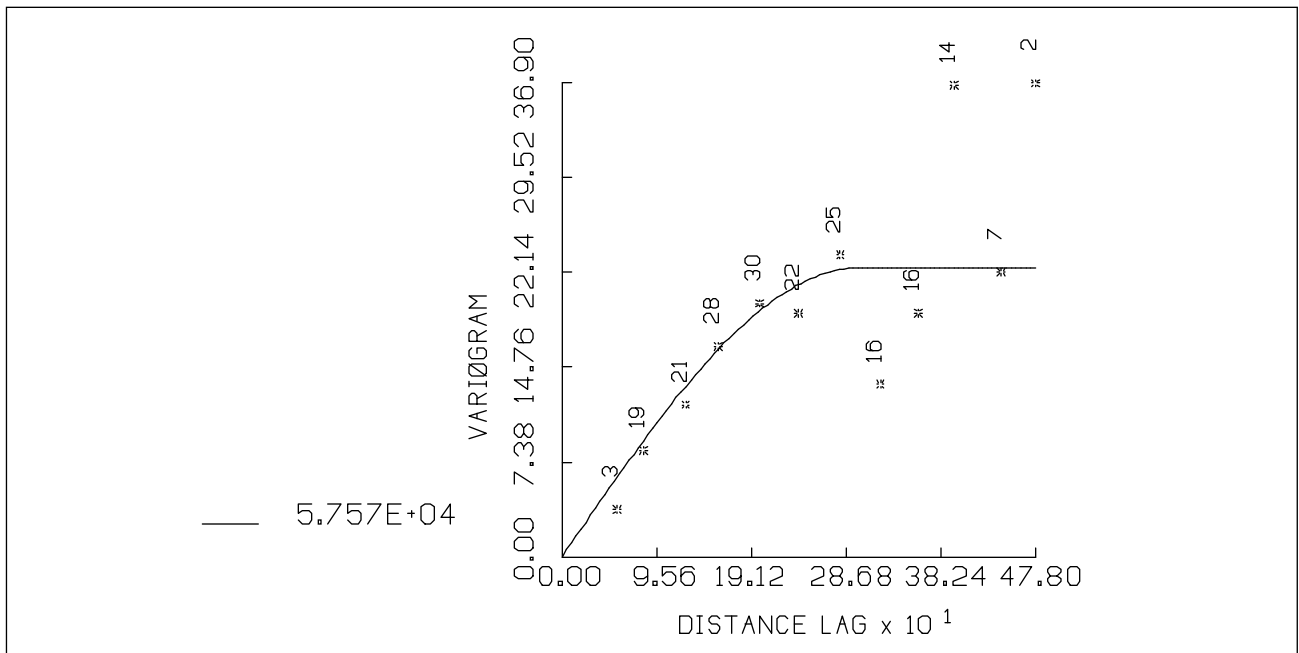Figure 3. (a, b, and c) Location of measurement points (example 2) and areas used to calculate $\sigma_k$ values.



Figure 4. Experimental and theoretical variogram of temperature (example 2).

| | |
|---|---|
| Nugget effect ($c_0$) | 0.0 |
| Sill ( c) | 22.5 $(^{\circ}F)^2$ |
| Range (a) | $300 \times 10^3$ ft |

The parameters of the variogram were cross-validated (Ahmed and Murthy, 1996). In addition to calculating the kriging variance on the center of the area from punctual ordinary kriging, as well as kriging of the data mean, the variance was calculated over the whole area as a block. To study change in the $\sigma_k(V)$ with the size of the area, the block area was increased by $50 \times 10^3$ ft on both the sides 5 times in steps. This increase was repeated in 3 ways (i) keeping the center of the initial area unchanged (Figure 3a), (ii) by retaining the same origin (Figure 3b), and (iii) by keeping the end opposite to the initial origin unchanged (Figure 3c). In all the 16 cases $\sigma_k(V)$ was calculated. The $\sigma_k(x_0)$ with $x_0$ as center of the area and $\sigma_{km}$ for the same network for comparison. The calculation of $\sigma_k$ values was repeated for all 16 cases after adding four additional observation points on the corners of the area. Table 2 shows all the $\sigma_k(V)$ values in this case.

Table 2. Values of $\sigma_k$ for Different Cases for the Second Example

| Case | Origin of the Area* | Center of the Area* | Size of the Area* | $\sigma_k(V)$ with old network | $\sigma_k(V)$ with revised network |
|---|---|---|---|---|---|
| 1 | 1980, -41 | 2225,47 | 490 x 576 | 0.6489 | 0.4837 |
| 2 | 1955, -66 | 2225,47 | 540 x 626 | 0.7464 | 0.5388 |
| 3 | 1930, -91 | 2225,47 | 590 x 676 | 0.8396 | 0.6066 |
| 4 | 1905, -116 | 2225,47 | 640 x 726 | 0.9280 | 0.6782 |
| 5 | 1880, -141 | 2225,47 | 690 x 776 | 1.0522 | 0.7900 |
| 6 | 1855, -166 | 2225,47 | 740 x 826 | 1.1541 | 0.8869 |
| 7 | 1980, -41 | 2250,272 | 540 x 626 | 0.7430 | 0.5317 |
| 8 | 1980, -41 | 2275,297 | 590 x 676 | 0.8861 | 0.6578 |
| 9 | 1980, -41 | 2300,302 | 640 x 726 | 1.0309 | 0.7934 |
| 10 | 1980, -41 | 2325,327 | 690 x 776 | 1.1399 | 0.8925 |
| 11 | 1980, -41 | 2350,332 | 740 x 826 | 1.2047 | 0.9530 |
| 12 | 1930, -91 | 2200,222 | 540 x 626 | 0.7239 | 0.5255 |
| 13 | 1880, -141 | 2175,197 | 590 x 676 | 0.8856 | 0.6768 |
| 14 | 1830, -191 | 2150,172 | 640 x 726 | 0.9755 | 0.7447 |
| 15 | 1780, -241 | 2125,147 | 690 x 776 | 1.1351 | 0.8356 |
| 16 | 1730, -291 | 2100,122 | 740 x 826 | 1.2103 | 0.9616 |

* all the values are in $\times 10^3$ ft

Note: The revised networks were derived by adding one measurement point at all the four corners

## Electrical Transverse Resistance of an Aquifer, Tunisia

*The studied aquifer and the data*

This example uses data on electrical transverse resistance from an alluvial aquifer in an interstream region of Medjerda and Rarai in Tunisia (Ahmed, 1987). The electrical transverse resistance (TR)
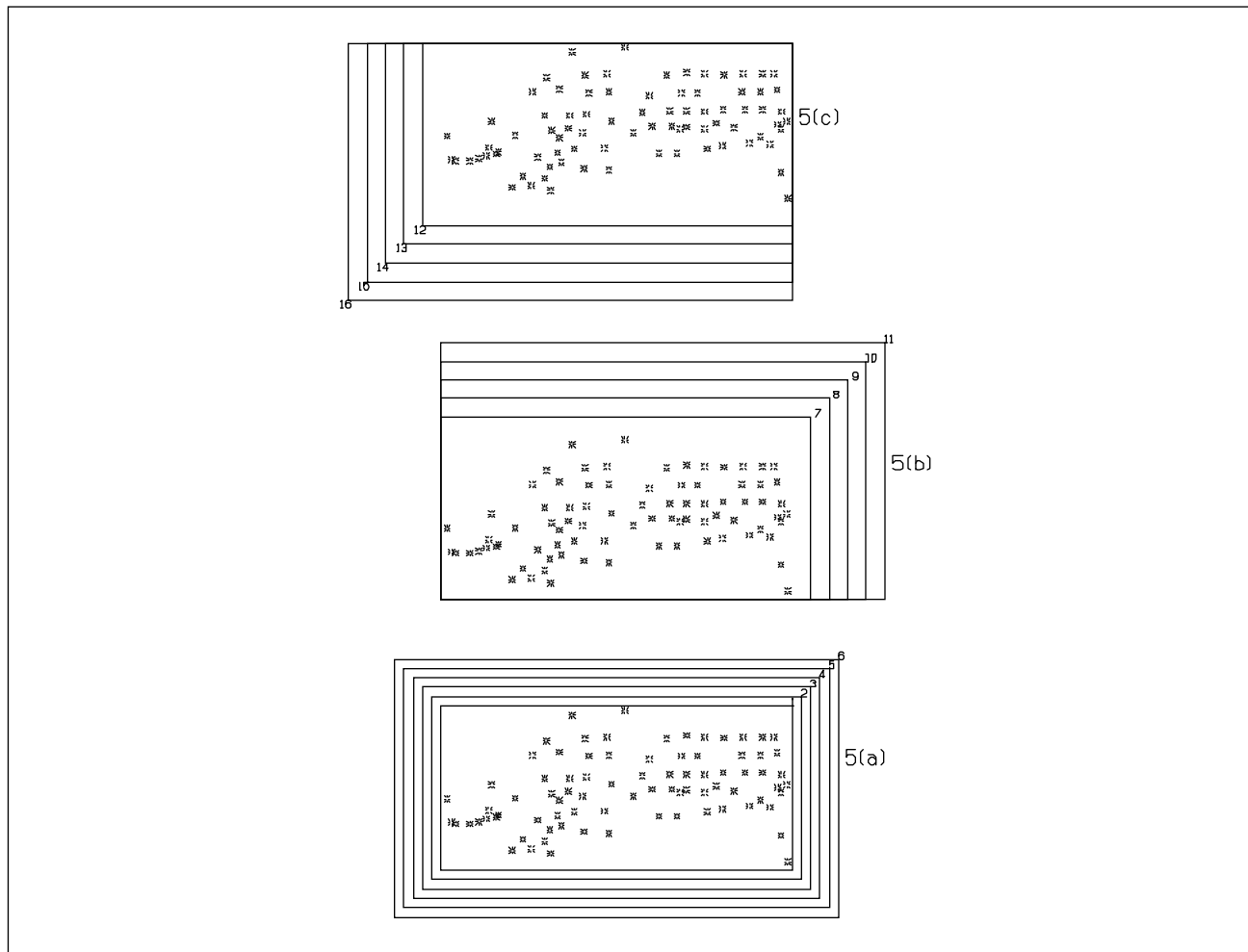
Figure 5.  Location of measurement points (example 3) and areas used to calculate $\sigma_k$ values.

was obtained from the vertical electrical soundings at 82 locations in an area of about 150 km$^2$ (Figure 5). All the TR values were corrected for variations in the water resistivity. TR values, since they could be obtained with comparatively easy experiments and correlated with the transmissivity of the aquifer, have been quite commonly used in obtaining the T distribution in an aquifer (Ahmed et al., 1988). The TR values range from 0.69 ohm m$^2$ to 14.0 ohm m$^2$ with a mean of 6.3 ohm m$^2$ and variance 12.1 (ohm m$^2$)$^2$.

*Variography and analysis of different variance of the estimation error*

The experimental variogram from 82 values of TR was calculated (Figure 6) which was fitted to a spherical model with following parameters.

Nugget effect (c$_0$)     0.0

Sill (c )     14.0  (ohm m$^2$)$^2$

Range (a)     3.8 km

Initially an area of 18 x 8 km wherein the sounding locations are spread, was taken as the block to calculate the standard deviation of estimation error ($\sigma_k$). Gradually this area was extended in both sides and the standard deviation was recalculated. The extended area was then shifted to both sides of the origin. Table 3 shows the $\sigma_k$ values calculated and Figures 5a, 5b and 5c show various areas
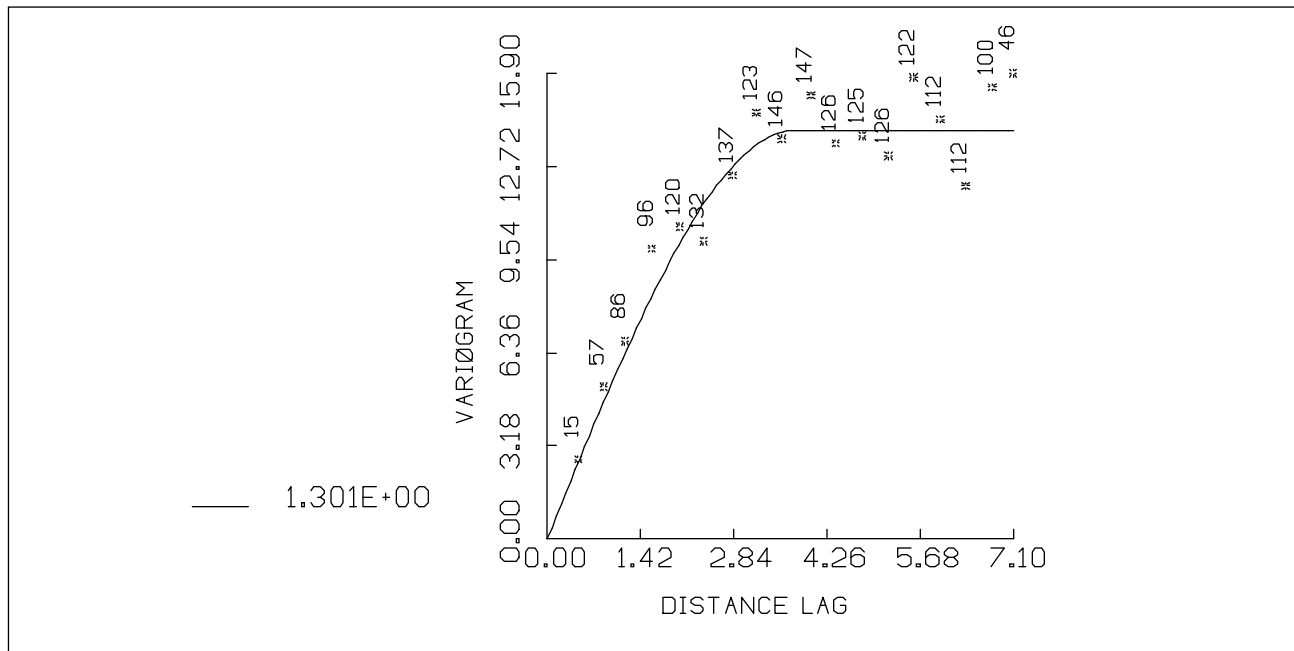
Figure 6. Experimental and theoretical variogram of electrical transverse resistance (example 3).

considered. The $\sigma_k(x_0)$ taking $x_0$ as the central point of the original area as well as $\sigma_{km}$ were also calculated.

Table 3.  Values of $\sigma_k$ for Different Cases for the Third Example

| Case | Origin of the Area* | Center of the Area* | Size of the Area* | $\sigma_k(V)$ with old network | $\sigma_k(V)$ with revised network |
|------|------|------|------|------|------|
| 1 | 363, 50 | 372, 354 | 18 x 8 | 0.4180 | 0.3690 |
| 2 | 363.5, 350.5 | 372, 354 | 19 x 9 | 0.4896 | 0.4252 |
| 3 | 364,351 | 372, 354 | 20 x 10 | 0.6014 | 0.5289 |
| 4 | 364.5, 351.5 | 372, 354 | 21 x 11 | 0.6619 | 0.5845 |
| 5 | 365, 352 | 372, 354 | 22 x 12 | 0.7216 | 0.6408 |
| 6 | 366, 353 | 372, 354 | 24 x 14 | 0.8142 | 0.7306 |
| 7 | 363, 350 | 372.5, 354.5 | 19 x 9 | 0.4474 | 0.3833 |
| 8 | 363, 350 | 373, 355 | 20 x 10 | 0.5367 | 0.4649 |
| 9 | 363, 350 | 373.5, 355.5 | 21 x 11 | 0.5703 | 0.4850 |
| 10 | 363, 350 | 374, 356 | 22 x 12 | 0.6274 | 0.5337 |
| 11 | 363, 350 | 375, 357 | 24 x 14 | 0.7027 | 0.6079 |
| 12 | 362, 349 | 371.5, 353.5 | 19 x 9 | 0.4826 | 0.4205 |
| 13 | 361, 348 | 371, 353 | 20 x 10 | 0.5391 | 0.4695 |
| 14 | 360, 347 | 370.5, 352.5 | 21 x 11 | 0.5880 | 0.5069 |
| 15 | 359, 346 | 370.352 | 22 x 12 | 0.6251 | 0.5386 |
| 16 | 358, 345 | 369.5, 351.5 | 24 x 14 | 0.7000 | 0.5994 |

* all the values are in x10³ ft

Note: The revised networks were derived by adding one measurement point at all the four corners

## DISCUSSION AND CONCLUSION

A large number of works use geostatistical methods in optimal data collection network design. However, very few have found application in the field. It is therefore useful to analyze and discuss the problems of their application. A number of ambiguities have been found in the methods so far applied; some of them are quite severe. Since most of the network designs are based on the reduction of kriging variance, which does not depend on the measured value of the parameter at a newly decided location, a common ambiguity is the maximum value allowed of the variance or the standard deviation of the estimation error (say a threshold). In the absence of an objective function directly involving the location of measurement points, it is difficult to minimize the variance of the estimation error ($\sigma^2_k$). Either this value is arbitrarily chosen or optimization of a data collection network may be terminated if the corresponding change in $\sigma^2_k$ is negligible.

The second point is where to calculate the $\sigma^2_k$, either on a point in the considered area or on the area itself. One can take the central point of the area to calculate and reduce the variance of the estimation error. However this central point has generally no significance with the objective of the study. Also the method of calculating estimation variance at the central point of the area has the ambiguity that any developed network can be valid for a much larger area provided the center remains unchanged. In addition $\sigma_k(x_0)$ will obviously be smallest if all the measurement points are located closest to the central point. These approaches are quite irrational.

The method of calculating estimation variance over an area of the system does not have the above ambiguity. The studied examples show that as the area increases, $\sigma_k$ increases, provided the center of the area remains unchanged. However, when the area was changed with a new center and a different origin, sometimes a reduction in the $\sigma_k$ was obtained depending upon the distribution of the density of the network. Therefore, it is concluded that a reduction in $\sigma_k$ calculated over the initial area may not be sufficient and, in addition, a few more areas obtained by shifting the size and origin must be checked to develop an adequate network. In all three examples, when a few measurement points were added, the revised $\sigma_k$ has shown reduction as expected, but the nature of ambiguities was retained.

Another method of calculating the variance of estimation error by kriging of the parameter mean and reducing its value based on the number and location of measurement points has been tried on the same data sets. It was found that the ambiguity of the same network representing an even larger area remains in this case also and the value of $\sigma_k$ has always been the least. However, theoretically the kriging of mean $m^*$ and $z^*(V)$ should be equal and the respective variances of the estimation error when the size of the block $V$ becomes infinity (Lantuéjoul, 1996). But in practice we do not work on an infinite area. Hence it is recommended that the method of estimating kriging variance on a block/area may be used in data collection network design but with the caution as described above. Of course, the better way of analyzing and designing a network is to discretize the area into a number of blocks and design a network by reducing the estimation variance on an average basis. This procedure could be repeated by reducing the size of discretized blocks until there is no change in the average statistics of the estimation variance.

## ACKNOWLEDGMENTS

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