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CORRECTING FOR NEGATIVE WEIGHTS IN ORDINARY KRIGING

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Abstract—Negative weights in ordinary kriging (OK) arise when data close to the location being estimated screen outlying data. Depending on the variogram and the amount of screening, the negative weights can be significant; there is nothing in the OK algorithm that alerts the kriging system about the zero threshold for weights. Negative weights, when interpreted as probabilities for constructing a local conditional distribution, are nonphysical. Also, negative weights when applied to high data values may lead to negative and nonphysical estimates. In these situations the negative weights in ordinary kriging must be corrected.

An algorithm is presented to reset negative kriging weights, and compensating positive weights to zero. The sum of the remaining nonzero weights is restandardized to 1.0 to ensure unbiasedness. The situations when this correction is appropriate are described and a number of examples are given. Copyright © 1996 Elsevier Science Ltd.

Key Words: Convex estimation, Kriging, Negative weights, Screen effect.

INTRODUCTION

Kriging is a nonconvex estimation technique. Negative kriging weights applied to "extreme" values can lead to kriging estimates outside the range of the observed data. This feature may be desirable when working with smooth variables such as surface elevations or isopach values. In other situations, a nonconvex estimator causes problems such as nonphysical estimates (negative probabilities, probabilities greater than one, negative porosities, or negative thicknesses). In these situations one would like an estimator that maintains the attractive features of kriging (declustering and variogram-distance weighting) and yet ensures no negative weights, thus ensuring convexity.

The approach taken here is to correct the kriging weights a posteriori. That is, the ordinary kriging weights are determined and then negative weights and some related small positive weights are reset to zero. The reason for correcting some positive weights is that data locations beyond the locations with negative weights may receive a small compensating positive weight; the weights can oscillate. These small positive weights should be reset to zero along with the negative weights.

THE PROPOSED ALGORITHM

Consider the estimate of an unsampled value $z(\mathbf{u})$ from neighboring data values $z(\mathbf{u}_\alpha)$, $\alpha = 1, \ldots, n$. The ordinary kriging (OK) estimator is written

$$z^*_{\mathrm{OK}}(\mathbf{u}) = \sum_{\alpha=1}^{n} \lambda_\alpha(\mathbf{u}) \cdot z(\mathbf{u}_\alpha). \tag{1}$$

The weights $\lambda_\alpha(\mathbf{u})$ are determined to minimize the error variance subject to the unbiasedness constraint $\Sigma_{\alpha=1}^{n} \lambda_\alpha(\mathbf{u}) = 1$, see Deutsch and Journel (1992, p. 63).

The subset of locations where the OK weight is negative ($\lambda_\beta < 0$) may be determined $\mathbf{u}'_\beta$, $\beta = 1, \ldots, n'$. The average absolute magnitude of the negative weights

$$\bar{\lambda}' = \frac{1}{n'} \sum_{\beta=1}^{n'} |\lambda_\beta| \tag{2}$$

and the average covariance between the location being estimated $\mathbf{u}$ and the locations receiving negative weight

$$\bar{C} = \frac{1}{n'} \sum_{\beta=1}^{n'} C(\mathbf{u} - \mathbf{u}'_\beta) \tag{3}$$

may be calculated. If the covariance function $C(\mathbf{h})$ decreases monotonically to zero then, for each direction, there is a distance d' such that $C(d') = \bar{C}$. When the covariance is isotropic then d' is a constant that does not depend on direction.

The set of OK weights λ_α, $\alpha = 1, \ldots, n$ are corrected as follows:

(1) $\lambda'_\alpha = \lambda_\alpha$
(2) if $\lambda_\alpha < 0$ then $\lambda'_\alpha = 0$

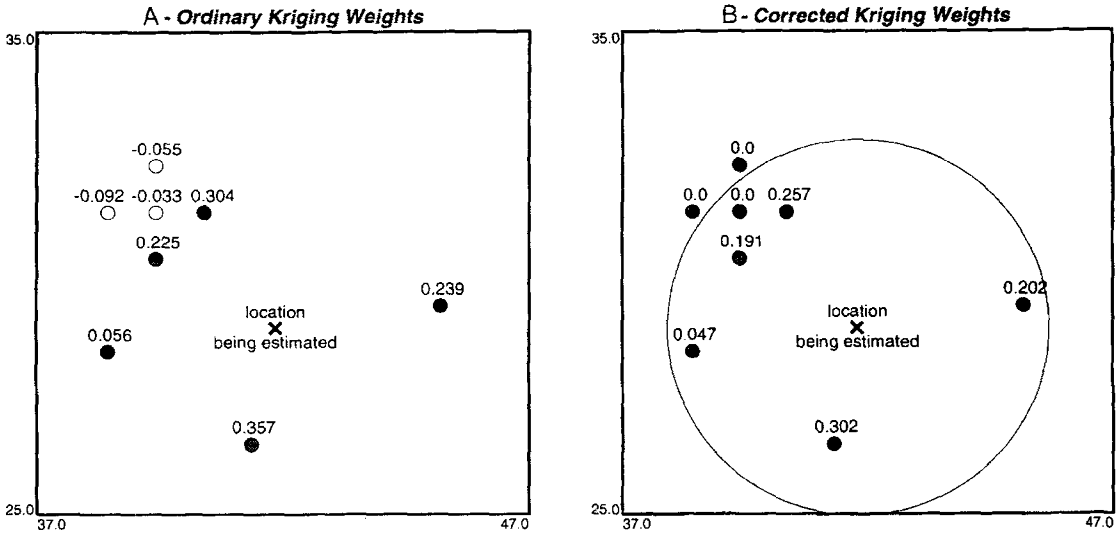

Figure 1. A. Ordinary kriging weights B. Corrected weights applied to eight-data configuration. Radius of circle around location being estimated corresponds to average covariance of samples receiving negative weights.

(3) if $\lambda_\alpha > 0$ and $C(\mathbf{u}-\mathbf{u}_\alpha) < \bar{C}$ and $\lambda_\alpha < \bar{\lambda}'$ then $\lambda'_\alpha = 0$.

The corrected weights are restandardized to sum to one

$$\nu_\alpha = \frac{\lambda'_\alpha}{\sum\limits_{\alpha}^{n} \lambda'_\alpha}, \quad \alpha = 1, \ldots, n. \tag{4}$$

The corrected estimate of the unsampled value $z(\mathbf{u})$ is then

$$z^{**}_{OK}(\mathbf{u}) = \sum_{\alpha=1}^{n} \nu_\alpha(\mathbf{u}) \cdot z(\mathbf{u}_\alpha). \tag{5}$$

The code required to implement this correction in the GSLIB software is available from the Computers & Geosciences ftp server, IAMG.ORG.

A SMALL EXAMPLE

Figure 1A shows the data configuration used in Part A of Problem Set Three in GSLIB, see Deutsch and Journel (1992, p. 108). The ordinary kriging weights shown on the left were obtained with an isotropic spherical variogram model with no nugget effect and a range of ten distance units equal to the side of the enclosing square. The location being estimated is annotated with the black cross. The three outermost sample locations in the cluster of five data receive negative weights.

These negative weights reflect the screening of the three remote data points by the set of two data locations in front of them. That screening effect is accentuated by the zero nugget effect of the variogram model adopted. There is nothing in the OK algorithm that alerts the kriging system about the importance of the zero threshold for the weights. Such negative weights if applied to elevated data values may lead to negative and nonphysical estimates. Such estimates are said to be nonconvex because they lie outside the range of data values used.

There are many options to impose a priori the convexity condition into the kriging system, either requiring that all weights be nonnegative or requiring that the resulting linear estimate be within the data range, Barnes and Johnson (1984). Another option consists of using the E-type estimate of indicator kriging, Journel (1986), although the probability estimates of indicator kriging itself might have

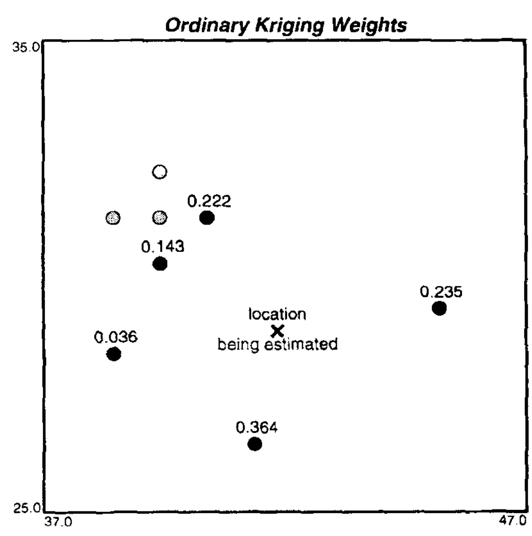

Figure 2. Five ordinary kriging weights excluding three data points that received negative weights in Fig. 1A.

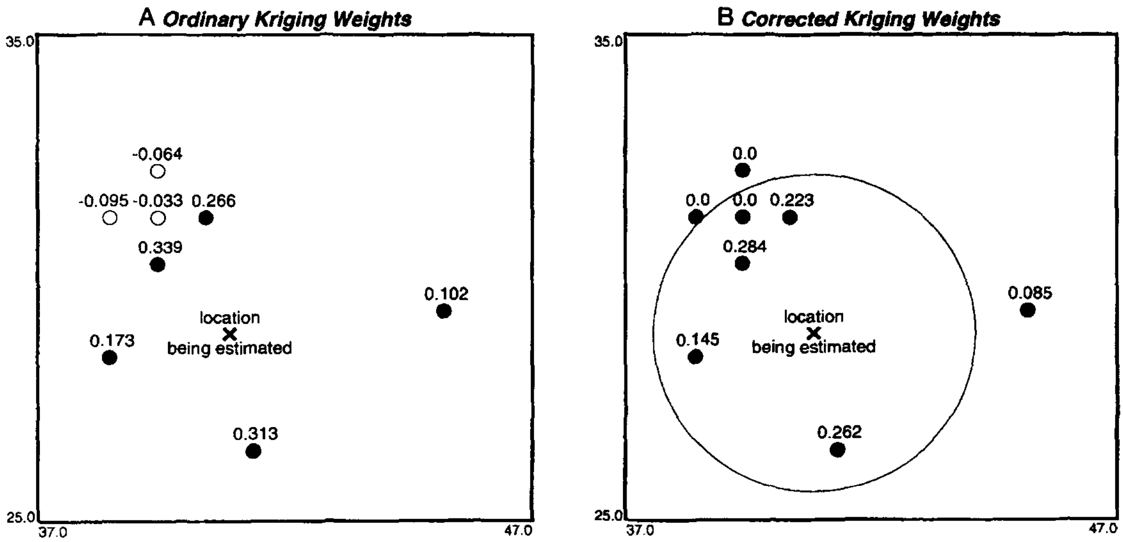

Figure 3. A. Ordinary kriging weights B. Corrected weights applied to eight-data configuration.

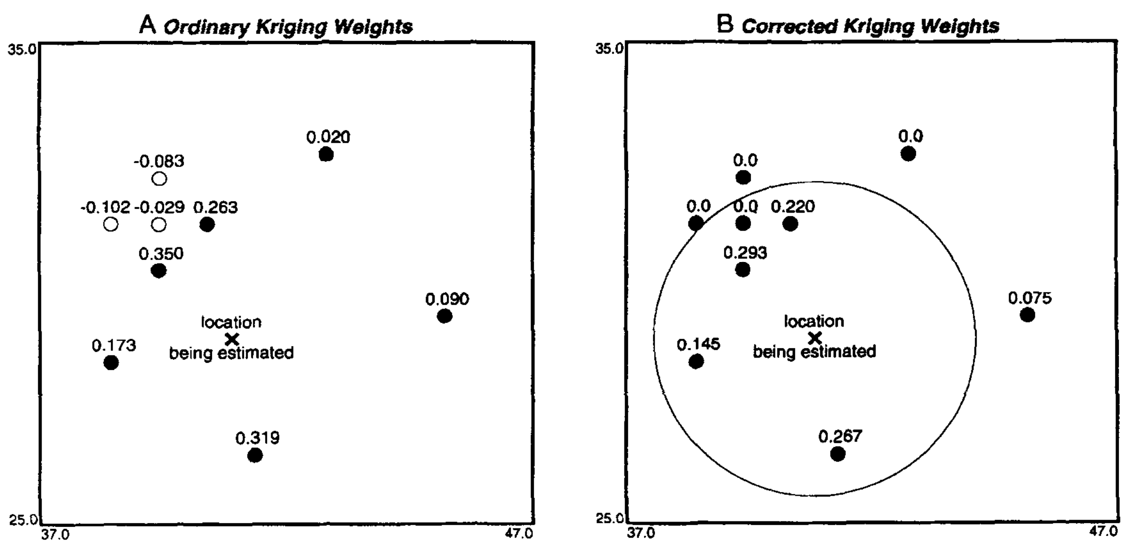

Figure 4. A. Ordinary kriging weights B. Corrected weights applied to nine-data configuration.

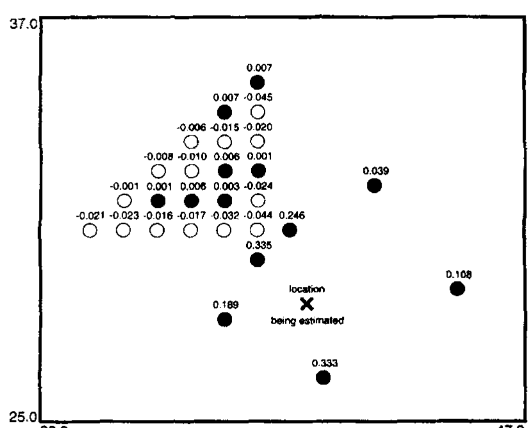

Figure 5. Ordinary kriging weights and corrected weights applied to 27-data configuration.

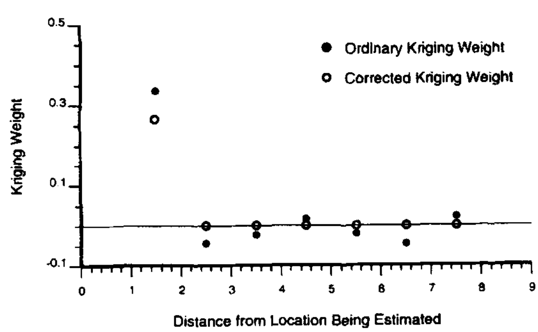

Figure 6. Profile of ordinary kriging weights vs distance (from Fig. 5).

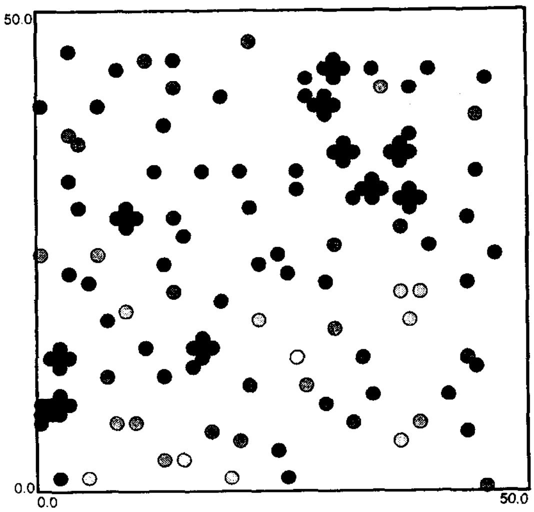

Figure 7. Location map of 140 data used for estimation of 50 by 50 grid.

to be corrected for nonconvexity-induced order relation problems. As another option, and a very fast one both to implement and CPU-wise, a direct (a posteriori) correction of the original OK weights is proposed here.

The correction amounts to resetting the negative weights to zero and restandardizing the remaining weights to sum to one; the corrected weights are shown on the right side of Figure 1. The radius of the circle around the location being estimated is the distance d' corresponding to the average covariance of the samples receiving negative weights. No location outside the circle is given a positive weight by the original OK system.

For comparison purposes, ordinary kriging was repeated after removing the three locations that originally received negative weight. These weights, shown on Figure 3, may be compared to the corrected weights shown on Figure 2. There is close agreement.

Figure 3 shows the OK and corrected weights that would be obtained for estimating a location one distance unit to the left of the previous example. The same variogram model and data were considered. Note that the datum to the extreme right (receiving an original OK weight of 0.102) is not reset to zero, even though it is less correlated to the location being estimated than the data receiving negative weight, that is $C < \bar{C}$. The weight is not reset because the kriging weight (0.102) is greater than $\overline{\lambda'}$, the average absolute negative weight (0.0064).

Figure 4 shows OK and corrected weights that would be obtained if a data point is added in the upper right quadrant (receiving an OK weight of 0.020). In this example, the new data location and the location to the far right (OK weight of 0.090) are beyond the distance corresponding to $\bar{C}$. Only the small weight is reset because it is smaller than the average absolute weight (0.071).

To illustrate further negative weights and their associated small compensating positive weights, consider the 27-point data configuration shown on Figure 5. Note the negative weights and the small positive weights (all positive weights are shown with a gray circle). A profile of these ordinary kriging weights through the dense cluster of data is shown on Figure 6. Also shown on Figure 6 are the corrected kriging weights.

```
                    Parameters for KB2D
                    *******************

START OF PARAMETERS:
parta.dat                          \file with data
1   2   3                          \   columns for X, Y, and variable
-0.01   9999.0                     \   trimming limits
kb2d.out                           \file for kriged output
3                                  \debugging level: 0,1,2,3
kb2d.dbg                           \file for debugging output
kb2d.loc                           \file for weights
1   42.0  10.0                     \X grid specification: nx, xmn, xsiz
1   29.0  10.0                     \Y grid specification: ny, ymn, ysiz
1    1                             \x and y block discretization
1    2.5                           \0=SK, 1=OK, 2=convex SK, 3=convex OK
4   16                             \min and max data for kriging
20.0                               \maximum search radius
1   0.0                            \nst, nugget effect
1   1.0    0.0 10.0   10.0  1.     \it, c, azm, a_max, a_min, power
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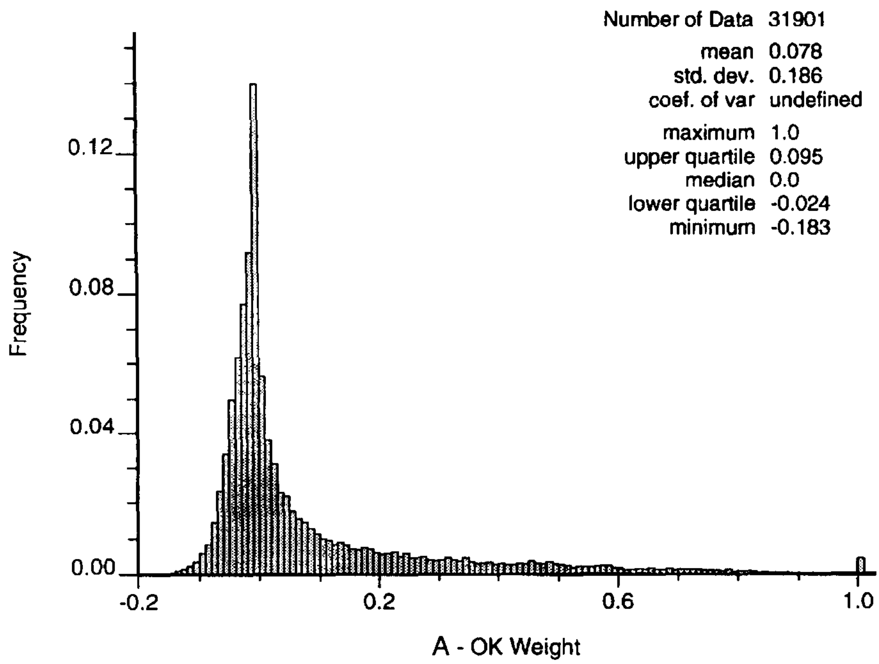
Figure 8. Parameter file for kb2d.



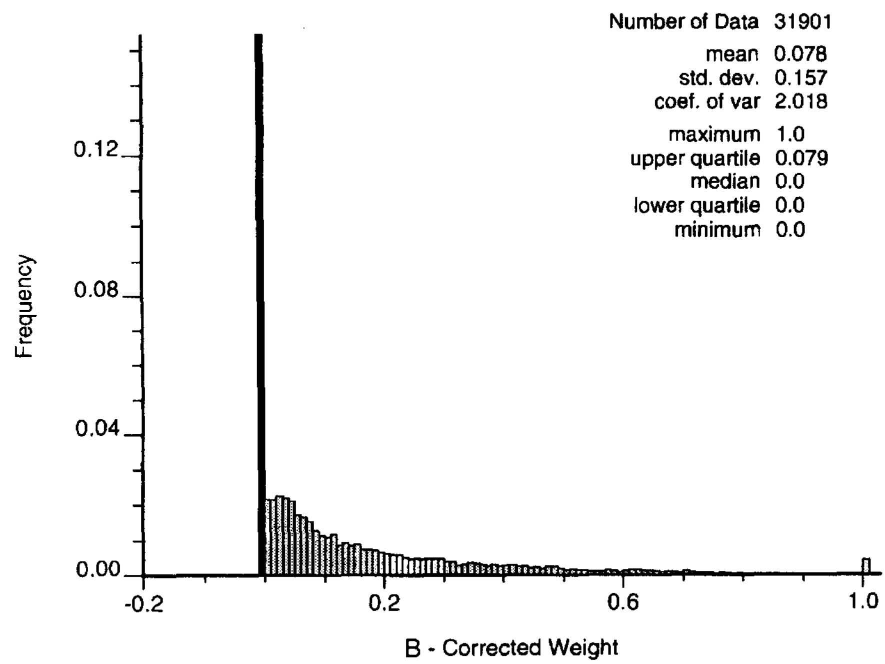


Figure 9. A. Histograms of original OK weights B. Histograms of corrected weights assigned to all data for kriging all locations of 50 by 50 grid shown on Figure 7.

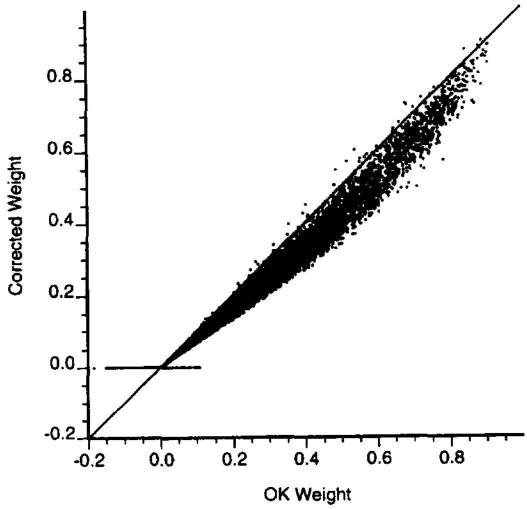


Figure 10. Scatterplot of OK estimates and corrected estimates.

KRIGING WITH THE GSLIB DATA

The set of 140 data used in the GSLIB book, Deutsch and Journel (1992, p. 37) and Figure 7, were used to estimate the attribute value on a regular 50 by 50 grid of points. The parameter file for kb2d (a second edition program replacing okb2d, Deutsch and Journel, 1992, p. 92) is shown on Figure 8. Out of the possible 2500 locations, 2485 were estimated; fifteen were left unestimated due to the minimum number of data constraint and the automatic octant search. On average, 12.8 data were used to make each estimate with 6.3 negative weights (average value of −0.032).

Figure 9A shows the histogram of all original OK weights and Figure 9B the corrected weights. Note that (i) the average is exactly the same since both sets of weights are subject to the constraint that the weights sum to one, (ii) 60% of the corrected weights are exactly 0.0, and (iii) the small spike of weights equal to 1.0 is due to estimating at a datum location. Figure 10 gives the scatterplot of corrected weights vs original OK weights. The horizontal line at a corrected weight of zero illustrates the significant number of weights being corrected.

Figure 11 shows the histogram of the OK estimates and the corrected estimates. There are 24 out of 2485

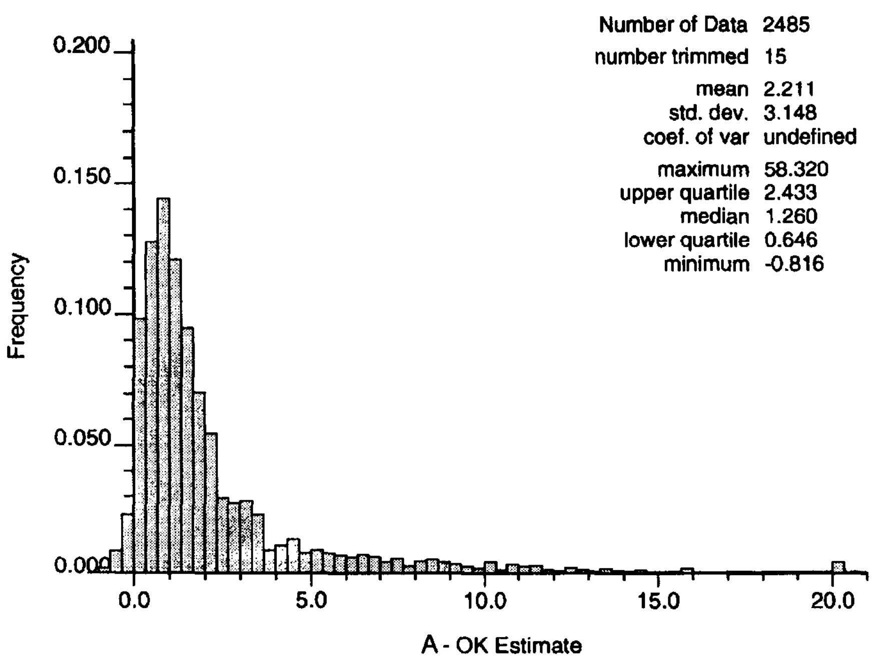


Figure 11 A. Histogram of OK-estimated values for all locations (15 out of 2500 were not estimated).

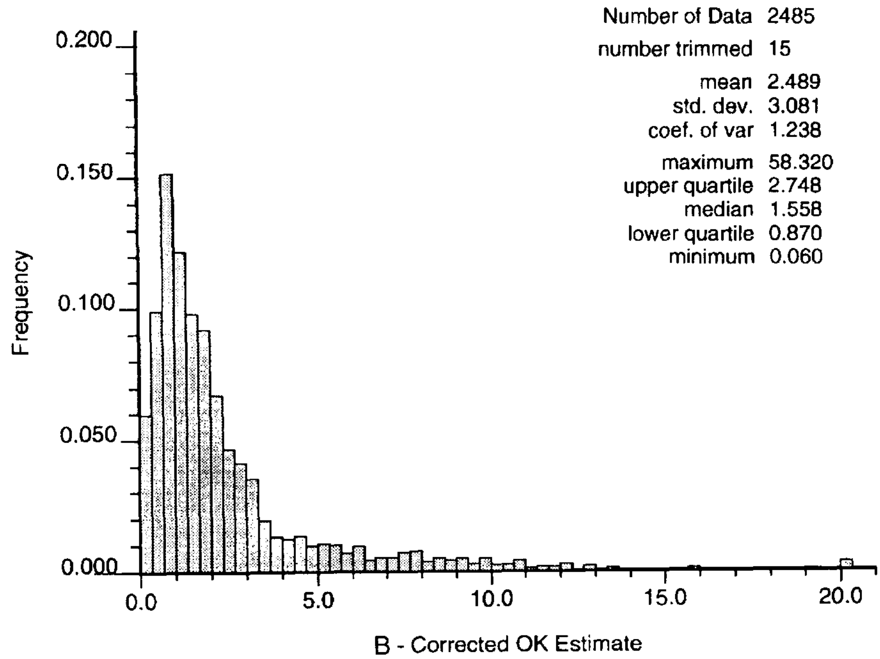


Figure 11 B. Histograms of corrected values for all locations (15 out of 2500 were not estimated).

estimates that are negative (3.4%). The average estimated value with the corrected weights is greater (2.49 vs 2.21) than the original OK estimates. The true mean is 2.58 and the declustered mean of the 140 data is 2.52. It should be pointed out that both OK and the corrected estimator are unbiased because the sum of the weights is constrained to be one.

A scatterplot of the corrected estimates vs the OK estimates is shown on Figure 12. As expected, there is a strong positive correlation (0.98) between the estimates. A cross validation (each sample location was estimated from its neighbors) was performed to

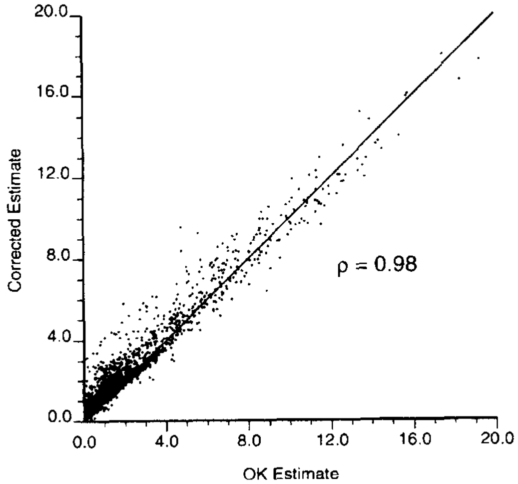


Figure 12. Scatterplot of corrected kriging estimate vs ordinary kriging estimate.

assess the difference between these two estimators. Figure 13 shows the histograms of errors. The mean squared error (MSE) was 41.5 for OK and 38.7 for the corrected estimator. Although the MSE for the corrected estimator is better, it has a larger average error (0.414 vs 0.250).

DISCUSSION

The correction proposed here should be limited to situations where there is a good reason to disregard negative weights, such as (i) when performing indicator kriging of either a categorical variable or an indicator transform of a continuous variable, (ii) when the weights are interpreted as probabilities for constructing a local conditional distribution, and (iii) when dealing with nonnegative attributes such as concentrations and when extreme data values are present.

The proposed correction could also be applied to simple kriging (SK) weights. The sum of the SK weights should be standardized along with the complement weight given to the global mean $[1 - \Sigma_{\alpha=1}^{n} \xi_\alpha]$, where ξ_α, $\alpha = 1, \ldots, n$ are the SK weights.

It should be noted also that the kriging variance increases when the corrected weights are used. The kriging variance of the corrected estimator may be calculated by the general equation $\mathrm{Var}\{Z^*(\mathbf{u})\} = \Sigma_{\alpha=1}^{n} \Sigma_{\beta=1}^{n} \nu_\alpha(\mathbf{u}) \cdot \nu_\beta(\mathbf{u}) \cdot C(\mathbf{u}_\alpha - \mathbf{u}_\beta)$. In the context of sequential Gaussian simulation (Deutsch and Journel, 1992; Journel, 1989), the original simple kriging variance should be used; otherwise, the

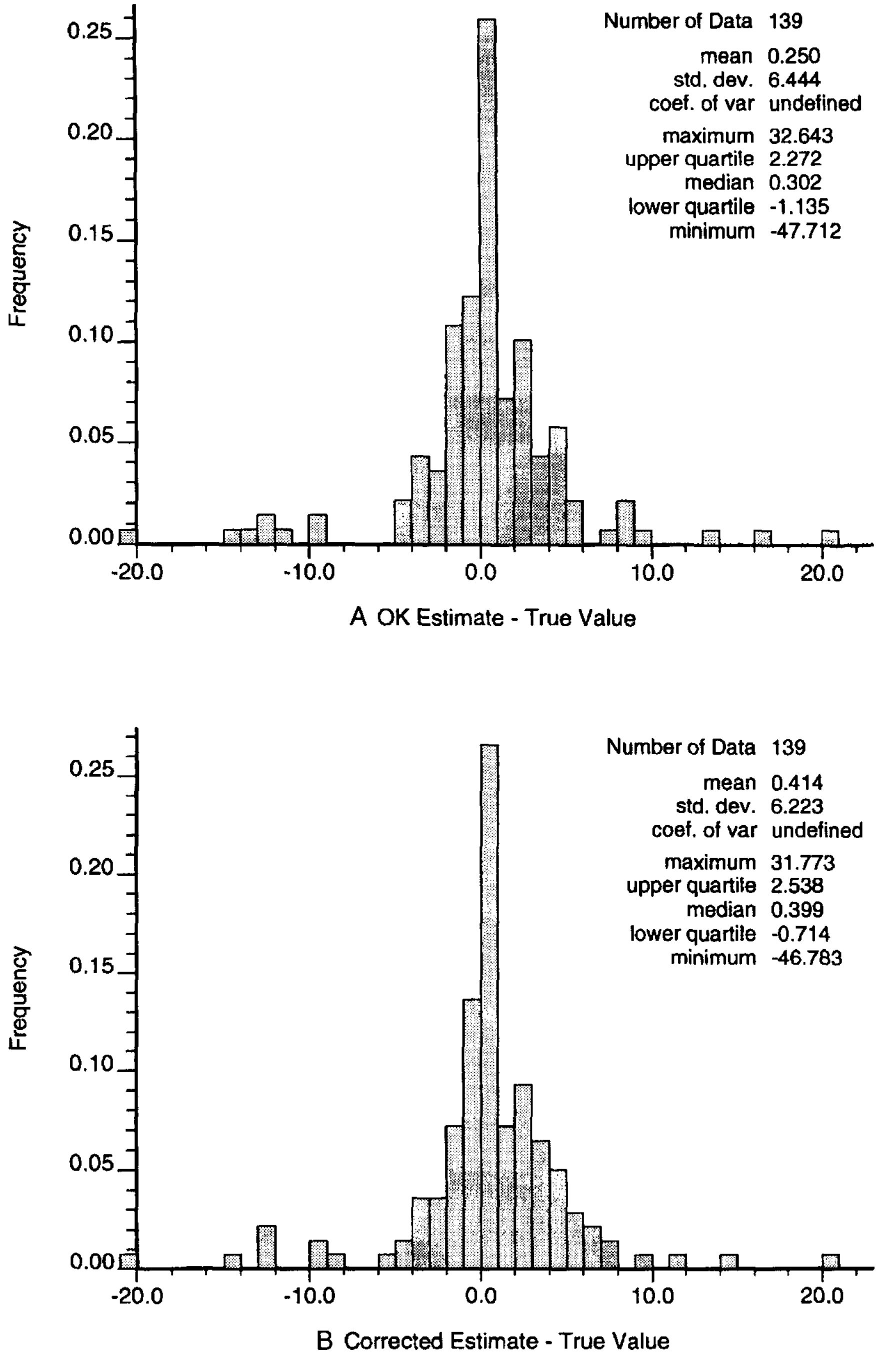


Figure 13. Histograms of error values obtained A. with OK and B. with corrected weights.

variance of the simulated realizations will be inflated due to using a kriging variance greater than the theoretical SK variance.

CONCLUSIONS

In many situations, negative kriging weights lead to nonphysical estimates. The algorithm proposed here to correct negative OK weights and the related small positive weights is simple and robust. The examples have shown that the weights do not differ greatly from the original OK weights and that the resulting estimate is within the bounds of the available data.

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