

On the reduction of the ordinary kriging smoothing effect

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Abstract

This study proposes a simple but novel and applicable approach to solve the problem of smoothing effect of ordinary kriging estimates. This approach is based on transformation equation in which Z scores are derived from ordinary kriging estimates and then rescaled by the standard deviation of sample data with addition of the mean value of original samples to the results. It bears great potential to reproduce the histogram and semivariogram of the primary data. Actually, raw data are transformed into normal scores in order to avoid the asymmetry of ordinary kriging estimates. Thus ordinary kriging estimates are first rescaled using the transformation equation and then back-transformed into the original scale of measurement. To test the proposed procedure, stratified random samples have been drawn from an exhaustive data set. Corrected ordinary kriging estimates follow the semivariogram model and back-transformed values reproduce the sample histogram, while preserving local accuracy.

Keywords: *ordinary kriging; smoothing effect; normal score transform; histogram reproduction; semivariogram model reproduction; local accuracy*

1. Introduction

Ordinary Kriging (OK), one of the most reliable local estimation methods, suffers from a main problem which has been known as “Smoothing Effect”. OK estimates do not reproduce the sample histogram because of reduced variance as a consequence of the smoothing effect. In the OK estimation process low values are overestimated and high values underestimated making the estimated histogram narrower than the sample histogram. Considering the sample as representative of the population from which was drawn, it is important that estimates follow the sample histogram in order to make inferences about the population. In the same way it is also important that estimates reproduce the spatial correlation model as described by the semivariogram. Actually the histogram and the semivariogram model characterize the population

or spatial phenomenon under study. Therefore, the challenge in geostatistics is to get estimated maps reproducing both the sample histogram and the semivariogram model. However, the reproduction of histogram and semivariogram model must be done without loss of local accuracy.

The solution for smoothing in kriging calls for some post-processing OK estimates in order to correct the smoothing effect and keeping the local accuracy that characterizes the OK estimation process.

The cornerstone of all research done to correct the smoothing effect is to apply some post processing to the Kriged values, instead of applying some changes to the Kriging equations themselves [1, 2, 3]. Guertin [1] proposed a nonlinear correction function based upon an analytical representation of the bivariate distribution of the true grade

against the estimated one. Olea and Pawlowsky [2] have proposed a procedure called compensated kriging in which through a numerical comparison they used cross-validation to detect and model such as the smoothing effects while the next inversion of the model produced a new estimator. Based on Olea and Pawlowsky [2] an intermediate state of Kriging and simulation was derived for the corrected estimates. A spectral approach proposed by Yao [4, 5] to conditional simulation capitalized on the speed of the Fast Fourier Transform (FFT). The strengths and weaknesses of a kriging approach vs. a simulation approach were recalled by Journel et al. [3]. However, according to these authors, semivariogram reproduction is achieved at a loss of local accuracy, confirming that global accuracy and local accuracy are conflicting objectives.

Yamamoto [6] proposed a four-step procedure for correcting the smoothing effect of ordinary kriging estimates that was shown to be effective for the reproduction of histogram and semivariogram without loss of local accuracy, sharing both local and global accuracies. Yamamoto [7] applied the post-processing algorithm for lognormal kriging estimates in order to avoid biased back-transformed estimates as given by conventional procedure proposed by Journel [8]. Yamamoto [9] compared the post-processing algorithm for correcting the smoothing effect of ordinary kriging estimates [6] with sequential Gaussian simulation realizations and showed the superiority of Corrected Ordinary kriging estimates to any individual simulation realization.

In this study a novel approach is proposed that yields global accuracy without loss of local accuracy. To apply the suggested procedure on the kriged estimates, a great deal of skills is needed which makes it hard at least for practitioners. The method presented in this study is easy to use while it reproduces sample histogram and the semivariogram model.

2. The post-processing algorithm for correcting kriging smoothing

The post-processing algorithm proposed by Yamamoto [6] and updated by Yamamoto [7] is based on four-step procedure. In the first step smoothing errors are derived from the cross-validation procedure. After this step, we have for every data point the estimated ($Z_{OK}^*(x_o)$) and actual ($Z(x_o)$) values and also the interpolation standard deviation (S_o) [10]. These values are

combined to derive a new random variable named number of interpolation standard deviations:

$$NS_o = \frac{-(Z_{OK}^*(x_o) - Z(x_o))}{S_o}$$

where $Z_{OK}^*(x_o)$ is the ordinary kriging estimate from cross-validation, $Z(x_o)$ is the actual value and S_o is the interpolation standard deviation.

In the second step, NS_o is estimated at nodes of a regular grid or unsampled locations resulting in $NS_o^*(x_o)$. In the next step, we run ordinary kriging to estimate the variable $Z(x)$ at nodes of the same regular grid as defined for NS_o . After doing these steps for every grid node we have: $Z_{OK}^*(x_o)$, S_o and $NS_o^*(x_o)$, that are combined for the post-processing in the fourth step as follows:

$$Z_{OK}^{**}(x_o) = Z_{OK}^*(x_o) + NS_o^*(x_o).S_o$$

On the right side the term $NS_o^*(x_o).S_o$ is the correcting amount that is added to or subtracted from the ordinary kriging estimate depending on the signal for $NS_o^*(x_o)$. But sometimes this term exceeds in such a way that the corrected estimate falls outside the range of neighbor data points, thus this term is replaced by a new variable usually less than $NS_o^*(x_o)$. Moreover, the correcting amount must be rescaled to reproduce the sample variance using a constant factor that multiplies all correcting amounts. It is important to note that this factor multiplies only the correcting amount and not the ordinary kriging estimate ($Z_{OK}^*(x_o)$). This procedure guarantees the local accuracy of corrected estimates. Details of this procedure can be found in Yamamoto [6, 7].

3. The new approach for correcting the smoothing effect

A completely new approach is proposed in this paper and it is based on a well-known transformation equation in statistics [11] that allows calculation of raw score when the Z score is known:

$$X = (Z).S_X + \bar{X} \tag{1}$$

where X is the raw score, and \bar{X} and S_X are the mean and standard deviation of the raw score. Replacing the terms in (1) to get corrected estimates we have:

$$Z_{OK}^{**}(x_o) = \left(\frac{Z_{OK}^*(x_o) - E[Z_{OK}^*(x_o)]}{\sqrt{Var[Z_{OK}^*(x_o)]}} \right) \cdot \sqrt{Var[Z(x)]} + E[Z(x)] \quad (2)$$

where $Z_{OK}^*(x_o)$ is the ordinary kriging estimate, $\left(\frac{Z_{OK}^*(x_o) - E[Z_{OK}^*(x_o)]}{\sqrt{Var[Z_{OK}^*(x_o)]}} \right)$ is the Z score and $\sqrt{Var[Z(x)]}$ is the sample standard deviation and $E[Z(x)]$ is the sample mean.

This equation gives corrected estimates presenting the sample standard deviation $\sqrt{Var[Z(x)]}$ and the sample mean $E[Z(x)]$ that are minimum requirements for histogram reproduction.

Before going further it is important to note that Equation 2 is based on Z score and therefore the distribution of $Z_{OK}^*(x_o)$ plays an important role in this process. Z score transformation retains the shape of $Z_{OK}^*(x_o)$, that is if $Z(x)$ follows a lognormal distribution, $Z_{OK}^*(x_o)$ will follow a lognormal distribution and consequently Z scores will present the same shape as the former distributions. Application of Equation 2 for skewed distributions can result in extreme values for corrected estimates. Thus, it is important to work with distributions as symmetric as possible. Evidently, it calls for a data transformation such as normal score transform as described by Deutsch and Journal [12]:

$$y(x_i) = G^{-1} \left(\frac{r(x_i)}{n+1} \right)$$

where $G(y)$ is the standard normal cdf and $r(x_i)$ is the rank for i th $z(x_i)$ associated with a set of n data values $\{z(x_i), i = 1, n\}$.

For illustration purposes Figure 1 shows distribution of Z scores for ordinary kriging estimates from raw data and normal score data. The range of Z scores for raw data is from -1.19 to 12.18 whereas for normal score data is from -3.14 to 3.40. Besides, the shape of raw data Z scores is positively skewed such as the sample histogram while the shape of normal data Z scores is almost symmetric because some asymmetry was introduced during the estimation process. Since Z scores are measured in a number of standard deviations, it is not convenient with scores less than -3 or greater than 3. Usually Z scores enlarge the range of normal score data from (-2.33 to

2.33) to (-3.14 to 3.40) and this may represent a problem when back-transforming corrected estimates to the original scale of measurement. However, the worst scenario comes from Z scores of raw data in which they range from -1.19 to 12.18. A large number of corrected estimates will likely fall outside the range of original data. This subject will be examined in the Section 5 Results and Discussion.

Further work takes place in the Gaussian domain. Statistics for sample data are then calculated:

$$E[Y(x)] = \frac{1}{n} \sum_{i=1}^n Y(x_i)$$

$$Var[Y(x)] = E[Y^2(x)] - E[Y(x)]^2$$

After computing and modeling the experimental semivariogram for $Y(x)$ we run ordinary Kriging for estimation at unsampled locations:

$$Y_{OK}^*(x_o) = \sum_{i=1}^n \lambda_i Y(x_i) \quad (3)$$

Once again we can compute the mean and variance for OK estimates $E[Y_{OK}^*(x_o)]$ and $Var[Y_{OK}^*(x_o)]$. Because the smoothing effect $Var[Y_{OK}^*(x_o)]$ will be less than $Var[Y(x)]$ and it is important to correct for the smoothing effect before back-transforming $Y_{OK}^*(x_o)$ into the original scale of measurement $Z_{OK}^*(x_o)$ as proposed by Yamamoto [7] for lognormal kriging estimates.

Equation 2 becomes:

$$Y_{OK}^{**}(x_o) = \left(\frac{Y_{OK}^*(x_o) - E[Y_{OK}^*(x_o)]}{\sqrt{Var[Y_{OK}^*(x_o)]}} \right) \cdot \sqrt{Var[Y(x)]} + E[Y(x)] \quad (4)$$

After this correction $Y_{OK}^{**}(x_o)$ is supposed to reproduce the sample histogram $Y(x)$ and the semivariogram model for $Y(x)$. Since we do not work with transformed values, it is important to check if the semivariogram model for $Y(x)$ is reproduced, because it guarantees that back-transformation will be carried out with the same spatial correlation.

Now $Y_{OK}^*(x_o)$ and $Y_{OK}^{**}(x_o)$ are back-transformed into the original scale using the inverse operation:

$$Z_{OK}^*(x_o) = F^{-1}(Y_{OK}^*(x_o)) \quad (5)$$

$$Z_{OK}^{**}(x_o) = F^{-1}(Y_{OK}^{**}(x_o)) \quad (6)$$

Back-transformed values after correcting the smoothing effect $Z_{OK}^{**}(x_o)$ should be close to the sample histogram of $Z(x)$. Therefore, in this paper we want to check Equation 4 for reproducing the semivariogram model and Equation 6 for reproducing the sample histogram.

4. Materials and methods

In this study we depart from an exhaustive data set composed of 50x50 values on a regular grid.

This exhaustive data set follows a lognormal distribution and it was derived from the public domain file true.dat [12]. The secondary variable of this data set was transformed into normal values using the normal score transform [12].

After that normal scores were transformed into a new variable using the exponential function:

$$Z(x) = e^{Y(x)}$$

This new variable presents a perfect lognormal distribution (Figure 2).

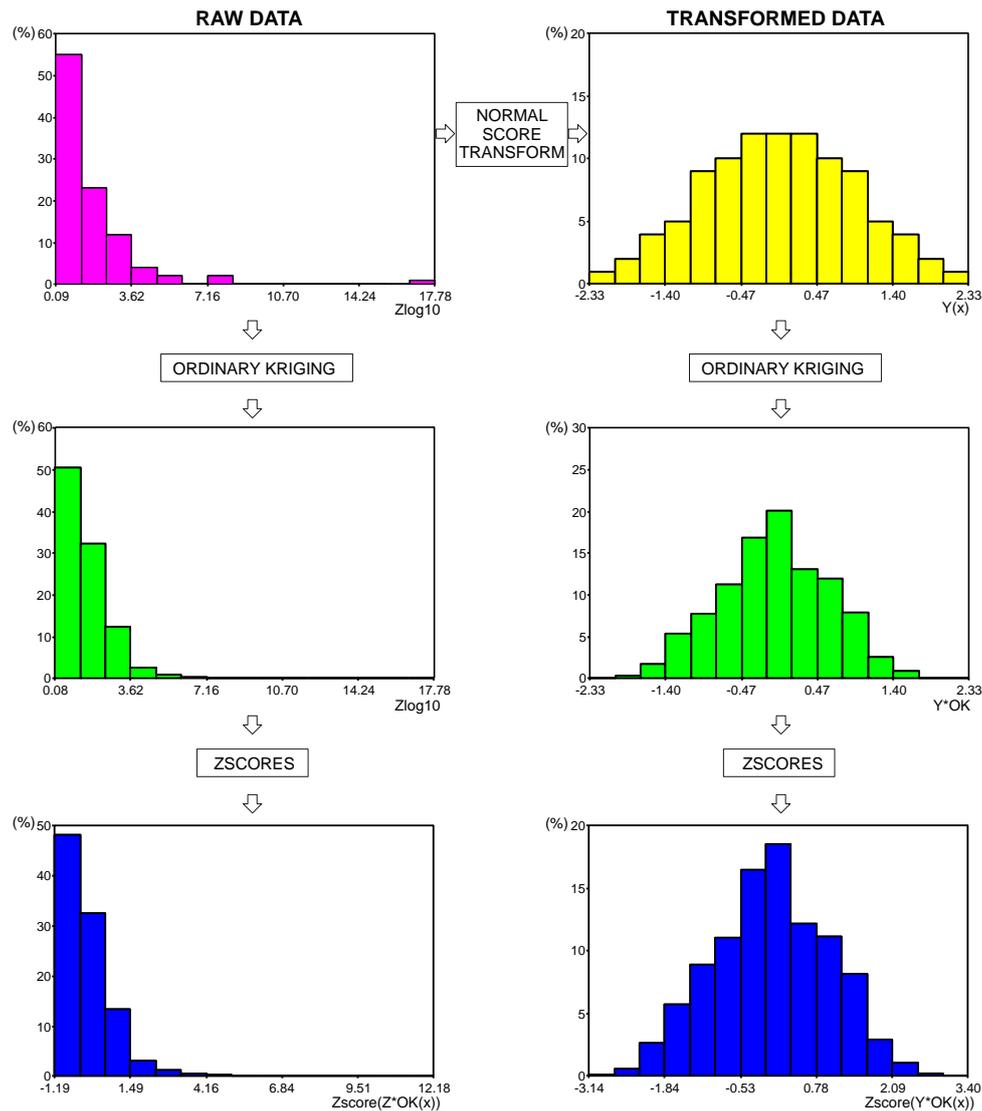


Figure 1. Histograms for Z scores calculated from both raw data and normal score data.

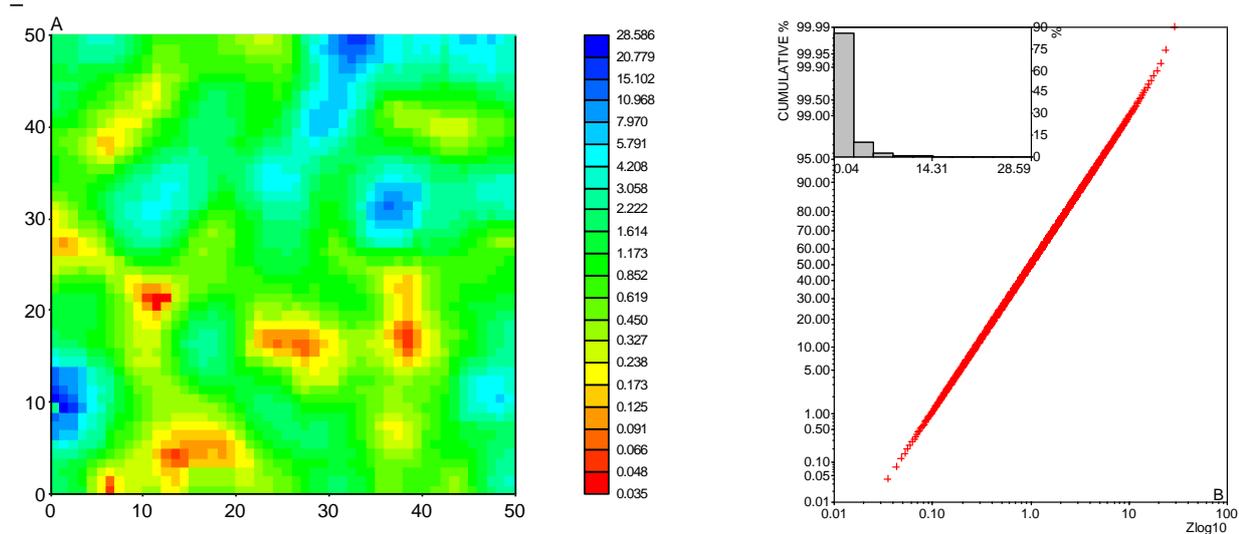


Figure 2. Spatial distribution of a lognormal variable (A); Cumulative frequency curve and histogram of the lognormal variable in exhaustive data set

Now, from this exhaustive data set we can draw samples for this study. In order to avoid clustering of sampled data points, we have used the stratified random sampling technique. Samples with 25, 49 and 100 data points have been drawn from the exhaustive data set. Since samples should give a good representation of the exhaustive data set, we compared sample distributions with exhaustive distribution (Figure 3).

It is clear that small size samples do not represent well the parent population or the exhaustive data set. On P-P plots we can measure an average distance to the reference line [6] that gives us an idea about how close points are to the reference line (Table 1).

Table 1: Average distances measured on P-P plots for stratified random samples.

Samples	Sample size		
	25	50	100
1	4.59	2.33	1.21
2	4.21	2.75	1.63
3	3.48	2.41	1.91
4	2.71	1.88	1.47
5	3.66	2.44	1.33
6	3.11	1.79	1.97

Looking at Figure 3 and Table 1, one readily concludes that samples with 100 data points are more representative of the exhaustive data set.

Even when sampling 100 points the maximum value was not reproduced, but this happens when we are working with lognormal distribution. In this study we will consider these samples as representative of the exhaustive data set and consequently they can be used to make statistical inferences about the exhaustive data set as well as the spatial distribution shown by the parent

population (Figure 2). Parameters for the exhaustive data set and statistics for samples are presented in Table 2.

As we can see in Table 2, samples follow either lognormal distribution with $CV > 1.2$ (samples 1-2-3) or positively-skewed distribution with $CV < 1.2$ (samples 4-5-6). Since sample distributions are not symmetric, we have to transform raw data into normal scores that follow a bell-shaped distribution presenting a mean zero and a variance equal to one. Thus, all data have been transformed into normal scores using the normal score transform as described in Deutsch and Journel [12, p. 138 and 209-211]. Experimental semivariograms have been calculated and modeled for normal scores data (Figure 4).

Thus, all calculations are made in the normal score domain in which we get the OK estimates after Equation 3. The grid on which further calculations are done is the same as primary exhaustive data set. It should be noted that the estimation is performed only on the nodes which belong to the convex hull [13]. Even in the Gaussian domain, OK estimates will present some smoothing that must be corrected using Equation 4. Corrected estimates can be back-transformed into original scale of measurement according to Equation 6.

Moreover, this procedure can be compared with the former procedure for correcting the smoothing in kriging as published by Yamamoto [6,7]. Actually, this paper will consider the same procedure for back-transforming lognormal kriging estimates [7]. OK estimates in the normal scores domain (Equation 3) will be corrected for

smoothing (Equation 4) and then back-transformed using the inverse operation as Equation 5 or 6. For comparison purposes back-transformed values from corrected estimates according to the former algorithm [6,7] will also be considered in this paper.

5. Results and discussion

Figure 5 presents the image maps of back-transformed values based on Equation 5 which are not corrected after kriging. These are given for comparison purposes. Results for corrected estimates from raw data will not be displayed but discussed accordingly.

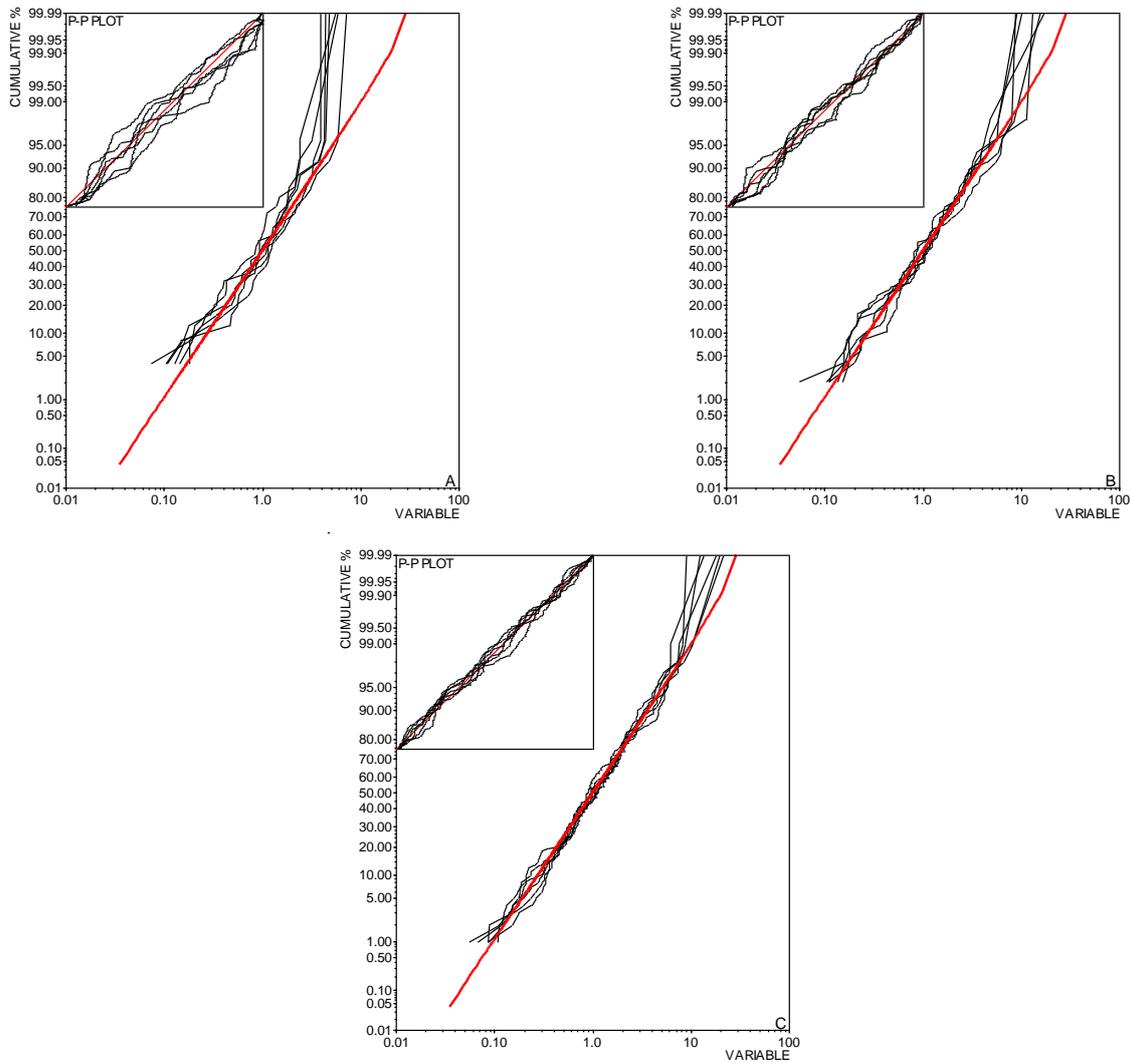


Figure 3. Cumulative frequencies for samples (thin black lines) compared with exhaustive distribution (thick red line) for samples with: 25 points (A), 49 points (B) and 100 points (C)

Table 2. Parameters and statistics for exhaustive data and samples.

Parameter/ Statistics	Exhaustive	Samples					
		1	2	3	4	5	6
N	2500	100	100	100	100	100	100
Mean	1.640	1.688	1.658	1.747	1.671	1.732	1.583
Std. Dev.	2.057	2.172	2.300	2.614	1.939	1.879	1.764
CV	1.254	1.286	1.387	1.496	1.160	1.085	1.114
Maximum	28.596	17.784	19.067	20.817	12.333	9.002	13.330
Upper Q.	1.961	1.954	2.080	1.954	1.918	1.971	1.750
Median	0.999	1.046	1.084	0.861	0.940	0.966	1.104
Lower Q.	0.509	0.542	0.555	0.514	0.592	0.580	0.604
Minimum	0.035	0.085	0.109	0.088	0.056	0.068	0.087

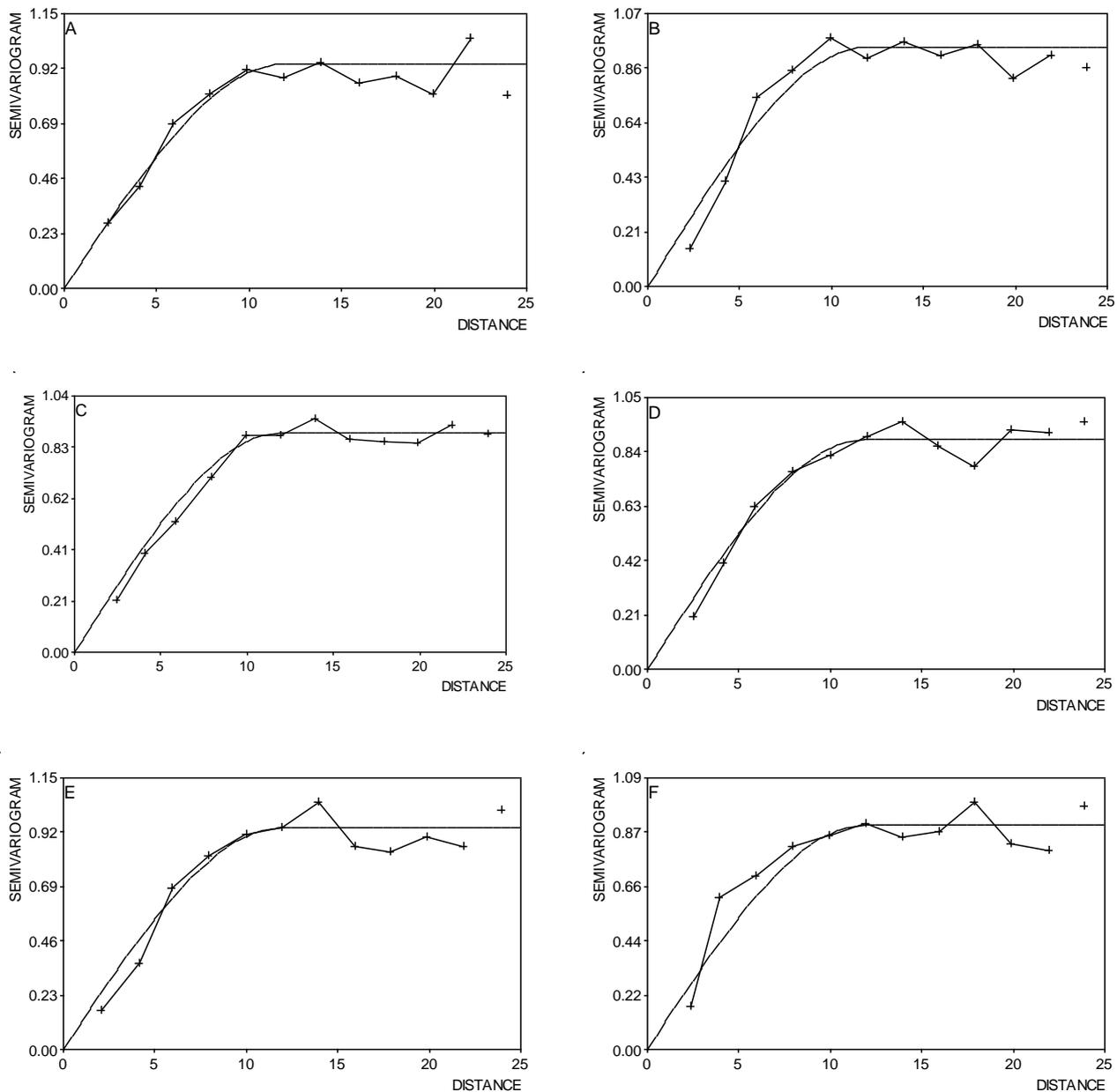


Figure 4. Experimental and modeled semivariograms for normal score data.

Figure 6 illustrates the image maps of back-transformed estimates (into original scale) for both approaches used in this study

It is very clear that corrected estimates produce enhanced maps in which low areas are lower and high areas are even higher. Moreover both approaches give similar and highly correlated results. Statistics calculated for back-transformed values after Equation 5 are in Table 3 and after Yamamoto [6-7] are presented in Table 4 and statistics for back-transformed values based on this paper's approach are listed in Table 5.

Comparing these statistics on Table 3 with sample statistics (Table 2), we realize back-transformed values after Equation 5 are biased. Actually, these values are mean biased and present reduced standard deviations. Besides, statistics of upper tails are strongly biased (maximum values and upper quartiles).

Both methods give similar results. Statistics for back-transformed values (Tables 4 and 5) are very close to the sample statistics (Table 2). Therefore, unbiased back-transform is only possible when estimates in the transform domain are corrected previously to the inverse operation as proposed by Yamamoto [7] for lognormal kriging estimates. It

is important to note that any correction based on the kriging variance or its square root will result in biased back-transformed values. Figure 7

presents cumulative curves and P-P plots comparing the sample distribution with back-transformed values.

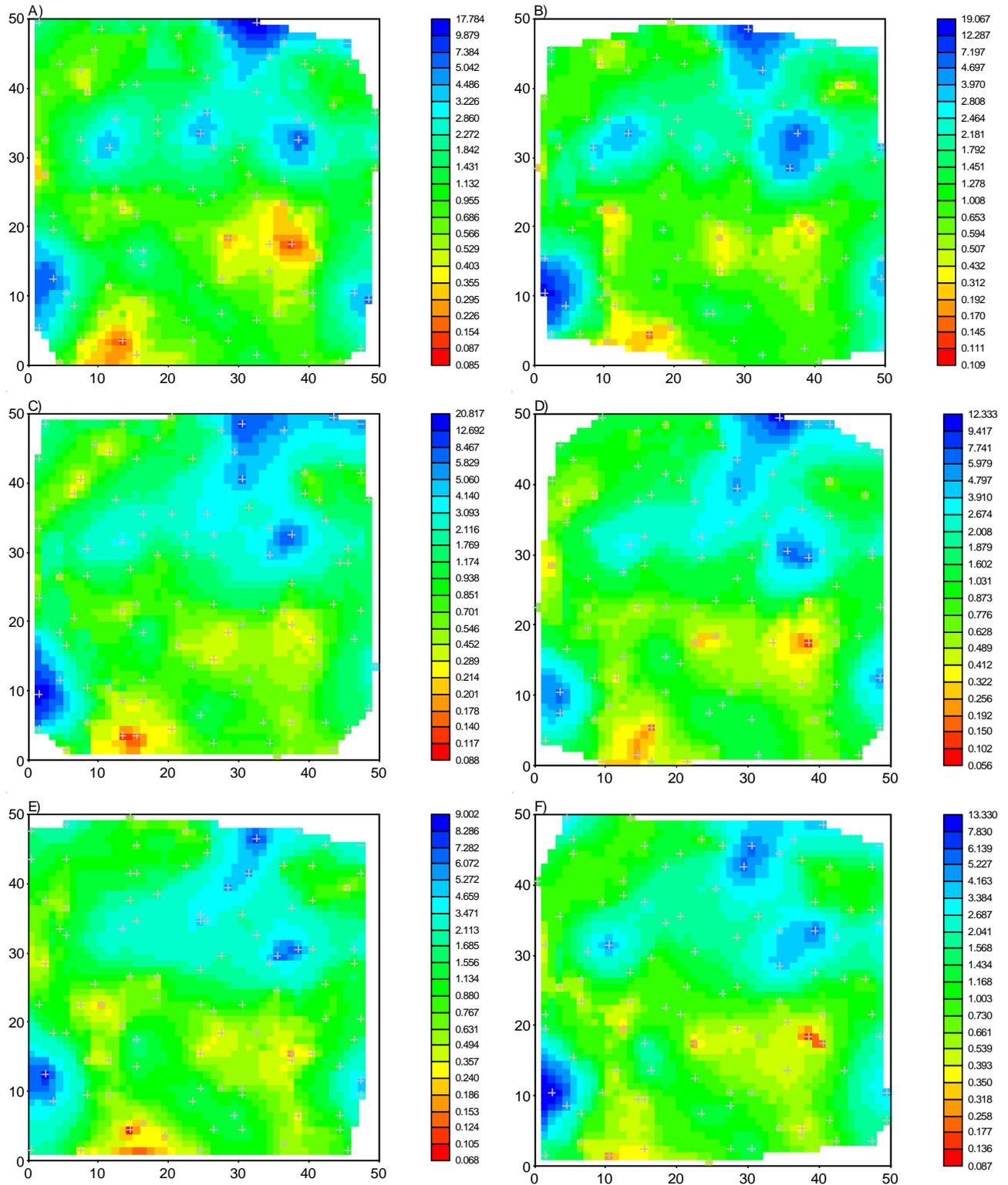
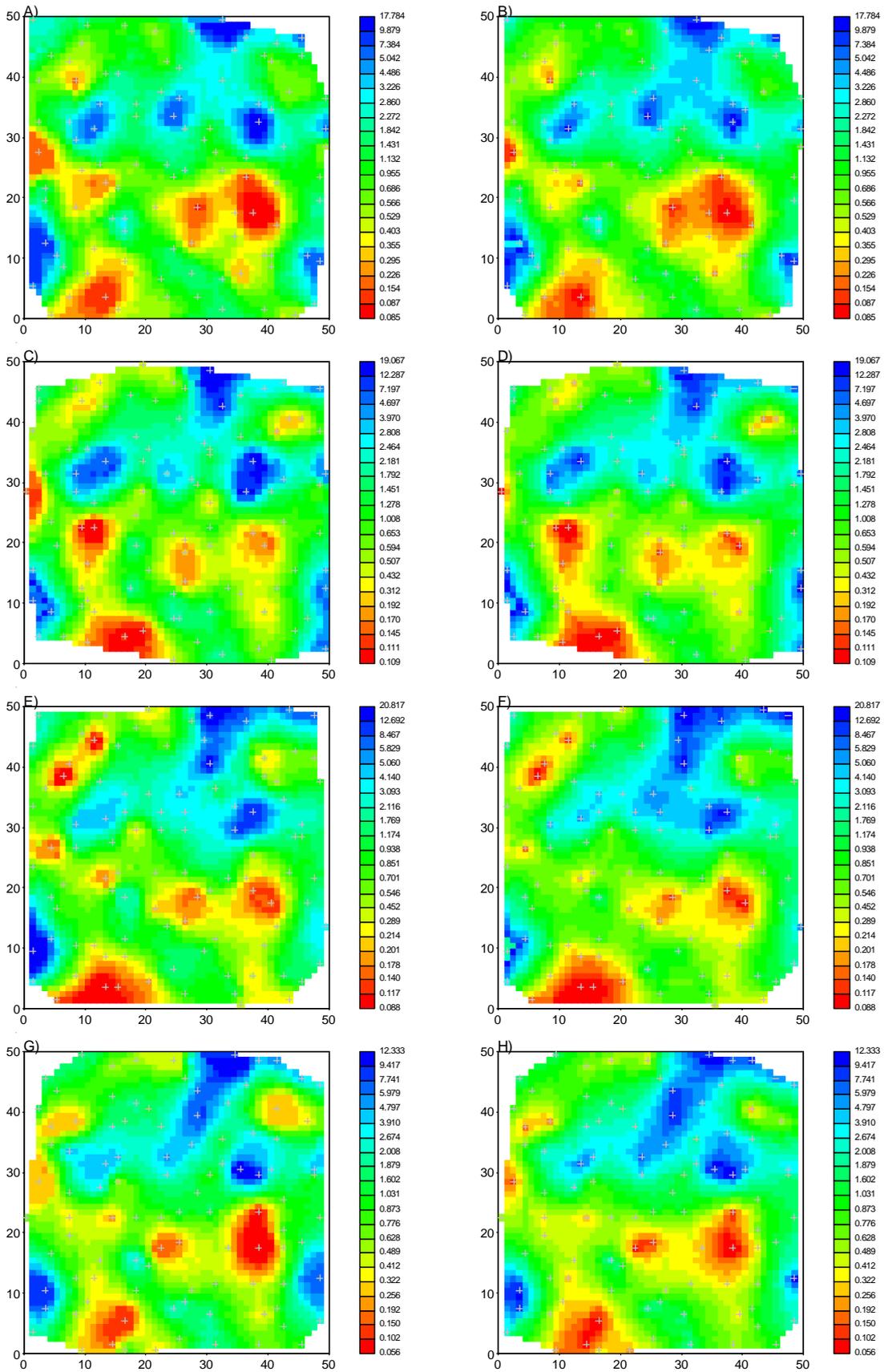


Figure 5. Image maps of back-transformed values after equation (4). Letters A-F correspond to samples 1-6. Legend: cross = sample data location



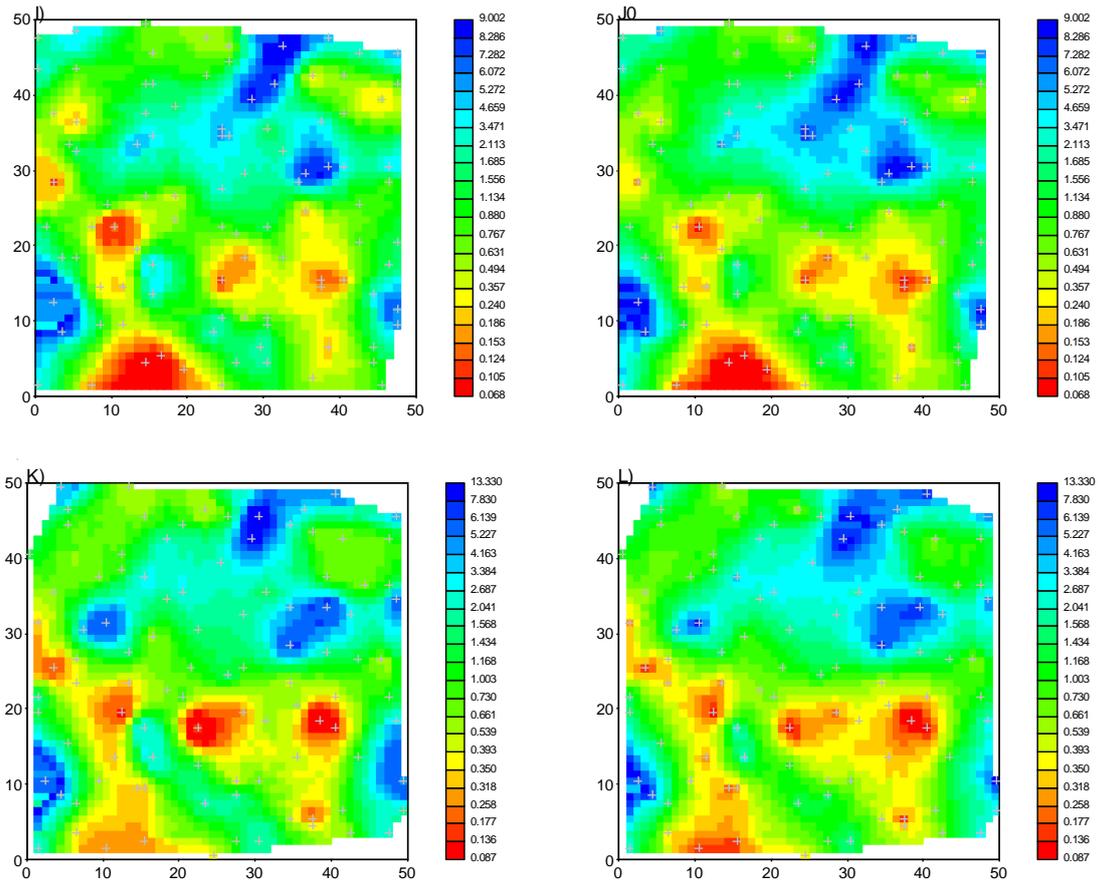


Figure 6. Image maps of back-transformed values to the original scale based on Yamamoto (2005 and 2007) are on the left (A-C-E-G-I-K – corresponding to samples 1 to 6) and on the right (B-D-F-H-J-L – corresponding to samples 1 to 6) are image maps back-transformed based on the new approach (this paper). Legend: cross = sample data location.

Table 4. Statistics for back-transformed values after Yamamoto (2005 and 2007).

Statistics	Samples					
	1	2	3	4	5	6
N	2332	2233	2285	2272	2253	2264
Mean	1.680	1.713	1.713	1.678	1.720	1.588
Std. Dev.	2.103	2.471	2.439	1.940	1.930	1.764
Coeff. Var.	1.252	1.442	1.424	1.156	1.122	1.111
Maximum	17.784	19.067	19.611	12.333	9.002	13.330
Upper Q.	1.943	2.079	2.039	1.917	1.972	1.920
Median	1.064	1.055	0.904	0.941	0.954	1.061
Lower Q.	0.547	0.556	0.517	0.589	0.575	0.607
Minimum	0.086	0.109	0.088	0.075	0.083	0.090

Table 5. Statistics for back-transformed values according to this paper's approach.

Statistics	Samples					
	1	2	3	4	5	6
N	2332	2233	2285	2272	2253	2264
Mean	1.653	1.615	1.738	1.674	1.755	1.589
Std. Dev.	2.020	2.115	2.404	1.875	1.935	1.750
Coeff. Var.	1.222	1.310	1.383	1.120	1.103	1.102
Maximum	17.784	19.067	20.817	12.333	9.002	13.330
Upper Q.	2.068	2.117	2.046	1.977	1.972	1.975
Median	1.049	1.027	0.849	0.909	0.949	1.065
Lower Q.	0.547	0.572	0.526	0.590	0.591	0.587
Minimum	0.085	0.109	0.088	0.056	0.068	0.087

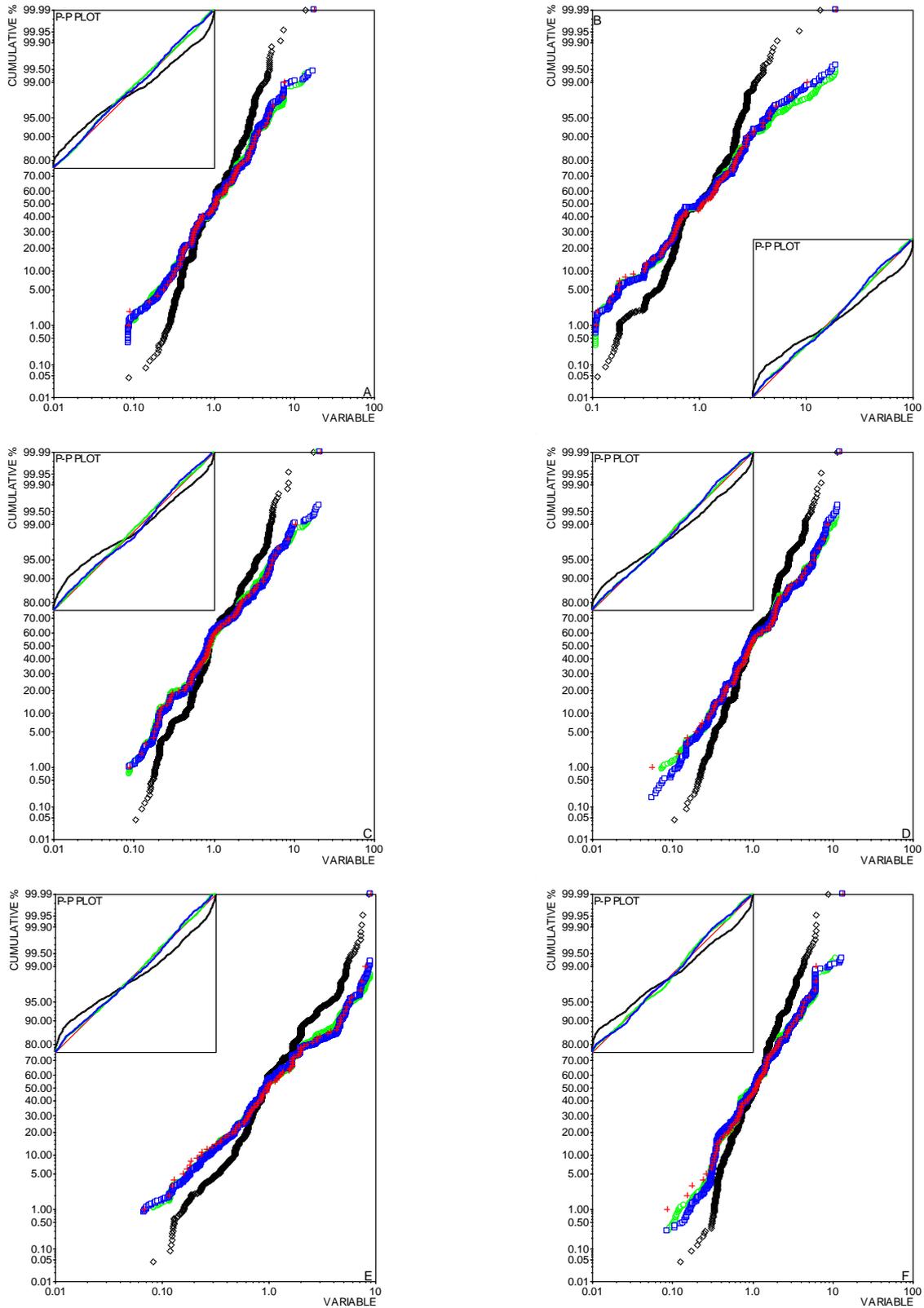


Figure 7. Cumulative curves and P-P plots comparing sample distribution with cumulative distributions of back-transformed estimates. Legend: red cross = sample data; green circle = back-transformed estimates after Yamamoto (2005 and 2007); blue square = back-transformed estimates according to this paper; black diamond = back-transformed after equation (5). Letters A-F correspond to samples 1-6.

Examining Figure 7, we conclude both approaches give very close results and consequently are valid approaches for correcting the smoothing effect of ordinary kriging estimates. Average distances on P-P plots confirm that both approaches give similar results (Table 5). However, back-transformed values after Equation 5 show different distributions to their respective sample distributions. Consequently, these values cannot be used to make statistical inference about the parent population.

Now we can check for semivariogram model reproduction after these approaches (Figure 8). Looking at this figure we conclude the former algorithm seems to reproduce the semivariogram model better. The new proposal also reproduces

the semivariogram model, but experimental semivariograms show more continuity than sample semivariograms.

Since we have the exhaustive data set, we can compare actual values with back-transformed estimates (Figure 9). This comparison gives an idea of the local precision as measured by the correlation coefficient in a scattergram.

Once again correlation coefficients are very close to each other proving both methods give a good correlation with actual values. Moreover, it also confirms that samples are representative of the exhaustive data set.

Now results provided by both approaches can also be compared on scattergrams and the correlation coefficient can be computed (Figure 10).

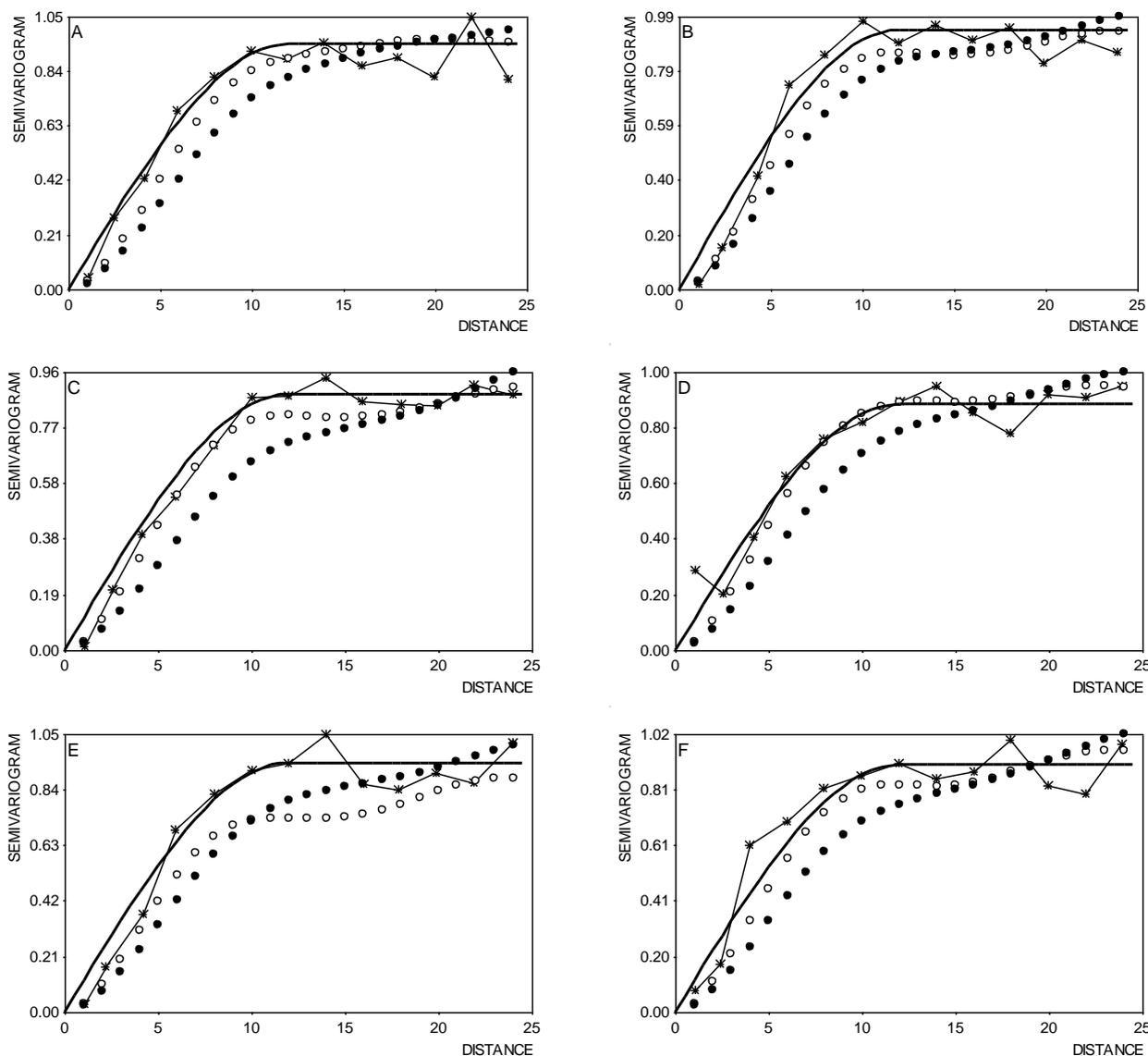
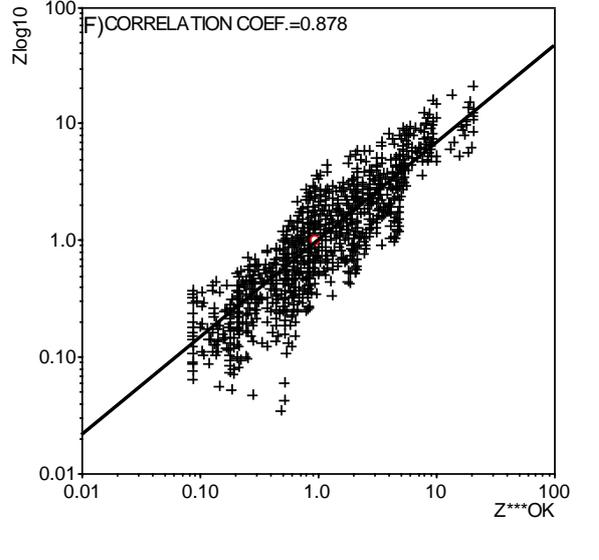
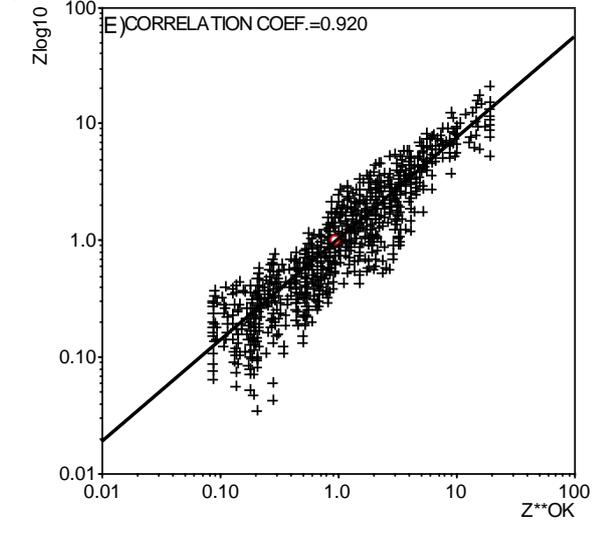
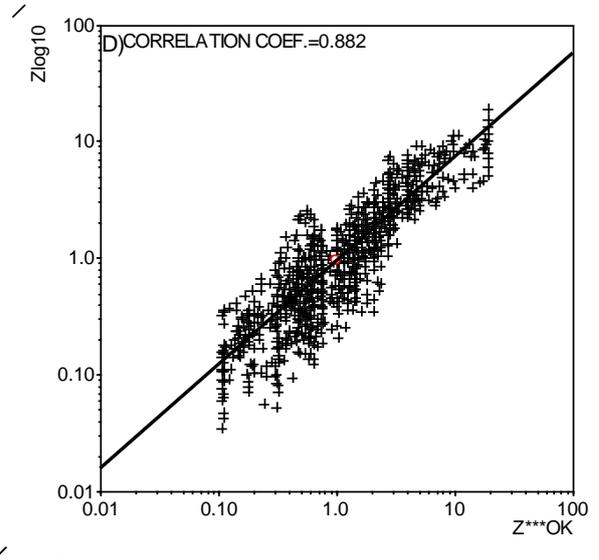
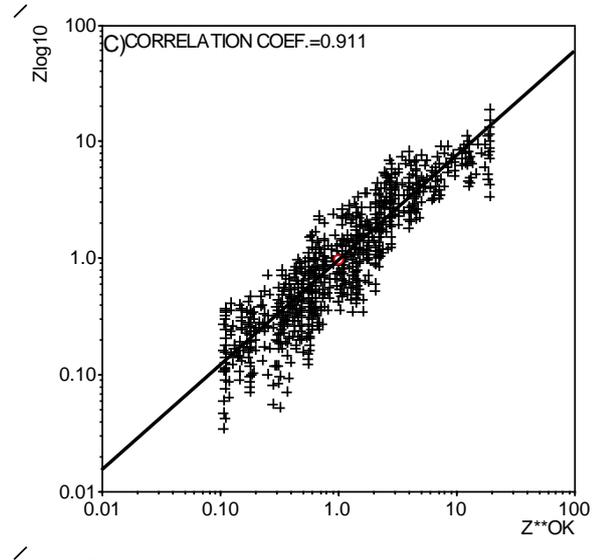
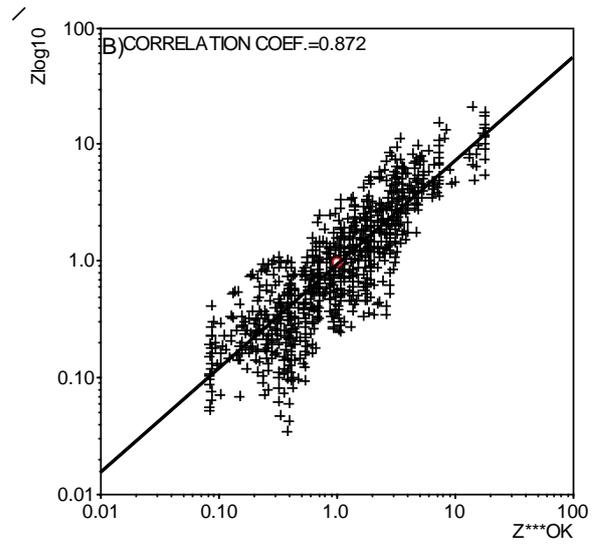
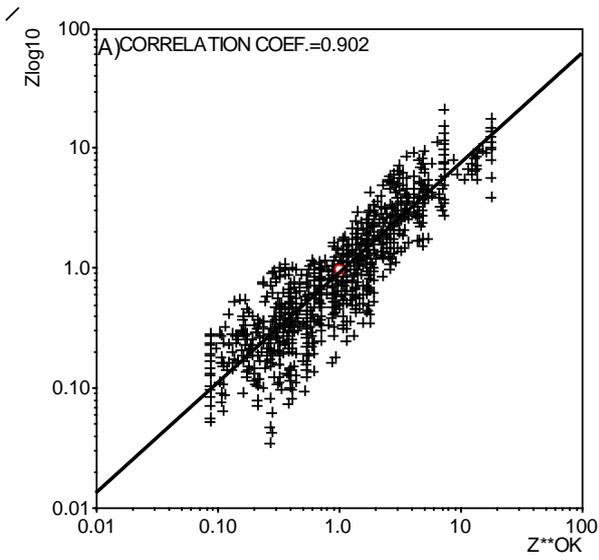


Figure 8. Experimental semivariograms computed from back-transformed estimates: open circle for values after Yamamoto (2005 and 2007); full circle for values after this paper; star = sample semivariogram; thick line = semivariogram model. Letters A-F correspond to samples 1-6.



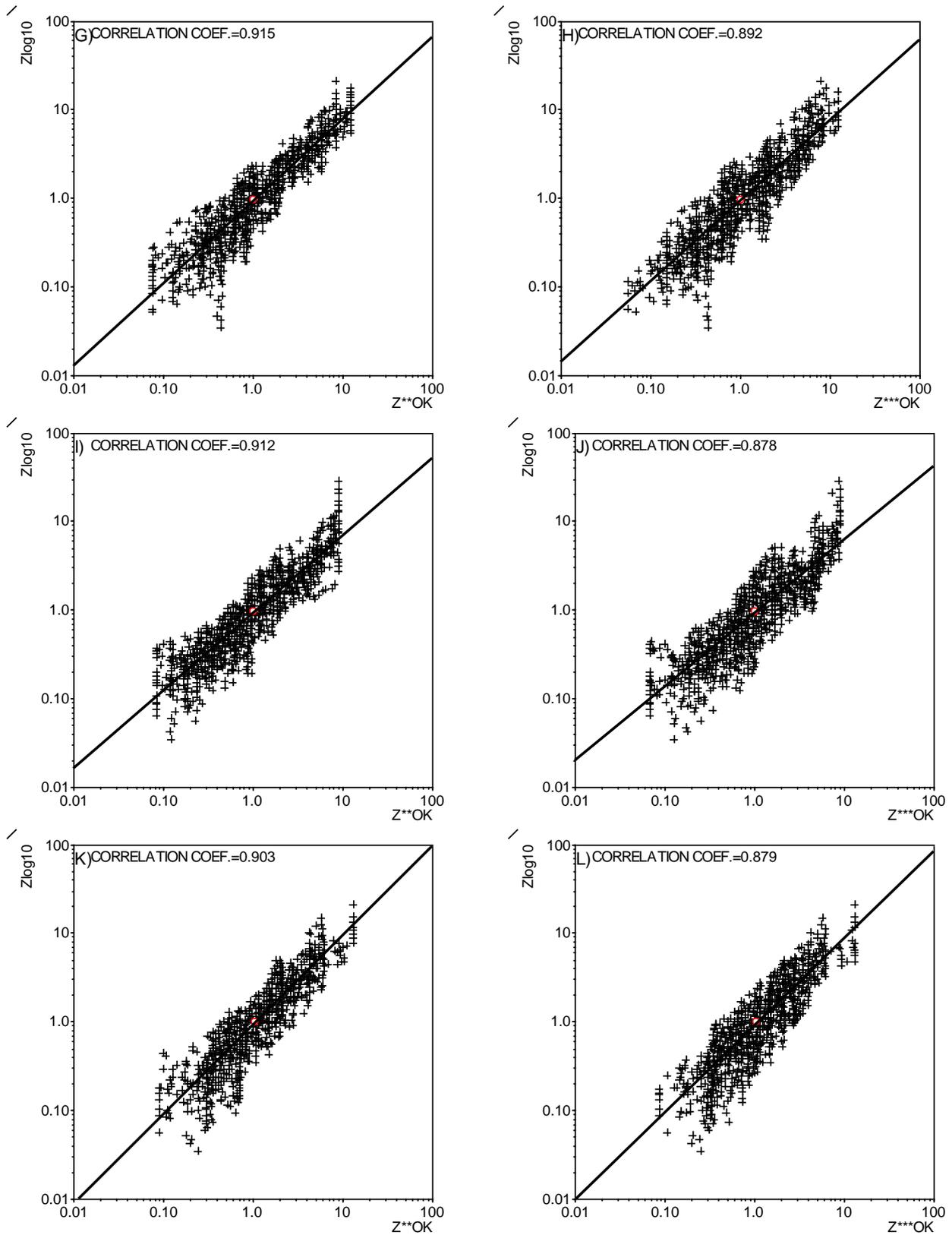


Figure 9. Scattergrams comparing actual values with back-transformed values to the original scale based on Yamamoto (2005 and 2007) are on the left (A-C-E-G-I-K – corresponding to samples 1 to 6) and on the right (B-D-F-H-J-L – corresponding to samples 1 to 6) are scattergrams comparing actual values with back-transformed based on the new approach (this paper).

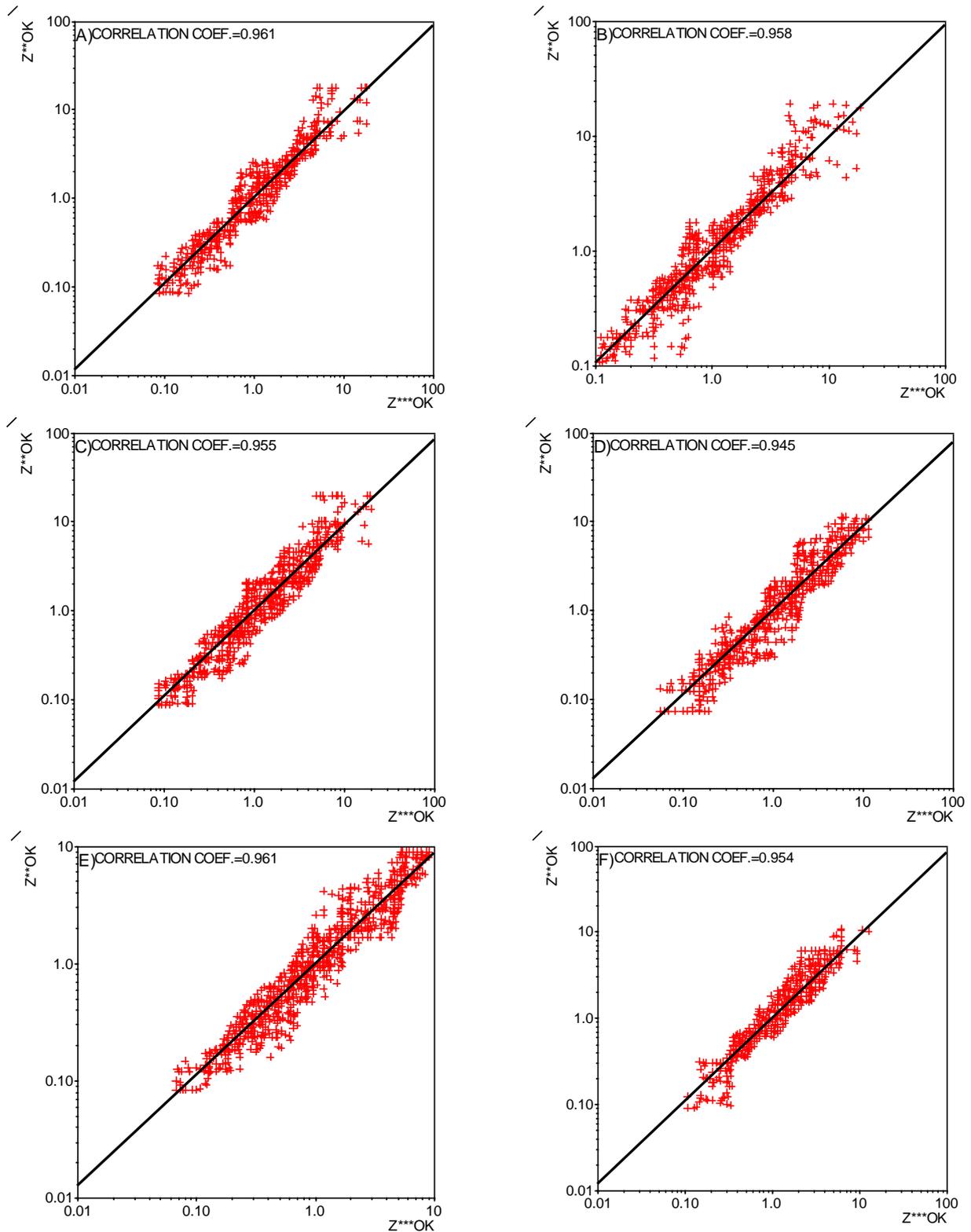


Figure 10. Scattergrams comparing back-transformed estimates after Yamamoto (2005 and 2007) with back-transformed estimates according to this paper. Letters A-F correspond to samples 1-6.

High correlation coefficients shown in Figure 10 confirm once again both methods give equivalent results. Evidently, back-transformed values are just close to each other but not equal because they are based on completely different approaches.

Finally we can check the effectiveness of the proposed method regarding corrected scores after the transformation equation. It can be tested by counting the number of times that corrected scores fall outside the permissible range (Tables 6 and 7,

respectively for raw data scores – Equation 2 and normal data scores – Equation 4).

Table 6 confirms that we cannot apply the transformation equation (Equation 2) for correcting Z scores from raw data because a large number of values are less than the sample

minimum. On the other hand, corrected Z scores from normal data present a little number of values falling outside the range of normal score data (-2.330 to 2.330) for samples considered in this study presenting 100 points.

Table 5. Average distances measured on P-P plots of sample data versus back-transformed values.

Procedure	Samples					
	1	2	3	4	5	6
Equation (5)	4.32	4.76	4.23	4.02	4.74	4.02
Yamamoto (2005)	0.81	0.66	0.54	0.45	0.56	0.96
This paper	0.66	0.94	1.17	0.88	0.98	0.90

Table 6. Counting of times falling outside range of sample data for raw data corrected scores.

Sample	Estimated values	Z_{min}	Z_{max}	$Z_{OK}^{**}(x_o) < Z_{min}$	$Z_{OK}^{**}(x_o) > Z_{max}$
1	2332	0.085	17.784	434	4
2	2233	0.109	19.067	444	4
3	2285	0.088	20.817	525	3
4	2272	0.056	12.333	286	3
5	2253	0.068	9.002	220	15
6	2264	0.087	13.330	247	6

6. Conclusions

This paper presented a new approach for correcting the smoothing effect of ordinary kriging estimates based on the well-known transformation equation used in statistics. Since this equation uses the Z score, it works better if data are transformed into a symmetric normal distribution. Calculations are then made in this domain and ordinary kriging estimates are corrected for smoothing before back-transforming into the original scale of measurement. Comparisons made with the former algorithm proved this new approach gives similar and equivalent results. The simplicity of this method is the most impressive feature.

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