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On Visualization for Assessing Kriging Outcomes[1]

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Extant opinion about kriging is that all weights should be positive. Visualizations rendered by converting kriged grids to digital images are presented to show that negative weights may be beneficial to some spatial problems. In particular, variogram models with zero-valued nuggets, already well known to minimize smoothing through kriging, result in a visual resolution substantially superior to that from kriging with a variogram model having a nonzero nugget value in application to satellite acquired data. Negative weights are more likely when using variogram models with zero-valued nuggets, but resultant visualizations often show a smoother transition between extreme data values. This is true even when a variogram model having a nugget value of zero is not optimum with respect to mean square error, as is demonstrated using a nitrate data set. An analogy to digital image processing is used to suggest that the influence of negative weights in kriging is similar to a high-boost kernel.

KEY WORDS: bitmap, kernel, Landsat, nitrate, variogram, weights.

INTRODUCTION

Positive [ordinary] kriging (Barnes and Johnson, 1984) involves a double constraint on kriging weights, $\sum \lambda = 1$, moreover $\lambda_i \geq 0, i = 1, 2, \ldots, N$ (closest surrounding estimation locations; see also Chiles and Delfiner, 1999, p. 225). Incentive for this work was Schaap and St. George (1981). Motivation is the avoidance of negative kriging weights that may impart unwanted artifacts in an estimated map. In particular, the range of estimates may, in some cases, exceed that of the sample data. Other authors addressing the issue of negative kriging weights include Szidarovsky, Baafi, and Kim (1987). Herzfeld (1989) provided an update to Barnes and Johnson (1984) by achieving the constraint of nonnegative weights through quadratic programming.

Negative kriging weights occur more frequently when using low-valued nuggets, zero-valued nuggets in particular. Unusual, estimated values often occur from negative kriging weights when a datum exists within the local estimation

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window that has a value much different than any of the other data falling within the estimation window. This is a particular consequence that prompted the advent of positive kriging. If, however, the range within the kriging neighborhood is small, unusual estimates are less likely. In this case, negative kriging weights do not yield unusual estimates.

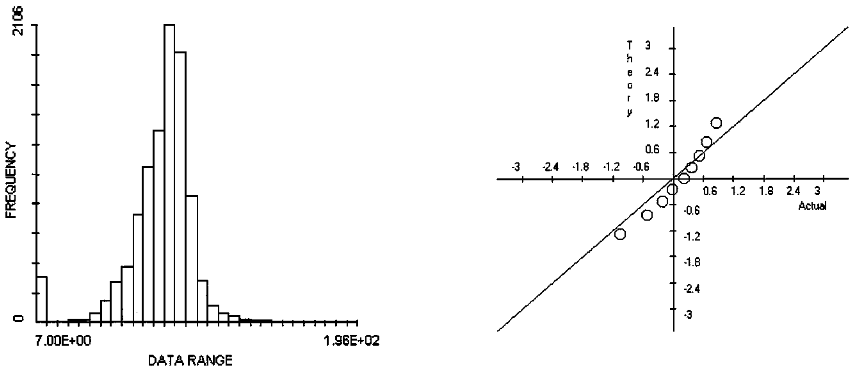
Visualizations are presented of two, different data sets to investigate the influence of negative kriging weights. Sampling geometry, data distribution, and variogram behavior distinguish these two sets of data.

APPLICATION TO DIGITAL SATELLITE IMAGE DATA

One of the most geometrically regular spatial data sets is that which is acquired by a scanner onboard an airborne or spaceborne platform. Visual demonstrations of kriging are forwarded based on a portion of a 1984 Landsat TM image of northern Mineral County, Nevada (Path 42, Row 33; July 7). Band 2 (visible green) data are chosen arbitrarily for demonstration. Original sampling resolution is 30 m $\times$ 30 m, consequently block sampling support is indicated. Each image pixel represents an average brightness, expressed as an integer value in the range [0, 255]. A spatial data set is developed by resampling the original image data to 120 m $\times$ 120 m by taking every fourth pixel along a row, then taking every fourth row of resampled pixels. A text file of pixel values and x, y coordinates is created of these resampled pixel values using a program, Visual_Data (Carr, 2002). The goal is to attempt the restoration of the original image data through kriging by interpolating to yield a 30 m $\times$ 30 m grid size. Visual comparison to the original image is used to assess the quality of interpolation via kriging for a range of variogram models.

Histogram analysis of these data suggests that a normal distribution model represents their distribution well (Fig. 1). Variogram analysis (Fig. 2) of the resampled image suggests a spherical model with a nugget equal to 20% of the sill value and a range of 240 pixels. Despite what the variogram suggests, experiments are designed to interpolate these data using nugget values ranging from 0 to 100% of the sill value. Four outcomes are visually compared to the original image data (Fig. 3(B) through (E)).

What is remarkable about this visual comparison is how strikingly clear the interpolation is that is based on a zero-valued nugget (Fig. 3(B)), whereas visualizations developed using nonzero nugget values are visually blurred (smoothed) and only subtly distinguishable (Fig. 3 (C) through (E)). This observation is supported by graphing mean square error versus nugget (Fig. 4). Error increases sharply with nugget from 0 to 20%. Thereafter, error is less affected by increases in the nugget value. A zero-valued nugget is optimum for these data, even though negative kriging weights are more likely, moreover variography suggests that a nonzero nugget value equal to approximately 20% of the sill value should be modeled.



A B

Figure 1. (A) Histogram of visible green reflectance, 10,000 total pixels. (B) Probability plot of *z*-scores of data quantiles (actual) versus *z*-scores of quantiles from a normal distribution model (theory).

The visual quality of kriging applied to satellite data using a zero-valued nugget was discovered accidentally in the writing of Carr (2002). Therein, a Matlab routine, pkrige (Middleton, 2000) was applied to the estimation of satellite data to demonstrate Matlab applications for visualizations of kriging. The manner

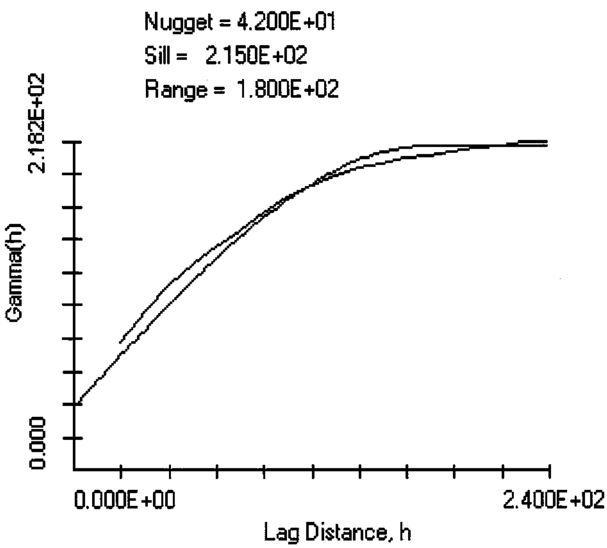


Figure 2. Variogram of visible green reflectance. Parameters of a spherical model fit to the data variogram are shown above the plot.

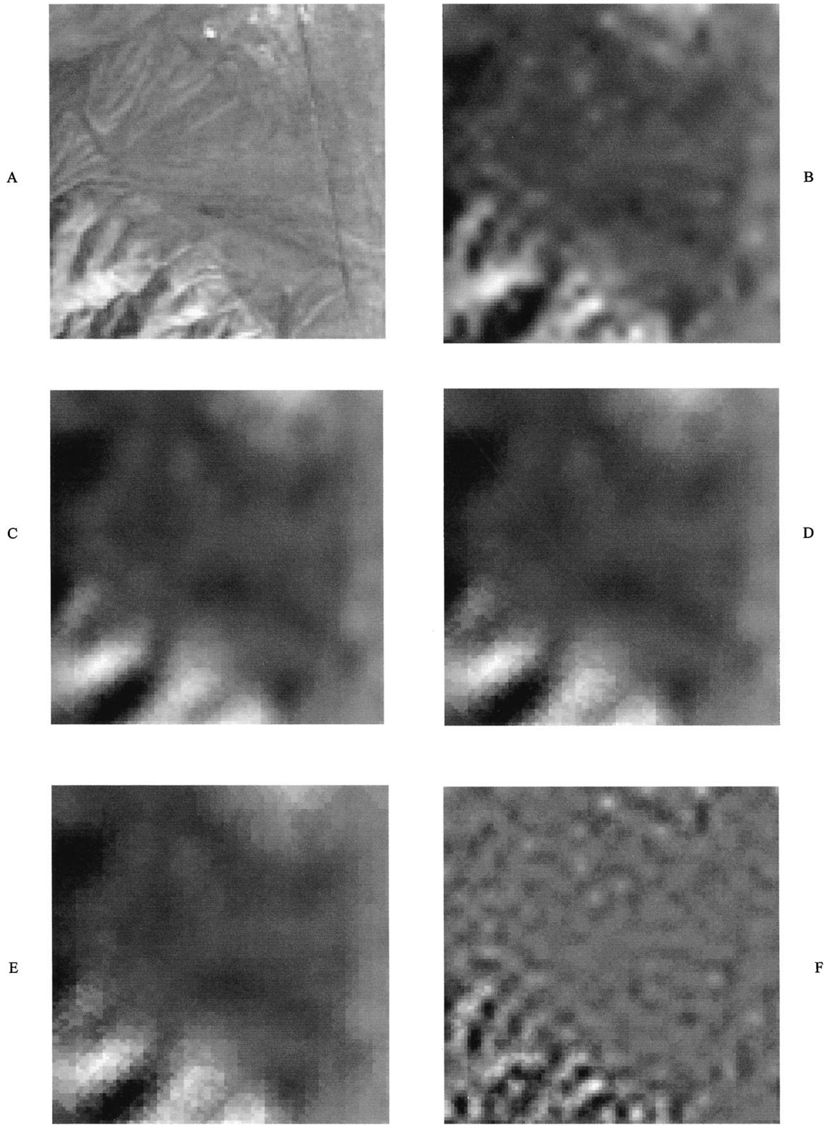


Figure 3. (A) Original image data, pixel resolution of 30 m. (B) Windows bitmap image of kriged estimates based on a zero-valued nugget applied to 4 $\times$ resampled pixel values. (C) Windows bitmap image of kriged estimates based on a nugget equal to 10% of the sill value. (D) Nugget value is 20% of the sill value. (E) Nugget value is equal to the sill value. (F) Difference image created by subtracting the bitmap image based on a nugget value equal to 10% of the sill value from that image created using a zero-valued nugget; this residual image is a visualization of higher spatial frequencies that are present in image (B), yet are filtered from image (C). Kriging neighborhood (N) is 10 for each image (B)–(E).

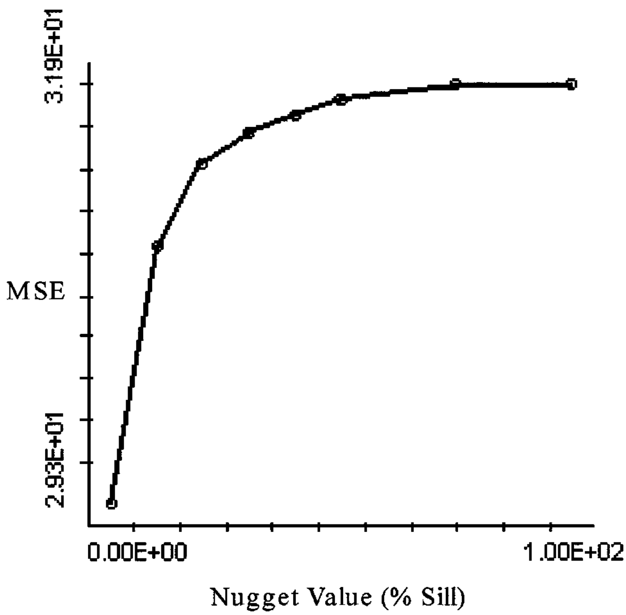


Figure 4. A plot of the change in mean square error (MSE) as the nugget value is increased from zero to the sill. In this particular case of Landsat TM data (visible green reflectance), a zero-valued nugget is associated with least error. Kriging neighborhood (N) is 10 for all nugget values.

in which the spherical model was embedded in this code resulted in a zero nugget value, even though a nonzero value was initially specified. A correction to pkrige is presented in Carr (2001). Nonetheless, the original Matlab code led to the development of a remarkable visualization identical to that shown earlier (Fig. 3(B)).

Inferences Drawn From Digital Image Processing

One kernel, or collection of weights, that is used in the spatial convolution filtering of digital images effects a *high boost*. Low spatial frequencies are not removed by this kernel. Instead, high spatial frequencies, such as lines and edges, are amplified. The visual outcome is a "crispening" or "sharpening" of the image. One example of a high-boost kernel is shown below (a 3×3 kernel size is assumed).

$$\begin{matrix} -1/9 & -1/9 & -1/9 \\ -1/9 & 27/9 & -1/9 \\ -1/9 & -1/9 & -1/9 \end{matrix}$$

Notice that outside weights are negative. The central weight is positive. Moreover, the sum of these [nine] weights exceeds one.

In contrast, a *low-pass* kernel, one that substantially removes high spatial frequencies, is associated with weights that sum to one. One example of a low-pass kernel is as follows.

$$\begin{array}{ccc} 1/9 & 1/9 & 1/9 \\ 1/9 & 1/9 & 1/9 \\ 1/9 & 1/9 & 1/9 \end{array}$$

Kriging, a weighted average in which weights sum to one (assuming this constraint is applied), is also a low-pass filter. The larger the nugget value is, the more severe is the filter. The optical result is a blurring of the original data (Fig. 3(C) through (E)).

Carr and Myers (1984) showed how to use the variogram with nonzero nugget values to design low-pass kernels for applications in digital image processing wherein noise attenuation is desirable with minimal blurring. Using a nugget value of zero and a 3×3 geometric configuration yields the following kernel (assuming a 3×3 size, moreover assuming a cross-validation-type application, estimation location is at center of 3×3 region; a range of 10.0 is used).

$$\begin{array}{rlr} -0.0047 & 0.2547 & -0.0047 \\ 0.2547 & 0 & 0.2547 \\ -0.0047 & 0.2547 & -0.0047 \end{array}$$

This kernel exhibits characteristics of both a low-pass and high-boost kernel. Although these weights sum to one, this outcome is likened to a high-boost kernel because central weights sum to a value greater than one, whereas more distant weights are negative. This combination of negative and positive weights tends to increase the numerical differences between pixels. The optical result is a boosting of high spatial frequencies (edges) in data, thus minimizing smoothing. Visually, this has the effect of crispening, or sharpening the kriging outcome (Fig. 3(B)). Higher spatial frequencies are preserved better than when kriging with a larger nugget. A difference image developed by subtracting the kriged result using a 10% nugget (Fig. 3(C)) from the result obtained using a zero-valued nugget (Fig. 3(B)) reveals the substantial amount of higher spatial frequencies preserved when using a zero-valued nugget (Fig. 3(F)).

Increasing the nugget value from 0 to 100% of the sill value eliminates negative weights, moreover causes weights to become equal. This is demonstrated in the following kernels (again assuming the same type of cross-validation procedure that is used earlier).

Nugget = 10% of the sill:

0.0644	0.1856	0.0644
0.1856	0	0.1856
0.0644	0.1856	0.0644

Nugget = 20% of the sill:

0.0886	0.1614	0.0886
0.1614	0	0.1614
0.0886	0.1614	0.0886

Nugget = 50% of the sill:

0.1135	0.1365	0.1135
0.1365	0	0.1365
0.1135	0.1365	0.1135

Nugget = 100% of the sill:

0.1250	0.1250	0.1250
0.1250	0	0.1250
0.1250	0.1250	0.1250

These kernels will vary with the range of the variogram model. Shorter ranges result in a larger numerical difference among kernel weights; longer ranges yield more parity among weights for larger nuggets. But, the relative outcomes remain the same, with zero-valued nuggets yielding a mixture of positive and negative weights. Nonzero nugget values yield positive weights. These kernels also show how rapidly weights change as the nugget is increased.

APPLICATION TO DATA EXHIBITING SPATIALLY IRREGULAR SAMPLING

Data associated with nitrate contamination of ground water in Washoe Valley, southern Washoe County, Nevada due to septic tank effluent are chosen for this demonstration (Zhan and McKay, 1998). These data are spatially, irregularly sampled and are associated with a highly skewed distribution (Fig. 5). Both Chiles and Delfiner (1999, p. 224) and Barnes and Johnson (1984, p. 231) acknowledge that negative weights can exacerbate geometric problems attributable to sampling, unusual data values in the local kriging neighborhood, and kriging implementation. These nitrate data are chosen as a test because their sampling is spatially random, coinciding with domestic water wells, and values often change rapidly over small spatial distances.

A comparison of visualizations (Figs. 6 and 7) based on zero-valued and nonzero-valued nuggets shows that unwanted artifacts are not introduced into the

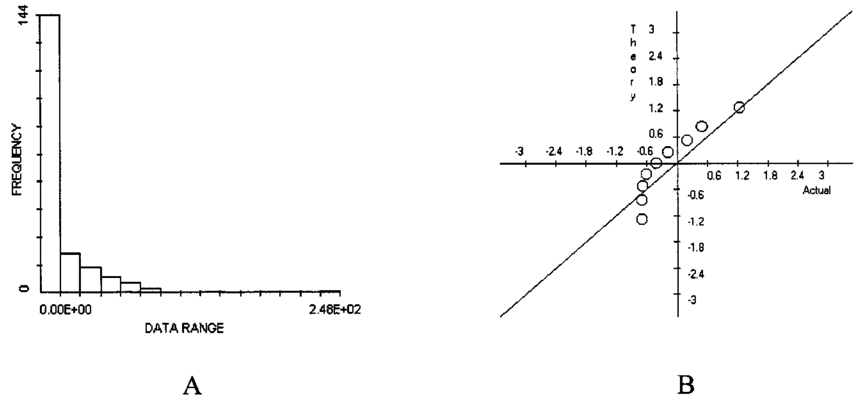


Figure 5. (A) Histogram of data associated with nitrate contamination of ground water, Washoe Valley, Nevada. (B) Probability plot of z-scores: data quantiles versus normal distribution quantiles. A normal distribution model does not represent the data distribution well.

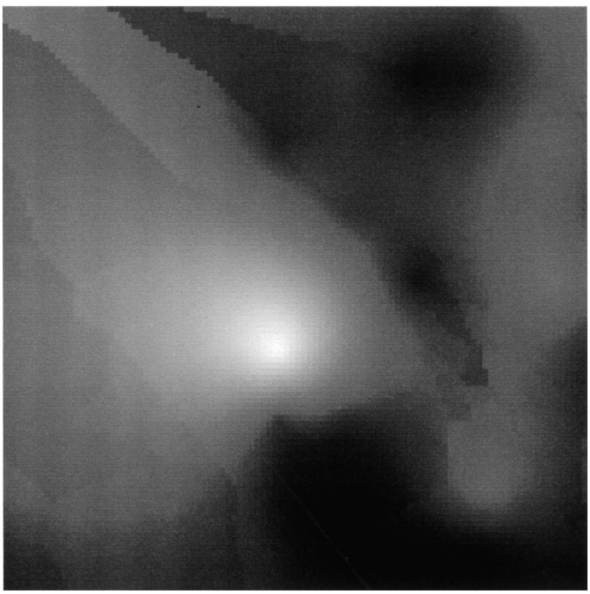


Figure 6. Windows bitmap image of kriged estimates of nitrate contamination. A nugget value of zero is used for estimation. Note the fairly smooth transition from higher (white) to lower (black) data values within the zone of highest sampling density (near the highest zone of nitrate contamination). Kriging neighborhood (N) is 10.

Figure 7. Kriged estimates of nitrate contamination, nugget value is equal to one-third the sill value. Transition from higher to lower data values is not as smooth, showing stepwise discontinuity. This visual artifact is most probably attributable to the small kriging neighborhood (N). Step discontinuities occur as sample data drop in or out of this neighborhood. Despite this visual artifact, analysis of mean square error (Fig. 9) shows that this image is associated with lower error in comparison to that which is obtained using a nugget value of zero. Kriging neighborhood (N) is 10.

final map. Moreover, the map based on a zero-valued nugget images the high zone of nitrate concentration more distinctly than does that which is based on nonzero nugget value. Furthermore, the transition from higher to lower data zones is smoother when using zero-valued nugget in comparison to the map that is based on nonzero nugget value. But, quantitative analysis of kriging performance shows that a zero-valued nugget is not optimal for these data (Fig. 8). In distinct contrast to the Landsat TM data, that which is associated with smallest mean squared error when modeling a zero-valued nugget and increasing error with nugget, these nitrate data exhibit the opposite result, with decreasing error with increasing nugget. The variogram (Fig. 9) is associated with a substantial nugget, suggesting either a high level of noise or limited to no representation in the spatial data of microspatial scales. That image (Fig. 7) which is based on a nugget value of approximately 33% of the sill value is a more accurate representation of these data, even though the visualization it rendered is, subject to personal preference, less appealing.

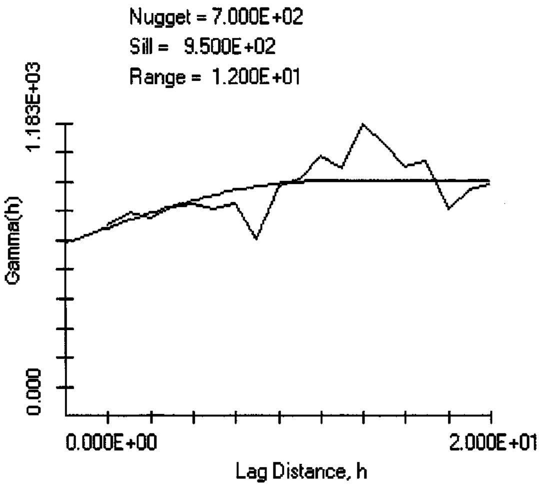


Figure 8. Variogram for nitrate data. Note the fairly large nugget value for these data.

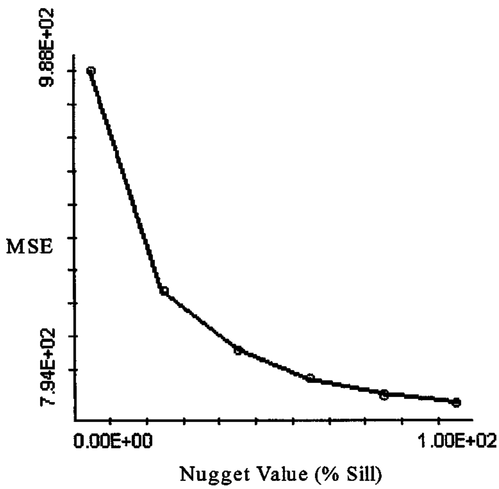


Figure 9. Plot of mean square error (MSE) versus nugget value for nitrate. Larger nuggets yield less error.

DISCUSSION

Mean Squared Error

Earlier figures (Figs. 4 and 9) demonstrate the influence of nugget value as a percentage of total sill on mean squared error. In the case of the Landsat TM data, best estimation performance is realized when the nugget value is zero. In contrast, best estimation performance is realized for the nitrate data when the nugget and sill values are equal. These conclusions resulted from using the 10 nearest neighboring sampling locations when kriging each point, both data sets.

This invokes an obvious question. What happens to error when more neighboring data locations are included when kriging each point? Several experiments are conducted as a test (Tables 1 and 2). Note that experiments on the Landsat TM data rely on 6 $\times$ (every sixth pixel and every sixth row) resampled data. Both experiments (Tables 1 and 2) yield results that are similar to the relative kriging performance that is based on using the 10 closest sampling locations.

Nitrate Data and the Robustness of Kriging

A highly skewed distribution is indicated for the nitrate data (Fig. 5). Application of kriging to such data seems contraindicated. Yet, kriging is adaptable to nonnormal data distributions provided the kriging neighborhood is constricted. The fact that kriging with zero nugget is the poorest model for these data is not related to their distribution. Rather, the variogram (Fig. 8) indicates a substantial nugget value. In fact, an argument can be made for a nugget-effect variogram model for these data. Indeed, estimation results (Fig. 9 and Table 2) show that a nugget-effect model is best for these data.

Visualization and the Human Mind

This paper emphasizes visualization when evaluating the outcome of spatial analysis. Aesthetic qualities of a resultant image, moreover their consequential

Table 1. Mean Squared Error as a Function of Kriging Neighborhood, Landsat TM Data

	Nugget (% sill)				
Neighborhood (N)	0	20	40	60	100
10	52	52	53	54	54
25	52	54	57	59	62
50	52	53	58	62	71

Table 2. Mean Squared Error as a Function of Kriging Neighborhood, Nitrate Data

	Nugget (% sill)				
Neighborhood (N)	0	20	40	60	100
25	993	849	807	784	770
50	1002	855	812	788	796

appeal to a viewer, can be a function of the brain's reaction to an image and not due to actual components of data displayed in the image. One way to test whether the difference between two images is substantial is to subtract one image from another and examine the resultant difference image. Such a difference image is shown earlier (Fig. 3(F)). Subtle differences in information content between images can substantially influence a brain's reaction to them.

CONCLUSION

A zero-valued nugget suggests that the spatial data it represents are error-free (not contaminated by white noise). Restating this implication, such a nugget value suggests that all spatial scales down to the most minute are sampled sufficiently and consequently are represented in the sample data. It is such a nugget value that, depending on sampling geometry and number of nearest, neighboring data locations that are used for estimation, causes negative weights to be associated with data locations in the kriging neighborhood that are more distant from the estimation location. The very closest data locations are boosted in value by positive weights that collectively sum to a value exceeding one. This is analogous to high-boost filtering in digital image processing that results in a sharpening of an image due to amplification of higher spatial frequencies.

A zero-valued nugget further suggests that high spatial frequencies in a set of data are an actual characteristic of a spatial phenomenon and not noise. Consequently, the N collective weights representing a mixture of positive and negative values work to boost these high frequencies. Visually, this weighting scheme yields a much sharper image of the actual data. In the case of the Landsat TM data, the visual outcome is substantially better in comparison to outcomes resulting from larger nugget values. But, in the case of the nitrate data, boosting high frequencies results in diminished estimation quality. For these data, the higher the nugget value is, the lower is the mean squared error. The variogram for these data indicates a substantial nugget value. This implies that smaller scale spatial variability is not well represented in the sample data, consequently weighting these data during estimation as if these smaller scales are present results in higher error.

That negative weights may occur in kriging for certain variogram parameters must be understood, moreover accommodated. Artifacts in a kriging outcome may be attributable to negative weights. These artifacts may also be related to sampling geometry and how kriging is implemented for data estimation. For some data sets, such as the Landsat TM data, a zero-valued nugget with associated negative kriging weights can substantially improve the visual outcome of estimation.

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