Kriging in a Finite Domain[1]

Clayton V. Deutsch[2,3]

*Adopting a random function model {Z(**u**), **u** ∈ study area A} and using the normal equations (kriging) for estimation amounts to assume that the study area A is embedded within a infinite domain. At first glance, this assumption has no inherent limitations since all locations outside A are of no interest and simply not considered. However, there is an interesting and practically important consequence that is reflected in the kriging weights assigned to data contiguously aligned along finite strings; the weights assigned to the end points of a string are large since the end points inform the infinite half-space beyond the string. These large weights are inappropriate when the finite string has been created by either stratigraphic/geological limits or a finite search neighborhood. This problem will be demonstrated with numerical examples and some partial solutions will be proposed.*

KEY WORDS: kriging, ergodicity, stratigraphic limits, finite domain.

INTRODUCTION

Two commonly encountered situations where finite strings of contiguously aligned data are used in kriging are shown on Fig. 1. In the first case, when strings of measurements taken along a drillhole are truncated by geological or stratigraphic boundaries, the study area *A* is clearly finite. In the second case, when strings of data are truncated by the boundaries of a local search ellipsoid, the area *A* may be infinite but the local neighborhood is not.

Figure 2 illustrates the counter-intuitive weighting scheme that will result when kriging (Journel and Huijbregts, 1978; Matheron, 1971) with a finite string of data. The profile of the ordinary kriging weights is shown next to the string. The variogram is a common spherical model with a range equal to the length of the string. Note that the point being estimated is beyond the range of the variogram and yet the implicit declustering of kriging causes the weights to change considerably along the vertical extent of the string with the outermost samples receiving a disproportionately large weight. Further note that the kriging

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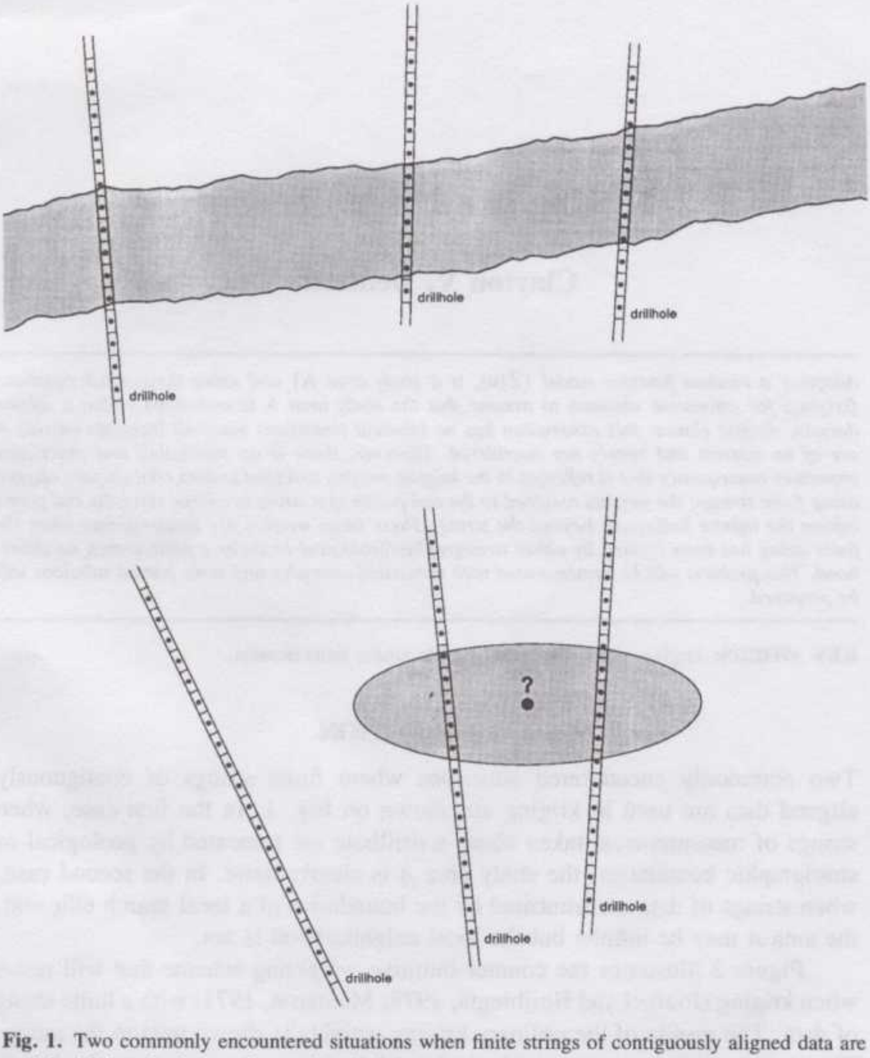

Fig. 1. Two commonly encountered situations when finite strings of contiguously aligned data are used in kriging. In the top figure, the shaded area represents a stratigraphic layer of interest. The shaded area in the bottom figure represents the limits of a local search neighborhood.

weights will remain unchanged as the point being estimated moves further away. Kriging yields this type of weighting because of the implicit assumption that the data are within an infinite domain—the outermost data inform the infinite half-space beyond the data string and hence receive greater weights. As the relative nugget effect increases the weight given to each end point decreases; that is, the central samples are considered relatively less redundant.

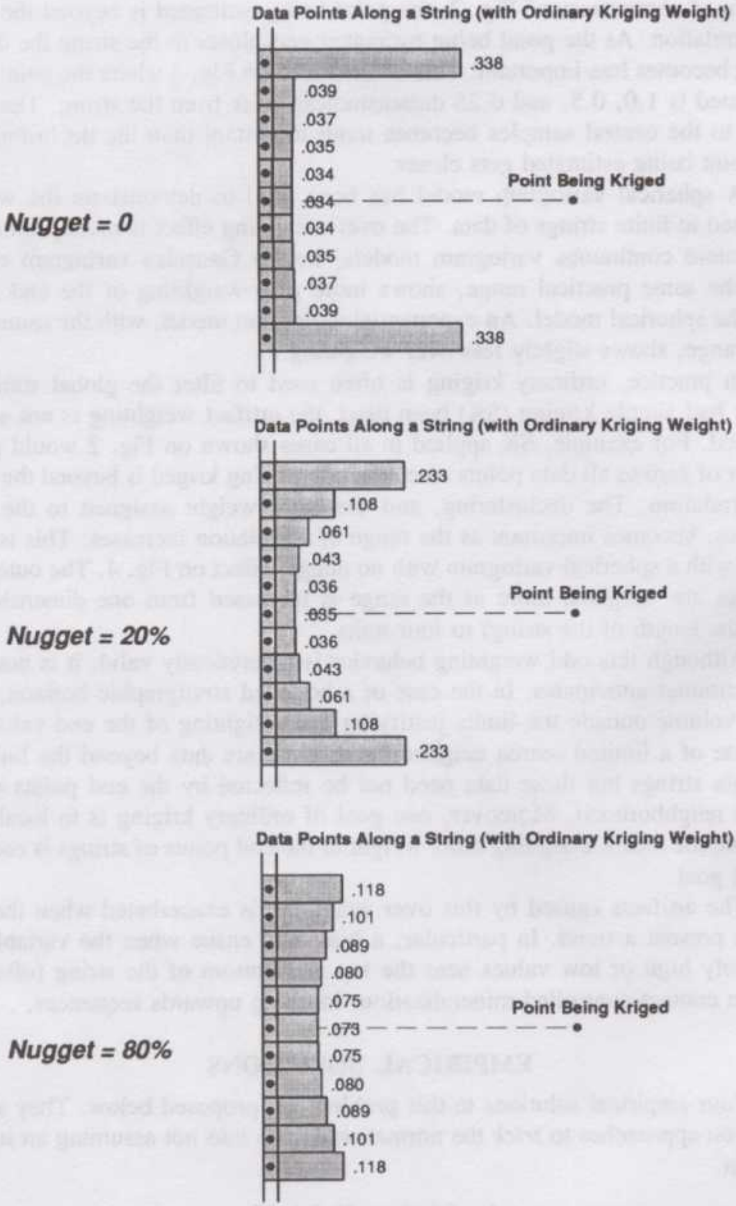

Fig. 2. A typical situation where the point being kriged is one or more dimensionless distance units (one dimensionless unit is the length of the finite string) away from the string, the spherical variogram has a range equal to one dimensionless unit, and there are 11 equally spaced data points along the string.

In all three cases of Fig. 2, the point being estimated is beyond the range of correlation. As the point being estimated gets closer to the string the declustering becomes less important. This is illustrated on Fig. 3 where the point being estimated is 1.0, 0.5, and 0.25 dimensionless units from the string. The proximity to the central samples becomes more important than the declustering as the point being estimated gets closer.

A spherical variogram model has been used to demonstrate the weights assigned to finite strings of data. The over-weighting effect is more pronounced with more continuous variogram models, i.e., a Gaussian variogram model, with the same practical range, shows more over-weighting of the end points than the spherical model. An exponential variogram model, with the same practical range, shows slightly less over-weighting.

In practice, ordinary kriging is often used to filter the global stationary mean; had simple kriging (SK) been used, the artifact weighting is not as pronounced. For example, SK applied in all cases shown on Fig. 2 would give a weight of zero to all data points since the point being kriged is beyond the range of correlation. The declustering, and the extra weight assigned to the outer samples, becomes important as the range of correlation increases. This is illustrated with a spherical variogram with no nugget effect on Fig. 4. The outermost samples are weighted more as the range is increased from one dimensionless unit (the length of the string) to four units.

Although this odd weighting behavior is theoretically valid, it is not what a practitioner anticipates. In the case of a bounded stratigraphic horizon, there is no volume outside the limits justifying overweighting of the end values. In the case of a limited search neighborhood, there are data beyond the limits of the data strings but these data need not be reflected by the end points of the search neighborhood. Moreover, one goal of ordinary kriging is to locally re-estimate the mean; assigning more weight to the end points of strings is contrary to that goal.

The artifacts caused by this over weighting is exacerbated when the data values present a trend. In particular, a bias may ensue when the variable has relatively high or low values near the top and bottom of the string (often the case in contact-controlled mineralization, in fining upwards sequences, . . .).

EMPIRICAL SOLUTIONS

Four empirical solutions to this problem are proposed below. They are all based on approaches to *trick* the normal equations into not assuming an infinite domain.

An Obvious Quick Fix

One obvious solution is to use only two samples from any one string of data. In this case, both samples are equally redundant and equally informative of the *infinite* domain. The principle disadvantage of this approach is that this

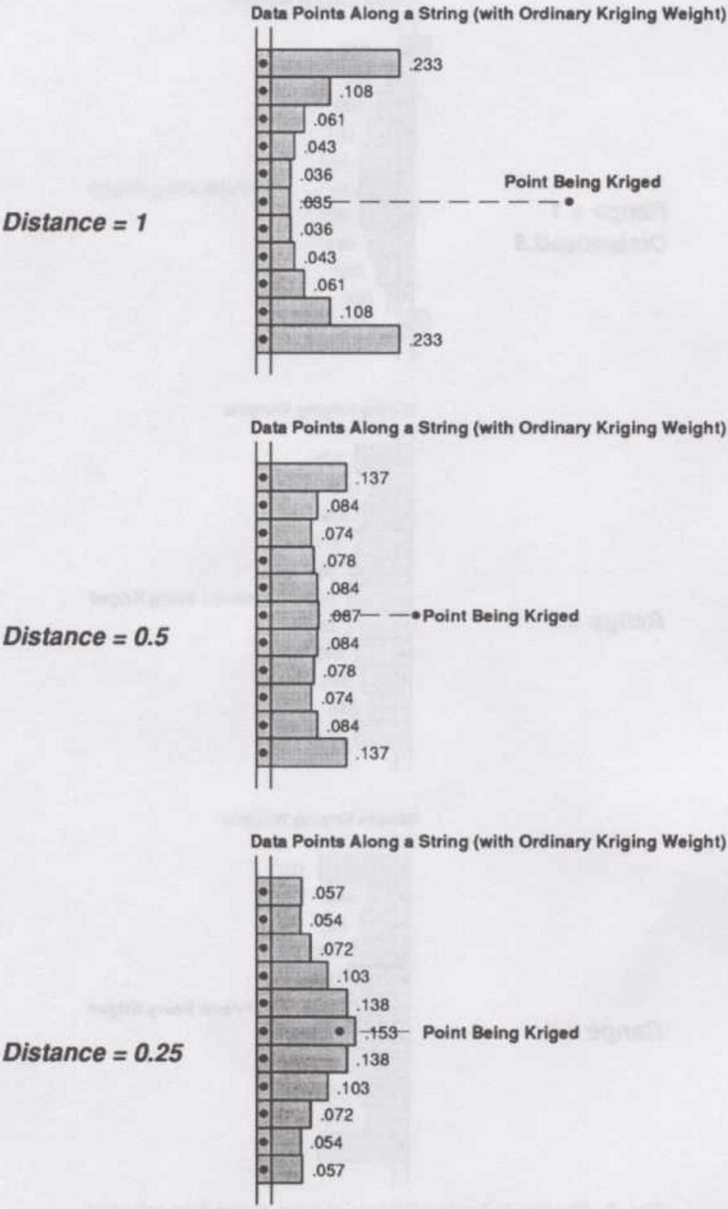

Fig. 3. The kriging weights are seen to change considerably as the point being estimated nears the string. The kriging weights are illustrated when the point is 1.00, 0.50, and 0.25 dimensionless units from the string. The nugget effect is 20% in all cases.

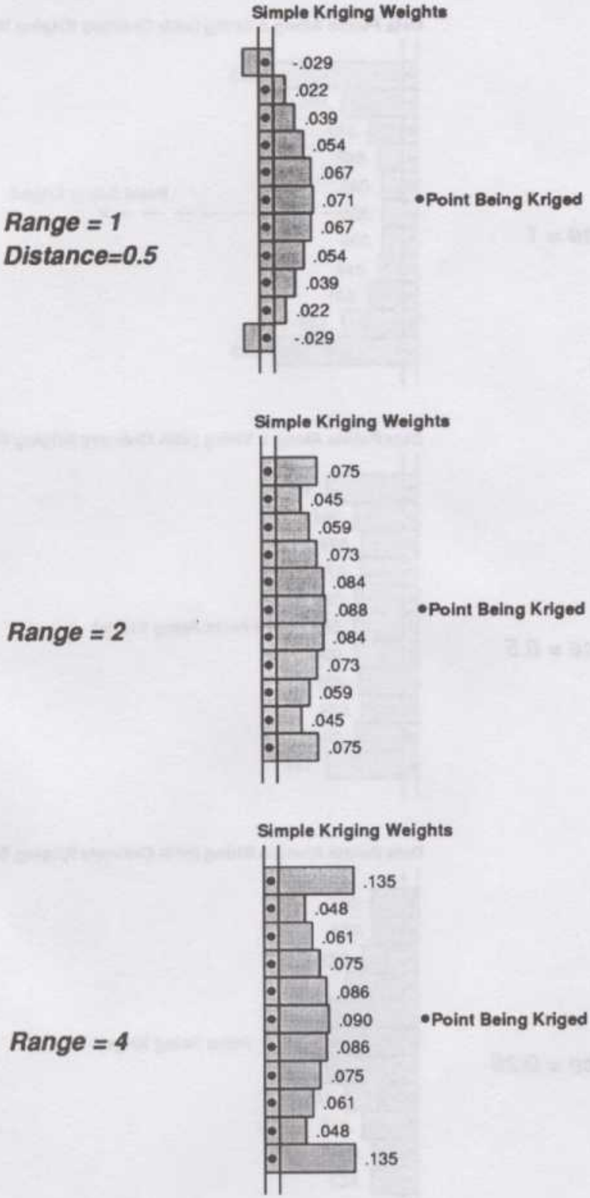

Fig. 4. The simple kriging (SK) weights are shown for a spherical variogram model as the range is increased from one dimensionless unit to four dimensionless units. The nugget effect is zero and the distance of the point to the string is 0.5 dimensionless units in all cases.

may result in too few data to allow a reliable estimate at each unsampled location.

Extend the String

The string can be extended by adding *phantom* data at each end and then removing the weights assigned to the phantom data. A larger ordinary kriging system with non-existent samples at each end point is solved, then the weights assigned to the non-existent samples are discarded and the remaining weights are restandardized to sum to 1.0. There are a number of implementation problems with this approach, some of these being:

- The "second" outer points may also receive a significant weight. Adding phantom data (with the same volume support) may not entirely remove the artifact weighting.
- The local direction vector of the string must be known so that the phantom samples are assigned the correct location.
- Any given data configuration may contain multiple strings with different numbers of data in each string. Adding phantom data with the same *support* to the end of each string would disproportionately weight the smaller strings. Ideally, the phantom samples would have a variable support dependent on the number of samples in a string.
- An octant search could generate multiple strings from the same drillhole or well. It would not be straightfoward to check all pathological cases of this situation. Moreover, missing samples in a string would further complicate the situation.

Use Simple Kriging:

The effect is not as pronounced with simple kriging; therefore, SK with the mean determined by local estimation over a finite volume V of interest could be applied. The idea is to proceed stepwise:

Identify the local mean to the ordinary kriging of a finite volume V centered near the point being estimated. Given n nearby data $z(\mathbf{u}_\alpha)$, $\alpha = 1, \ldots, n$, an estimate of the local mean is written as:

$$m^* = \sum_{\alpha=1}^{n} \nu_\alpha z(\mathbf{u}_\alpha) \tag{1}$$

with m^* the local mean, $z(\mathbf{u}_\alpha)$, $\alpha = 1, \ldots, n$, the local data, and ν_α, $\alpha = 1, \ldots, n$, the weights given by the ordinary kriging system:

$$\begin{cases} \sum_{\beta=1}^{n} \nu_\beta(\mathbf{u})C(\mathbf{u}_\beta - \mathbf{u}_\alpha) + \mu_{oV} = \overline{C}(V, \mathbf{u}_\alpha), \quad \alpha = 1, \ldots, n \\ \sum_{\beta=1}^{n} \nu_\beta(\mathbf{u}) = 1 \end{cases} \tag{2}$$

with $\overline{C}(V, \mathbf{u}_\alpha) = 1/|V| \int_V C(\mathbf{u} - \mathbf{u}_\alpha)d\mathbf{u}$ being the average V-data location covariance.

Compute the local estimate with simple kriging using the local mean estimated from the prior ordinary kriging. The estimate at local **u** is written as:

$$z^*(\mathbf{u}) = \sum_{\alpha=1}^{n} \xi_\alpha[z(\mathbf{u}_\alpha) - m^*] + m^* \tag{3}$$

with $\xi_\alpha, \alpha = 1, \ldots, n$ the simple kriging weights given by the SK system:

$$\sum_{\beta=1}^{n} \xi_\beta(\mathbf{u})C(\mathbf{u}_\beta - \mathbf{u}_\alpha) = C(\mathbf{u} - \mathbf{u}_\alpha), \; \alpha = 1, \ldots, n \tag{4}$$

The final weight assigned to each of the local data may be obtained from expression (3) above:

$$z^*(\mathbf{u}) = \sum_{\alpha=1}^{n} \xi_\alpha \left[z(\mathbf{u}_\alpha) - \sum_{\beta=1}^{n} \nu_\beta z(\mathbf{u}_\beta) \right] + \sum_{\beta=1}^{n} \nu_\beta z(\mathbf{u}_\beta)$$

Thus, the final weight $\lambda_\alpha, \alpha = 1, \ldots, n$, assigned to each datum is:

$$\lambda_\alpha = \xi_\alpha + \left[1 - \sum_{\beta=1}^{n} \xi_\beta \right] \cdot \nu_\alpha \tag{5}$$

Note that the sum of the final weights $\Sigma_{\beta=1}^{n} \lambda_\alpha$ is equal to one, i.e., the estimator $z^*(\mathbf{u})$ (3) has the same unbiasedness properties as ordinary kriging. Further, note that as the sum of the SK weights ξ_α approaches 1.0 the effect of the prior ordinary kriging of the mean is filtered from the estimate.

The hope with this approach is that the weights for estimating a finite block V will not show the same artifact overweighting of the outermost points on the string. However, the artifact overweighting is due to the declustering in the left hand side of the kriging system (2) and the final weights λ_α still show the artifact over-weighting. This is illustrated on Fig. 5 where a zero nuggest effect spherical variogram with a range equal to the length of the string has been used. The kriging weights for the block mean, at the top, show a significant overweighting of the outermost samples. The simple kriging weights, in the center of the figure, do not show the effect because of the relatively short range and the importance of the right hand side *closeness* covariance values $C(\mathbf{u} - \mathbf{u}_\alpha), \alpha = 1, \ldots, n$. The final weights, at the bottom of the figure, are a combination of the two previous sets of weights.

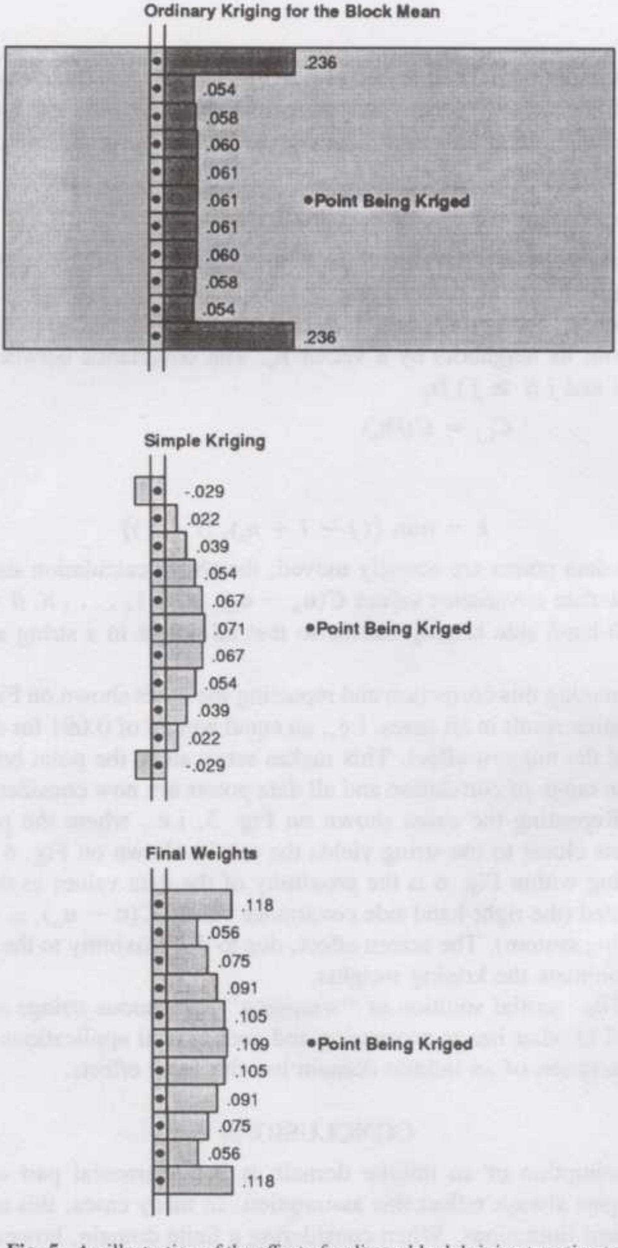

Fig. 5. An illustration of the effect of ordinary block kriging to estimate the local mean followed by point a simple kriging using that local mean. The variogram is a spherical model with no nugget effect and a range equal to one dimensionless unit (the length of the data string). The block V is one unit by two units and the point being estimated is 0.5 unit from the string.

The combination of ordinary kriging to estimate m^* and then simple kriging (with m^*) to estimate the local value does not entirely remove the extra weight given to the end points. However, this overweighting is significantly less when using ordinary kriging.

Wrap the String

Another idea is to wrap each finite string of data, i.e., connect the two end points when building the declustering (left hand side) kriging matrix[4].

Consider n_s contiguous data $i = 1, \ldots, n_s$, aligned in a string each separated from its neighbors by a vector $\mathbf{h}_s$. The covariance between any two data points i and j ($i \geq j$) is,

$$C_{i,j} = C(k\mathbf{h}_s)$$

with:

$$k = \min \{(j - i + n_s), (i - j)\} \tag{6}$$

None of the data points are actually moved; the above calculation simply modifies the data–data covariance values $C(\mathbf{u}_\alpha - \mathbf{u}_\beta)$, $\alpha = 1, \ldots, n$, $\beta = 1, \ldots, n$, in the left-hand side kriging matrix so that all points in a string are equally redundant[5].

Implementing this correction and repeating the cases shown on Fig. 2 yields exactly the same result in all cases, i.e., an equal weight of 0.091 for all samples regardless of the nuggest effect. This makes sense since the point being kriged is beyond the range of correlation and all data points are now considered equally redundant. Repeating the cases shown on Fig. 3, i.e., where the point being estimated gets closer to the string yields the results shown on Fig. 6. The only thing changing within Fig. 6 is the proximity of the data values to the location being estimated (the right-hand side covariance values $C(\mathbf{u} - \mathbf{u}_\alpha)$, $\alpha = 1, \ldots, n$ in the kriging system). The screen effect, due to the proximity to the unknown, is seen to dominate the kriging weights.

The *ad hoc* partial solution of "wrapping" continuous strings of data has been adopted in other image processing and geophysical applications where the implicit assumption of an infinite domain has the same effects.

CONCLUSIONS

The assumption of an infinite domain is a fundamental part of kriging. Kriging weights always reflect this assumption. In many cases, this assumption has no inherent limitations. When considering a finite domain, however, that is

[4] Wrapping the data is equivalent to the "circular stationary" decision adopted by certain techniques in statistics and geophysics (Aki and Richards, 1980).

[5] Interestingly, this correction imparts a perfect banding to the data-data covariance matrix. This may allow a faster numerical inversion.

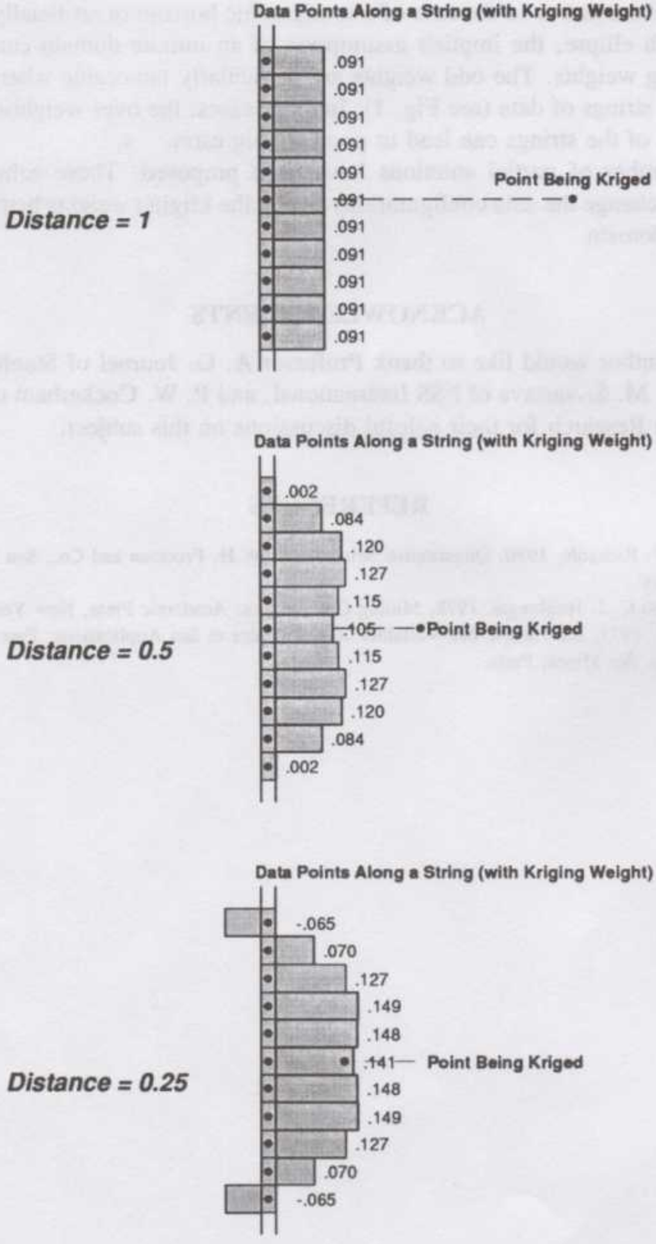

Fig. 6. The same cases as Fig. 3 are shown on this figure. The difference is that the declustering of kriging has been removed. The kriging weights are seen to change considerably as the point being kriged nears the data.

physically bounded as in the case of a stratigraphic horizon or artificially created by a search ellipse, the implicit assumption of an infinite domain can lead to odd kriging weights. The odd weights are particularly noticeable when dealing with finite strings of data (see Fig. 1). In these cases, the over-weighting of the end points of the strings can lead to poor kriging estimates.

A number of partial solutions have been proposed. These solutions all attempt to change the data configurations so that the kriging weights better reflect the finite domain.

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