A Recall of Factorial Kriging with Examples and a Modified Version of `kt3d`

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Factorial kriging is a technique that aims to either extract features for separate analysis or filter features from spatial data. The technique was proposed by Matheron in the early days of geostatistics. Factorial kriging is of greatest interest to geophysicists and those concerned with image analysis; however, there are a number of applications in geostatistics. This note recalls the theory and practice of factorial kriging with a version of `kt3d` *that implements a flexible version of factorial kriging.*

Setting

Consider a regionalized variable $\{Z(\mathbf{u}),\ \mathbf{u}\ in\ A\}$. We adopt a linear model of regionalization, that is, the $Z(\mathbf{u})$ variable consists of a sum of independent factors and a non-stationary mean:

$$Z(\mathbf{u}) = \sum_{l=0}^{L} a_l Y_l(\mathbf{u}) + m(\mathbf{u}) \tag{1}$$

The $L+1$ standard factors $Y_l(\mathbf{u})$ all have a mean of 0 and a variance of 1. By convention, the 0^{th} factor is reserved to an uncorrelated pure nugget effect factor. The a_l parameters are stationary, that is, they do not depend on location. The mean and variance of the $Z(\mathbf{u})$ variable are given by:

$$E\{Z(\mathbf{u})\} = E\left\{\sum_{l=0}^{L} a_l Y_l(\mathbf{u}) + m(\mathbf{u})\right\} = \sum_{l=0}^{L} a_l E\{Y_l(\mathbf{u})\} + m(\mathbf{u}) = m(\mathbf{u}) \tag{2}$$

$$Var\{Z(\mathbf{u})\} = \sum_{l=0}^{L} a_l^2 Var\{Y_l(\mathbf{u})\} + 0 = \sum_{l=0}^{L} a_l^2$$

The variance of $Z(\mathbf{u})$ follows such a simple expression because $m(\mathbf{u})$ is a constant and the Y factors are standard and independent. These characteristics of m and Y also lead to a straightforward expression for the variogram of the $Z(\mathbf{u})$variable:

$$\gamma(\mathbf{h}) = \sum_{l=0}^{L} a_l^2 \gamma_l(\mathbf{h}) \tag{3}$$

The $Z(\mathbf{u})$ regionalized variable is fully specified by $m(\mathbf{u})$, the $L+1$ a_l values, and the $L+1$ variograms $\gamma_l(\mathbf{h})$. We do not, of course, have any direct measurements of the Y factors. Nor do we have any direct measurements of the a_l parameters that specify the importance (variance explained) by each of the factors. We have access to the mean, variance and variogram of Z. We potentially have access to an understanding of the Z variable and the processes that led to the current regionalization. The mean and variance are unlikely to help us understand the factors, but the variogram may provide a means to distinguish the factors. We will be able to better distinguish the factors if the constituent variograms $\gamma_l(\mathbf{h})$ are different from one another. In fact, an essential feature of factorial kriging is to use the fitted nested structures to identify the factors. The reasonableness of factorial kriging depends entirely on the fitted nested structures. Ideally, this variogram is based on fitting a well-defined experimental variogram; however, we could use an arbitrary model based on an understanding of the variable under consideration.

Factorial Kriging

The aim of factorial kriging is to estimate each factor individually, that is, extract different features. Another aim of factorial kriging is to filter certain factors. Factorial kriging consists of estimating the *L+2* factors that constitute the random variable. The true factors:

$$m(\mathbf{u}), \left(Z_l(\mathbf{u}) = a_l Y_l(\mathbf{u})\right), l = 0, \ldots, L \tag{4}$$

These factors are estimated by linear combinations of the original data ($z(\mathbf{u}_i), i=1,\ldots,n$):

$$m^*(\mathbf{u}) = \sum_{i=1}^{n} \lambda_{m,i} z\left(\mathbf{u}_i\right) \tag{5}$$

$$z_l^*(\mathbf{u}) = \sum_{i=1}^{n} \lambda_{l,i} z\left(\mathbf{u}_i\right), \quad l = 0, \ldots, L$$

The weights are location dependent, but the (**u**) has been dropped for cleaner notation. There are no obvious reasons why simple kriging or cokriging could not be used; however, the conventional approach to factorial kriging is to adopt an ordinary kriging paradigm. The constraints on the weights are established to ensure unbiasedness:

$$\sum_{i=1}^{n} \lambda_{m,i} = 1 \tag{6}$$

$$\sum_{i=1}^{n} \lambda_{l,i} = 0, \quad l = 0, \ldots, L$$

The constraint that the sum of the weights in the estimation of a factor equals zero is strong. This is reminiscent of ordinary cokriging where the sum of weights to secondary data are constrained to zero to ensure unbiasedness. This possible limitation will be revisited below.

The estimation variances are minimized subject to the constraints given in (6) leading to the factorial kriging equations:

$$\sum_{i=1}^{n} \lambda_{m,i} C(\mathbf{u}_i - \mathbf{u}_j) - \mu_m = 0, \; i = 0, \ldots, n \qquad \sum_{i=1}^{n} \lambda_{m,i} = 1 \tag{7}$$

$$\sum_{i=1}^{n} \lambda_{l,i} C(\mathbf{u}_i - \mathbf{u}_j) - \mu_l = C_l(\mathbf{u}_i - \mathbf{u}), \; i = 0, \ldots, n \qquad \sum_{i=1}^{n} \lambda_{l,i} = 0, \quad l = 0, \ldots, L$$

Note that the right hand side covariances on the estimation of the mean (first equation) are zero since the mean is a constant albeit unknown. The right hand side covariances in the estimation of each factor are the covariance corresponding to the particular nested structure/factor being estimated. This is a result of the factors being independent. The redundancy between the data in the left hand side of the kriging equations is the covariance between the *Z* data, that is, the sum of all nested structures. These *L+2* sets of equations are solved to arrive at the *L+2* estimates of the different factors. It is interesting to note that the sum of the estimates is the conventional ordinary kriging estimate:

$$z_{OK}^*(\mathbf{u}) = m^*(\mathbf{u}) + \sum_{l=0}^{L} z_l^*(\mathbf{u}) \tag{8}$$

Like all kriging estimators, the estimates will be smooth in presence of sparse data. This will undermine the usefulness of the results for interpretation.

Implementation Details

The *itrend* option in kt3d permits estimation of the variable (*itrend=0*) or the mean (*itrend=1*). Estimation of the mean is a form of factorial kriging. A third option was added: *itrend=2*. This option specifies factorial kriging. Ordinary kriging will be performed even if it is not specified. All factors are estimated and the estimate is constructed with each factor filtered from the estimation.

The technique could be applied for exhaustive data; however, because of the unbiasedness constraints used, the estimate of the mean will be the collocated gridded data value. The factors will be positive and negative (because they must sum to one) and the weights will be constant for all locations.

A First Example

A synthetic example is shown first to show how the approach works. A synthetic 256x256 2-D Gaussian variable was simulated with a small nugget effect (10%) and two isotropic spherical structures equally explaining the remaining 90% of the variability. The ranges of the spherical structures are 16 and 64 units. A search radius of 64 units and a large number of previously simulated grid nodes (50) were used to ensure that the simulated values reproduce both nested structures. Data were sampled from the reference grid at a very close 5x5 spacing. The reference grid and sample data are shown on Figure 1.

As developed above, conventional factorial kriging is based on ordinary kriging. The sum of the estimate of each factor adds up to the ordinary kriging estimate. This was checked. The ordinary kriging estimates are shown on Figure 2. The reference variogram was used. The map appears close to the reference true values because of the dense grid of sample data. Note that the ordinary kriging estimates are smoother than the reference values – a characteristic property of all kriging. Note also that the data are reproduced exactly, but with an apparent discontinuity because of the nugget effect.

The Factorial kriging in kt3d estimates the mean and each factor independently and the estimate filtering each factor in turn. In this example there is the mean and three factors. Maps of the factors are shown on Figure 3. Although the nugget effect map looks constant, it is not. There is a discontinuity at each data point. Note that the estimate of the mean reflects the most variability because of the unbiasedness constraints.

Figure 4 shows the estimates with each factor filtered from the estimate. In the first case (upper left), the mean is filtered, then the nugget effect and the two nested structures. Note that the map filtering the nugget effect does not show the discontinuities hear the data values. The results with the short and long scale structures filtered make sense, that is, we reveal more long range structures when we filter the short scale and we reveal more short scale structures when we filter the long scale.

This example shows how factorial kriging works. It is interesting to look at each factor and at the maps filtering each factor. Although the mean is not supposed to be variable, estimates of the mean show almost all of the variability even with a large dense grid of data. This is a result of the unbiasedness constraints used in ordinary factorial kriging.

A Second Example

This example is known to many readers. It was originally published in Deutsch's Ph.D. thesis (1992) and is based on a scanned rock acquired by André Journel in 1990. The data consist of a 164x85 grid of gray scale values that have been transformed to a standard normal distribution.

All distances are relative to the discretization units of the image with the image being 164 pixels by 85 pixels. The variogram model consists of four nested structures with (h_1, h_2) being the coordinates in the two directions corresponding to the sides of the image. The spherical and exponential structures are classical in geostatistics. The dampened hole effect cosine model is not as commonly used; it is defined as:

$$DH_{d,a}(h) = 1.0 - \exp\left(\frac{-ha}{d}\right)\cos(ha)$$

There are four components in the semivariogram model that correspond to factors in the interpretation of factorial kriging:

1. A short scale anisotropic spherical structure that explains 40% of the total variability (the longer range is in the horizontal h_2 direction and the shorter range is in the vertical h_1 direction).
2. A second short scale anisotropic spherical structure (with a more pronounced anisotropy along the same horizontal and vertical directions) that explains an additional 20% of the variability,
3. A third anisotropic long range exponential structure (the range parameter is 40.0, thus, the effective range is 120.0 in the horizontal direction and 0.0 in the vertical direction) that explains 40% of the variability, and
4. Finally, a dampened hole effect model in the vertical direction to account for the periodicity.

Factorial kriging leads to six factors: the mean, the nugget effect and the four specified above. The variogram model has no nugget effect effect, but the program automatically treats the mean and nugget effect. Figure 6 shows the factors when kriging with 16 data. The ordinary kriging estimates are, of course, the values in the initial image – kriging is exact. The mean explains most of the variance. The amount of variance used in each nested structure affects the variability of the factor. Some features are evident, for example, the anisotropic exponential structure does reveal more continuity in the horizontal direction. There are quite a few large negative values in the factor representing the dampened hole effect.

Conclusions

Factorial kriging is a well established technique that has been available for many years. The theory of conventional ordinary factorial kriging is recalled and an implementation in the GSLIB kt3d program is described. The program is of interest for geophysical and image analysis applications where there is a goal to filter noise or other artifact features from certain data sources.

There are some evident areas of future work. The most important is to relax the unbiasedness constraints. Forcing the sum of the weights to equal zero in the estimation of each factor amounts appears to underestimate the contribution of each factor. The mean explains the majority of the variance even with exhaustive measurements. There is also the inherent smoothing of kriging with sparse data and the possibility of factorial simulation.

Significant work has been done in multivariate factorial (co)kriging, which warrants further investigation and implementation in, perhaps, cokb3d.

References

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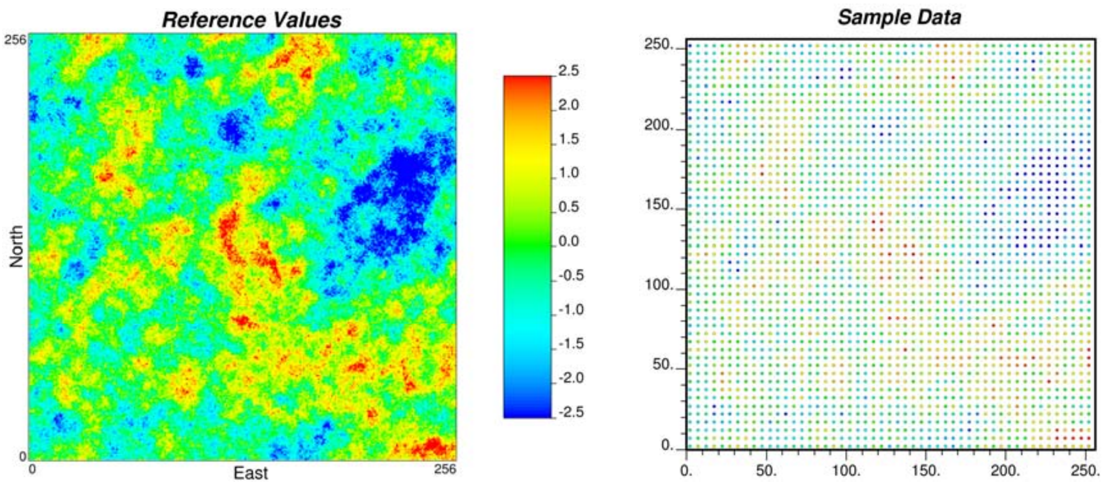


Figure 1: Reference values and sample data for first example.

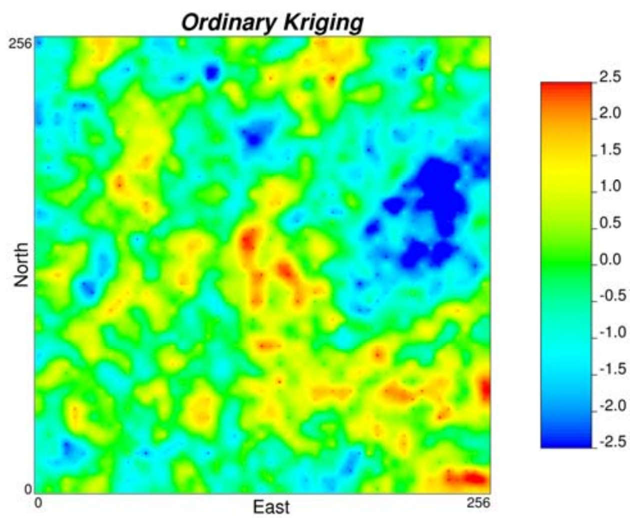


Figure 2: Ordinary kriging for first example.

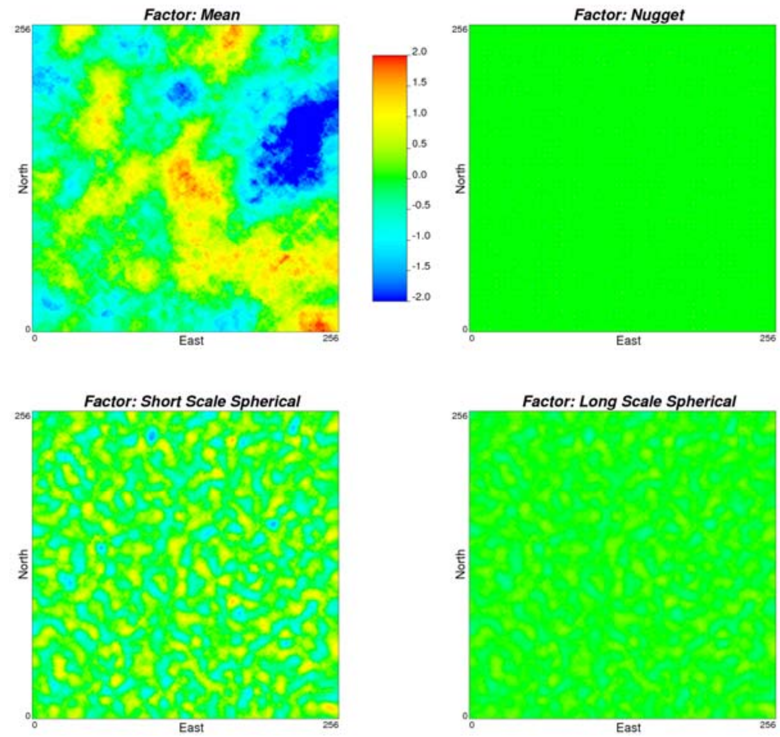


Figure 3: Factors for the first example.

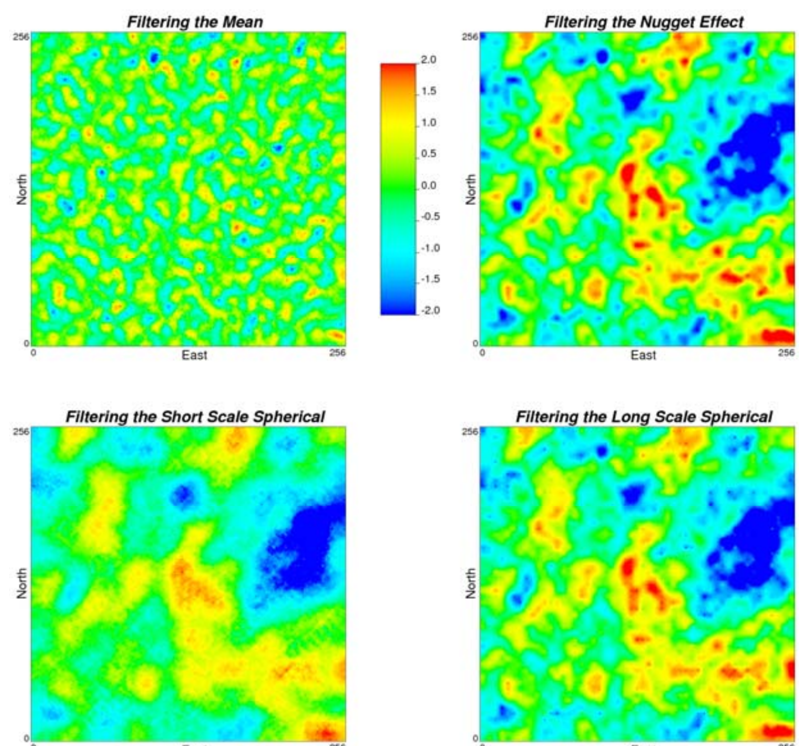
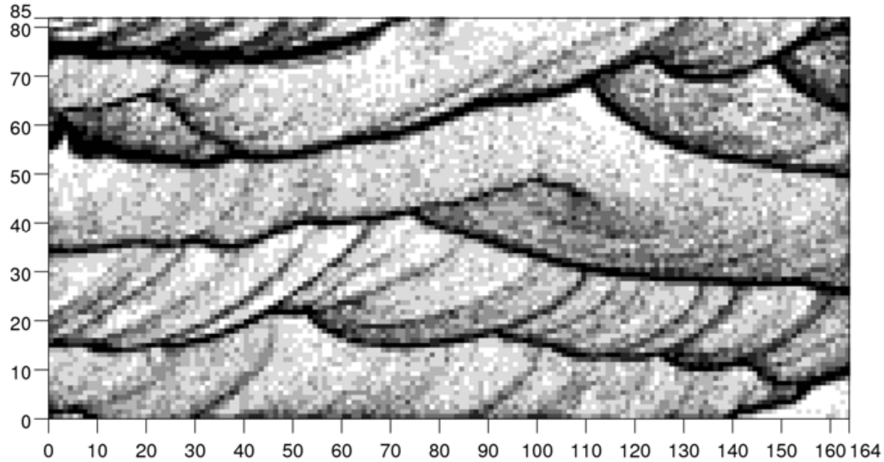
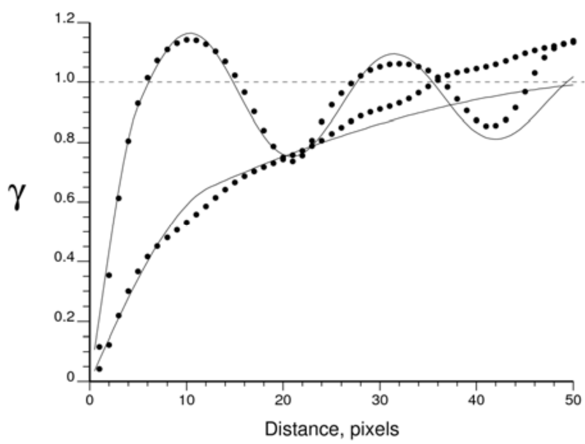


Figure 4: Filtering each factors for the first example.





$$
\begin{aligned}
\gamma_Y(\mathbf{h}) \;=\;& 0.45 \cdot Sph\left(\sqrt{\frac{h_1^2}{2.0^2} + \frac{h_2^2}{5.0^2}}\right)\\
+\;& 0.22 \cdot Sph\left(\sqrt{\frac{h_1^2}{0.5^2} + \frac{h_2^2}{5.0^2}}\right)\\
+\;& 0.45 \cdot Exp\left(\sqrt{\frac{h_1^2}{0.00001^2} + \frac{h_2^2}{40.0^2}}\right)\\
+\;& 0.27 \cdot DH_{17.0,0.298}\left(\sqrt{h_1^2}\right)
\end{aligned}
$$

Figure 5: Reference data and variogram for the second example.

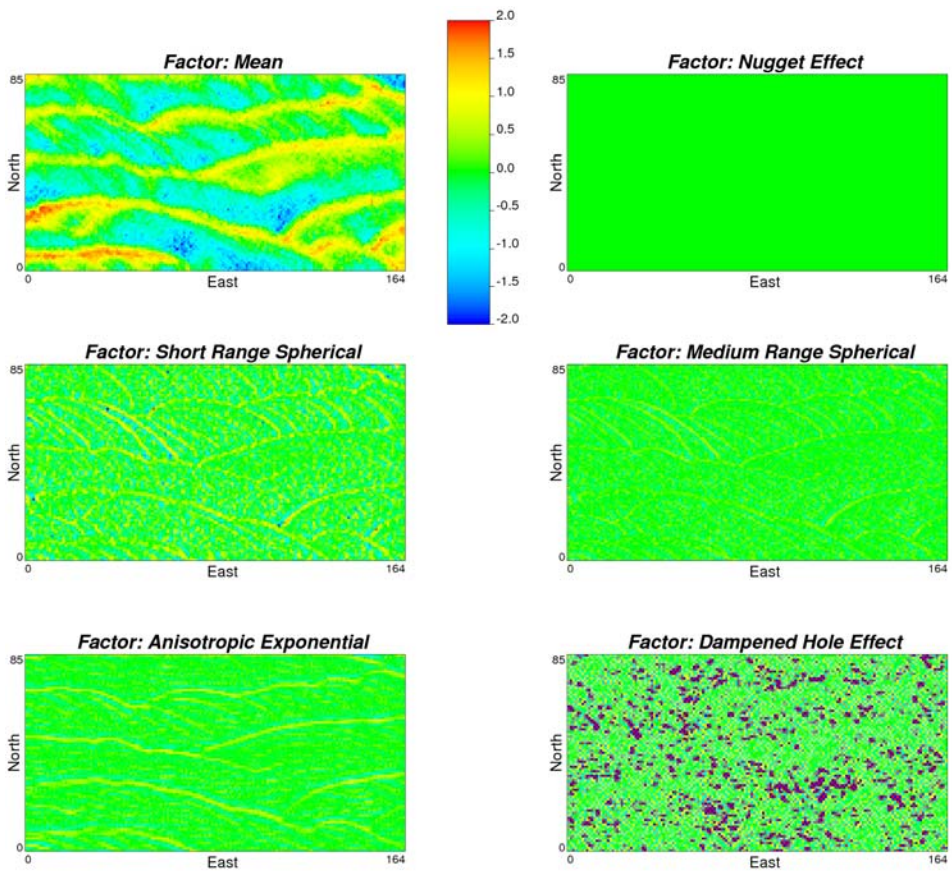


Figure 6: Factors for the second example.