A Program for Global Kriging in the Presence of Locally Varying Anisotropy

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Kriging with locally varying anisotropy allows geologic knowledge to be incorporated in the calculation of kriging estimates. Global kriging involves using all of the data to estimate at all locations. Combining these two methods provides a powerful estimation methodology. Geological knowledge can be incorporated in the kriging estimates while any artifacts due to a local search are removed by eliminating the search. A program called `kt3d_gl_lva` *combines these two methods and is documented herein.*

Introduction

Kriging in the presence of locally varying anisotropy (LVA) has been shown to be a useful method for incorporating expert knowledge into the kriging estimates (Boisvert and Deutsch, 2009a). The expert knowledge is incorporated by the use of locally varying anisotropy. Locally varying anisotropy is a field where locally varying directions and magnitudes of continuity are specified. Global kriging refers to using all of the data to estimate at all estimation locations. This eliminates the need for a search which in turn eliminates artifacts due to the search. This note briefly reviews the theory of kriging with LVA and the theory of global kriging as well as documenting a program, `kt3d_gl_lva`, which performs global kriging in the presence of LVA.

Kriging with LVA Review

Kriging consists of calculating distances between data and estimation locations which are converted to covariances using a variogram model. The covariances make up the kriging system of equations which minimizes the estimation error. This field of locally varying anisotropy modifies the distances between data and estimation locations. These distances are not necessarily linear or straight line distances; this methodology can consider non-linear paths between locations. The distances are determined by using the Dijkstra algorithm (Boisvert and Deutsch, 2008a). These distances account for the geological setting of the data.

Once these distances are known, the coordinates of the locations are embedded into a high dimensional space using multidimensional scaling (MDS). This is done to ensure that the kriging system of equations is positive definite (Boisvert and Deutsch, 2008b).

Once the locations have been embedded into the high dimensional space, the process of estimating at unknown locations can begin. At each unknown location, the following takes place (Boisvert and Deutsch, 2009b):

1. Determine the nearest *n* neighbors
2. Calculate the required *n* by *n* distance matrix
3. From the *n* by *n* distance matrix, calculate the covariance matrix
4. Solve the resulting system of equations to determine weights for each datum
5. Calculate the kriging mean and error variance

After each location has been estimated, the locations of the estimates are back-transformed to original Cartesian space to be written in typical GSLIB (Deutsch and Journel, 1998) style.

Global Kriging Review

Global kriging refers to using all of the data to estimate at every location (Neufeld and Wilde, 2005). With the traditional implementation of kriging, this would be very expensive computationally as a large system of equations would have to be built and solved at each unknown location. Global kriging is made feasible by the realization that the large left-hand side (LHS) matrix of data-to-data covariances is constant at all locations. As such, this matrix must only be built and inverted once. Also, because all of the data are used at every location, no search is performed. The lack of search means that no search artifacts are present.

Search Artifacts

Searching for nearby data to inform the estimate at the unknown location is a necessary part of the traditional implementation of kriging. The size and shape of the search is controlled by the user. Parameters such as search radii, search orientation, and minimum and maximum number of data to use determine which data are used to inform each estimate. Artifacts occur when the procession from one unknown location to another causes a change in the data used to inform the estimates. Proceeding from one unknown location to another can exclude a sample previously within the search window or include a sample previously outside the search window. This change in conditioning data can cause the solution to the kriging system of equations to vary significantly between adjacent locations. An example of this is shown in Figure 1. There are many instances in this figure where adjacent locations have significant difference in estimate values. The differences are due to changes in the data which fall within the search window.

Global Kriging in Presence of LVA

Kriging in the presence of locally varying anisotropy can be performed globally. This prevents artifacts that can arise from the search for nearby data in the high dimensional space. Once the data and unknown locations have been embedded in the high dimensional space, the n by n distance matrix is determined. It is populated by the multi-dimensional distances between data. From this distance matrix, the n by n covariance matrix is derived. The n by n covariance matrix is calculated only once and remains constant for all estimation locations. The right-hand side (RHS) covariance vector changes at each estimation location as it is comprised of the covariances between the data and the unknown location.

Solving Systems of Equations

There are a number of methods for solving systems of equations, depending on the characteristics of the system. Inverting the LHS matrix and multiplying this inverse by the RHS vector at each location is not necessarily the most efficient. This is particularly true with regard to the kriging system of equations which is symmetric and positive definite. These characteristics make the system amenable to being solved by the Cholesky factorization of the LHS matrix. This results in a triangular matrix. A system with a triangular matrix can be solved quickly in few operations.

Consider the kriging system $K\lambda = k$. The Cholesky factorization of K yields $K = R^TR$ such that R is upper triangular and has all main diagonal entries positive. Substituting into the previous equation yields $R^TR\lambda = k$. Let $y = R\lambda$. λ is unknown and therefore y is unknown also. However, y satisfies $R^Ty = k$. Since R^T is lower triangular, y can be determined by forward substitution (Cormen et al., 2009). Once y is determined, the upper triangular system $R\lambda= y$ is used to solve for λ by back substitution (Watkins, 2002).

Program

A program which performs global kriging in the presence of locally varying anisotropy is available. It is called `kt3d_gl_lva`. It reads in a data file and LVA field and calculates estimates using all of the data. An example parameter file is shown in Figure 2. The file with the input data is specified on line 6. The columns for the coordinates and variable are specified on line 7. Line 8 specifies the trimming limits while line 9 specifies whether to perform kriging on a grid or cross validation. If cross validation is performed, a drillhole ID must be specified. The debugging level is specified on line 10 with the debug file specified on line 11. The file for the kriged output is specified on line 12. Lines 13 to 15 specify the estimation grid. Line 16 specifies the file with the LVA field. Line 17 specifies the columns for the three angles and two ratios within the LVA field. Lines 18 to 20 specify the LVA grid. The number of offsets is specified on line 21. Using more offsets is recommended as paths will be smoother and shorter but this requires more memory and may be infeasible for large 3D models. Line 22 specifies whether to calculate the distances between locations or to read the previously calculated distances from a file. If the distances have already been calculated once, a significant speed advantage can be had by reading them from a file for subsequent runs. If the number of offsets, the grid, or the configuration of landmark points are changed the distances must be calculated again. Line 23 specifies the number of landmark points in x,y,z. The number of dimensions to use is specified on line 24. Specifying -1 indicates to use the maximum. Line 25 specifies the type of kriging to perform and the simple kriging mean. If the kriging type is negative, inverse distance is performed. Lines 26 and 27 specify the variogram. As the variogram is isotropic, no angles need be specified and one range is sufficient.

Conclusions

Kriging using locally varying anisotropy is a useful method for incorporating geologic knowledge in kriging estimates. The use of distances between points that are not necessarily straight-line distances allows the most relevant data to inform each estimation location. Global kriging, that is, kriging using all of the data at all locations, has the advantage of eliminating artifacts that can arise due to the search for nearby data. As kriging with locally varying anisotropy takes place in a high-dimensional coordinate system, it can be beneficial to eliminate the search for nearby data and use all of the data at every location. This eliminates any artifacts that may have been present using local search neighborhoods. A program called `kt3d_gl_lva` implements global kriging with locally varying anisotropy. This program is very similar to the original implementation of kriging with locally varying anisotropy: `kt3d_lva`. The parameters controlling the search are removed and the LHS matrix is built and decomposed only once.

References

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Figures

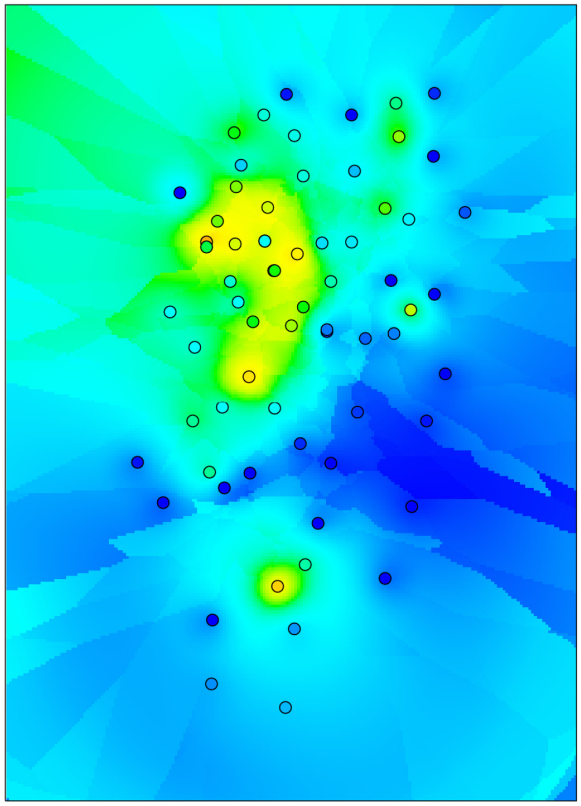

Figure 1: An example of a kriged model with search artifacts.

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                        Parameters for KT3D_GL_LVA
                        **************************

START OF PARAMETERS:
data.out                -file with data
1 2 0 3                 -columns for X,Y,Z,var
-998   1.0e21           -trimming limits
0 0                     -option (0=grid 1=cross), col for  DHID
0                       -debugging level: 0,1,2,3
kt3d.dbg                -file for debugging output
kriging.out             -file for kriged output
51  0.5 1               -nx,xmn,xsiz (ESTIMATION GRID)
51  0.5 1               -ny,ymn,ysiz (ESTIMATION GRID)
1   0.5 1               -nz,zmn,zsiz (ESTIMATION GRID)
grid_anticline.out -file containing the locally varying anisotropy grid
1 2 3 4 5               -LVA columns for ang1, ang2, ang3, anis1,anis2
51  0.5 1               -nx,xmn,xsiz (LVA GRID)
51  0.5 1               -ny,ymn,ysiz (LVA GRID)
1   0.5 1               -nz,zmn,zsiz (LVA GRID)
3                       -noffsets for graph
2                       -use MDS? 2=L-ISOMAP 3=read dist from  grid_cpp.out
10 10 1                 -number of landmark points in x,y,z (evenly spaced grid nodes)
-1                      -max number of dimensions to use (set -1 to use max)
0      0                -[0=SK 1=OK <0 inverse distance, simple kriging mean
1 0.00                  -# of nested structures, nugget effect (1D variogram)
2 1 1935                -it,cc,range
```

Figure 2: An example parameter file for `kt3d_gl_lva`.