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Computational properties of min/max autocorrelation factors

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Abstract

Minimum/maximum autocorrelation factor (MAF) is a suitable algorithm for orthogonalization of a vector random field. Orthogonalization avoids the use of multivariate geostatistics during joint stochastic modeling of geological attributes. This manuscript demonstrates in a practical way that computation of MAF is the same as discriminant analysis of the nested structures. Mathematica software is used to illustrate MAF calculations from a linear model of coregionalization (LMC) model. The limitation of two nested structures in the LMC for MAF is also discussed and linked to the effects of anisotropy and support. The analysis elucidates the matrix properties behind the approach and clarifies relationships that may be useful for model-based approaches.

Keywords: Orthogonalization; Spatial components; Nested structures; Discriminant analysis

1. Introduction

Geostatistical simulation of a stationary and Gaussian vector random field $\mathbf{Z}(x) = [Z_1(x)Z_2(x)\ldots Z_n(x)]$ may be performed without the use of cross-covariances. The already classic idea is to rotate the data $\mathbf{Z}(x_\alpha)$ to get factor scores as $\mathbf{Y}(x_\alpha) = \mathbf{Z}(x_\alpha)\mathbf{A}$ (e.g., Davis, 1986). Note that the components in $\mathbf{Z}(x)$ are centered with respect to the mean. After estimation or simulation is independently performed for the PCA factor scores, results are back rotated into the space of the original attributes. This very attractive proposal introduced by Davis and Greenes (1983) has not been completely achieved yet because there is no a general rotation method that may orthogonalize any general case of $\mathbf{Z}(x)$ for all separation lag distances. Davis and Greenes (1983), David et al. (1984), Wackernagel (1988), Goovaerts (1993), Myers (1994), have considered this problem with principal component analysis (PCA), and coregionalized PCA. Switzer and Green (1984), Wackernagel (1995) and Desbarats and Dimitrakopoulos (2000) have used min/max autocorrelation factors (MAF) for this problem.

Principal component analysis (PCA) orthogonalization computes eigenvectors $\mathbf{Q}$ and eigenvalues $\mathbf{\Lambda}$ by the spectral decomposition $\mathbf{Q}\mathbf{C}(0)\mathbf{Q}^{\mathrm{T}} = \mathbf{\Lambda}$ for the matrix of multivariate covariances $\mathbf{C}(0)$ at zero lag distance. This approach has the limitation that it can orthogonalize the multivariate covariance matrix $\mathbf{C}(h)$ only if all covariance and cross-covariance structures are proportional to each other, that is $\mathbf{C}(h) = \mathbf{B}\,c(h)$ and the attributes have the same elementary covariance structure $c(h)$. This is called intrinsic coregionalization (e.g., Wackernagel, 1995).

Another alternative is the orthogonalization of the q nested structures in the linear model of coregionalization (LMC) as

$$\mathbf{C}(h) = \sum_{u=1}^{q} \mathbf{B}_u c^u(h). \tag{1}$$

The total vector random function is made of spatial components, this is $\mathbf{Z}(x) = \sum_{u=1}^{q} \mathbf{Z}^u(x)$ The coregionalization matrices $\mathbf{B}_u$ in Eq. (1) are diagonalized by the spectral decomposition $\mathbf{Q}_u\mathbf{B}_u\mathbf{Q}_u^{\mathrm{T}} = \mathbf{\Lambda}^u$ and the scalar elementary model covariance $c^u(h)$, with unit variance, has no effect on the eigenvectors; it just multiplies the

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eigenvalues in the covariance of coregionalized factors (e.g., Wackernagel, 1995). This approach does not provide a single matrix as desired that can orthogonalize $\mathbf{C}(h)$ for all lag distances. The coregionalized factors are $\mathbf{Y}^u(x) = \mathbf{Z}^u(x)\mathbf{Q}_u$ for each nested spatial component. Simulation of coregionalized factor scores $\mathbf{Y}^u(x)$ may be made separately. This approach is limited because the data for conditional simulations require previous factorial kriging filtering (Matheron, 1971; and Wackernagel, 1988). A numerical approach that searches average matrix of factors is the simultaneous diagonalization (Myers, 1994).

Minimum/maximum autocorrelation factors (MAF) method (Switzer and Green, 1984) is a double rotation approach that allows for orthogonalization of $\mathbf{Z}(x)$ for the case where modeling of the sample matrix covariance is adequate with up to two nested structures in the LMC in Eq. (1). Desbarats and Dimitrakopoulos (2000) have used MAF in geostatistics for simulation of fifteen joint attributes. MAF is explained in detail in Section 2 and is classically performed on sample covariance values using the so-called delta lag covariance matrices.

This paper aims to revisit MAF approach to derive a model-based approach that can be used with Mathematica software. The approach is shown to be equivalent to classic discriminant analysis of the coregionalization matrices of the LMC. Results are numerically the same than the usual MAF performed with the delta lag distances (Switzer and Green, 1984; Berman, 1985). The paper also addresses MAF computational properties such as support effects, the inclusion of anisotropy in computations, and the reasons for limitation of orthogonalization to just two nested structures.

2. The computation of MAF factors revisited

2.1. The MAF algorithm and discriminant analysis

Minimum/maximum autocorrelation factors were introduced as a filtering technique into remote sensing imagery. Webster (1978) computed the spectral decomposition of a ratio of variances for the variability between and within soil series. Based on this proposal Switzer and Green (1984) developed a rotation that maximizes and minimizes the autocorrelation of the factors MAF. This is

$$\mathbf{Q}_2\mathbf{\Gamma}(\Delta)(\mathbf{Q}_1\mathbf{B}\mathbf{Q}_1^{\mathrm{T}})^{-1}\mathbf{Q}_2^{\mathrm{T}} = \mathbf{\Lambda}, \tag{2}$$

where $\mathbf{\Gamma}(\Delta)$ is the matrix variogram for non-standardized PCA factor scores $\mathbf{Y}(x)$ at a $\mathbf{\Delta}$ lag distance smaller than the range, $\mathbf{Q}_1\mathbf{B}\mathbf{Q}_1^{\mathrm{T}}$ is a matrix of PCA eigenvalues, $\mathbf{B}$ is the sum of the coregionalization matrices for the original attributes, same as $\mathbf{C}(0)$, $\mathbf{Q}_2$ is the matrix of eigenvectors for the standardized variogram $\mathbf{\Gamma}(\Delta)(\mathbf{Q}_1\mathbf{B}\mathbf{Q}_1^{\mathrm{T}})^{-1}$ at some lag $\mathbf{\Delta}$, and $\mathbf{\Lambda}$ is a matrix of eigenvalues. The approach have been shown (Berman, 1985) to be related to discriminant analysis or diagonalization of an asymmetric covariance matrix as follows:

$$\mathbf{Q}[\mathbf{B}_1\mathbf{B}^{-1}]\mathbf{Q}^{\mathrm{T}} = \mathbf{\Lambda}, \tag{3}$$

where $\mathbf{B}_1$ is the coregionalization matrix for one nested structure. See Wackernagel (1995) for a review. The discriminant analysis of Eq. (3) is based on the property that $\mathbf{B}_1\mathbf{B}^{-1} = I - \mathbf{B}_2\mathbf{B}^{-1}$. This means that any matrix $\mathbf{Q}$ that diagonalizes $\mathbf{B}_1\mathbf{B}^{-1}$ simultaneously diagonalizes $\mathbf{B}_2\mathbf{B}^{-1}$. However, it does not necessarily imply that it also diagonalizes $\mathbf{B}_1$ or $\mathbf{B}_2$ simultaneously. Both ratio matrices are asymmetric and that complicates calculations.

2.2. From LMC to MAF

MAF is applied to two nested structures as follows. The multivariate matrix of covariance is

$$\mathbf{C}(h) = \mathbf{B}_1 c^1(h) + \mathbf{B}_2 c^2(h). \tag{4}$$

For $h = 0$ this is

$$\mathbf{B} = \mathbf{B}_1 + \mathbf{B}_2. \tag{5}$$

The covariance becomes

$$\mathbf{C}(h) = \mathbf{B}_1 c^1(h) + \mathbf{B} c^2(h) - \mathbf{B}_1 c^2(h). \tag{6}$$

Computing the eigenvectors $\mathbf{Q}$ gives a symmetric rotation

$$\mathbf{Q}_1\mathbf{B}\mathbf{Q}_1^{\mathrm{T}} = \mathbf{Q}_1[\mathbf{B}_1 + \mathbf{B}_2]\mathbf{Q}_1^{\mathrm{T}}. \tag{7}$$

Scaling the eigenvectors by the standard deviation of the factors yields

$$\mathbf{A}_1 = \mathbf{Q}\mathbf{\Lambda}^{-1/2}. \tag{8}$$

This is a key step because the PCA factors become standardized. Thus, the covariance matrix for the PCA scores for lag distance zero $\mathbf{C}_Y(0)$ (i.e., variance) is the identity matrix that cannot be affected by any subsequent rotation. The PCA factors $\mathbf{A}_1$ are applied to the coregionalization matrices as

$$\mathbf{A}_1\mathbf{B}\mathbf{A}_1^{\mathrm{T}} = \mathbf{A}_1[\mathbf{B}_1 + \mathbf{B}_2]\mathbf{A}_1^{\mathrm{T}}. \tag{9}$$

Since the eigenvalues are the variances of the factors, they standardize the factor scores $\mathbf{Y}(\mathrm{x})$ of Eq. (3).

$$\mathbf{C}_Y(h) = \mathbf{A}_1\mathbf{B}_1\mathbf{A}_1^{\mathrm{T}} c^1(h) + \mathbf{A}_1\mathbf{B}\mathbf{A}_1^{\mathrm{T}} c^2(h) - \mathbf{A}_1\mathbf{B}_1\mathbf{A}_1^{\mathrm{T}} c^2(h). \tag{10}$$

Note $\mathbf{C}_Y(0) = \mathbf{I}$ is a diagonal identity matrix, and the factor scores are still correlated at lag distance $h \neq 0$. Then,

$$\mathbf{C}_Y(h) = \mathbf{A}_1\mathbf{B}_1\mathbf{A}_1^{\mathrm{T}} c^1(h) + \mathbf{I}c^2(h) - \mathbf{A}_1\mathbf{B}_1\mathbf{A}_1^{\mathrm{T}} c^2(h). \tag{11}$$

Using $\mathbf{V}$ for notation of the new coregionalization matrices, $\mathbf{C}_Y(h)$ becomes

$$\mathbf{C}_Y(h) = \mathbf{V}_1 c^1(h) + (\mathbf{I} - \mathbf{V}_1)c^2(h). \tag{12}$$

This is an important property of the PCA factors where the variances of two non-orthogonal nested components are complementary and the off-diagonal terms (cross-covariances) have opposite signs to provide the identity matrix $\mathbf{C}_Y(0)$. Arraying the multivariate matrix of covariances for factors yields

$$\mathbf{C}_Y(h) = \mathbf{V}_1(c^1(h) - c^2(h)) + \mathbf{I}c^2(h). \tag{13}$$

Deviations from orthogonality of the PCA factors are clearly the difference between nested structures $c^1(h) - c^2(h)$ scaled by the off-diagonal terms of $\mathbf{V}_1$. The matrix $\mathbf{C}_Y(h)$ is usually asymmetric and has an odd and even component for any given $h \neq 0$. The next step of MAF builds on the assumption that the covariance matrix $\mathbf{C}_Y(h)$ can be substituted by the multivariate matrix variogram that is symmetric.

The asymmetry of the covariance for PCA factors can be explicitly removed using the variogram for factors. This is

$$\mathbf{\Gamma}_Y(h) = \mathbf{I} - ([\mathbf{C}_Y(h)]^{\mathrm{T}} + [\mathbf{C}_Y(h)])\tfrac{1}{2}. \tag{14}$$

The matrix $\mathbf{V}_1$ is made symmetric, this yields

$$\mathbf{\Gamma}_Y(h) = \mathbf{I} - [(\mathbf{V}_1^{\mathrm{T}} + \mathbf{V}_1)\tfrac{1}{2}](c^1(h) - c^2(h)) - \mathbf{I}c^2(h). \tag{15}$$

Assuming a lag distance $h = \mathbf{\Delta}$ and $\Delta \neq 0$, MAF are obtained from a second computation of eigenvectors as

$$\begin{aligned}\mathbf{\Gamma}_{\mathrm{MAF}}(\Delta) &= \mathbf{Q}_2\mathbf{\Gamma}_Y(\Delta)\mathbf{Q}_2^{\mathrm{T}} = \mathbf{I} - \mathbf{Q}_2[(\mathbf{V}_1^{\mathrm{T}} + \mathbf{V}_1)\tfrac{1}{2}] \\ &\quad \times \mathbf{Q}_2^{\mathrm{T}}(c^1(\Delta) - c^2(\Delta)) - \mathbf{I}c^2(\Delta).\end{aligned} \tag{16}$$

The new eigenvectors $\mathbf{Q}_2$ are the same for any lag distance Δ. However, the eigenvalues depend on Δ, and in general they make the new covariance for the spatially orthogonal factors. The term $\mathbf{D} = \mathbf{Q}_2[(\mathbf{V}_1^{\mathrm{T}} + \mathbf{V}_1)\tfrac{1}{2}]\mathbf{Q}_2^{\mathrm{T}}$ is perfectly diagonal. Then, the last rotation diagonalizes both the total variogram for PCA factors and the matrix of the rotated components. The variogram for MAF factors for two nested structures is perfectly diagonal for all lag distances. This is

$$\begin{aligned}\mathbf{\Gamma}_{\mathrm{MAF}}(h) &= \mathbf{Q}_2\mathbf{\Gamma}_Y(h)\mathbf{Q}_2^{\mathrm{T}} \\ &= \mathbf{I} - [\mathbf{D}c^1(h) + (\mathbf{I} - \mathbf{D})c^2(h)].\end{aligned} \tag{17}$$

The diagonal matrix $\mathbf{D}$ may be written also as

$$\mathbf{D} = \mathbf{Q}_2[[\mathbf{Q}_1\mathbf{B}_1\mathbf{Q}_1^{\mathrm{T}}]\mathbf{\Lambda}^{-1} + ([\mathbf{Q}_1\mathbf{B}_1\mathbf{Q}_1^{\mathrm{T}}]\mathbf{\Lambda}^{-1})^{\mathrm{T}}]\mathbf{Q}_2^{\mathrm{T}}. \tag{18}$$

Note that due to asymmetry $\mathbf{Q}_2[[\mathbf{Q}_1\mathbf{B}_1\mathbf{Q}_1^{\mathrm{T}}]\mathbf{\Lambda}^{-1}]\mathbf{Q}_2^{\mathrm{T}}$ is not strictly diagonal as could be assumed. However, the term $\mathbf{D}$ is a diagonal matrix, then the property of eigenvectors $\mathbf{Q}_2$ is that they diagonalize $[(\mathbf{V}_1^{\mathrm{T}} + \mathbf{V}_1)\tfrac{1}{2}]$ and $\mathbf{I} - [(\mathbf{V}_1^{\mathrm{T}} + \mathbf{V}_1)\tfrac{1}{2}]$ also. The division by two may not be required in the eigenvector computation; also the variogram may be avoided if an average covariance is utilized. Eq. (17) may also be written as a covariance, this is

$$\mathbf{C}_{\mathrm{MAF}}(h) = \mathbf{D}c^1(h) + (\mathbf{I} - \mathbf{D})c^2(h). \tag{19}$$

Up to Eq. (19), the rotation is perfect and the averaging of the asymmetric cross-covariances $\mathbf{C}_Y(h)$ to make the variogram is a very important step for it. It is evident that the average covariance suffices. Theoretically, no deviations from orthogonality exist, numerically MAF provides a perfect orthogonalization if performed on covariance models with two nested structures. However, to avoid the modeling of cross-covariances MAF is usually done on numerical sample covariances.

Data can be rotated in two stages, as shown above, or a single matrix of loadings for factors may be built as

$$\mathbf{A}_{\mathrm{MAF}} = \mathbf{Q}_2\mathbf{\Lambda}_1^{-1}\mathbf{Q}_1. \tag{20}$$

An important point is that the linear model of coregionalization LMC in Eq. (1) has been used for demonstration purposes here, but in the common remote sensing practice of MAF modeling the LMC has been avoided. MAF has been a data-based approach because in remote sensing the objective is filtering and not stochastic modeling. In most cases, an exhaustive data set or complete image is assumed available. However, in geostatistics one needs to generalize the concept using random field theory for modeling data from sampling. This implies that MAF is computed in geostatistics from sample covariances obtained basically from sample data analysis. In the cases where a good fit to a multivariate covariance model is available, performing MAF on models may be a preferred alternative. Another reason for using the LMC previous to MAF approach is to test whether the assumption that there are only two unknown nested components in the problem is applicable. In other words, if MAF does not provide reasonable orthogonal factors, then a check for the amount of nested structures present should be carried out.

3. Analysis of computational limitations and spatial characteristics of MAF

3.1. Computational oscillations in the extension of MAF

Extending MAF approach for three nested structures may be attractive but appears non-trivial within a linear framework. Extension to three nested structures could allow for a spatial orthogonality of the factor scores for cases where two nested structures are not sufficient enough in the LMC. For theoretical purposes, we use the linear model of coregionalization. This is

$$\mathbf{C}(h) = \mathbf{B}_1 c^1(h) + \mathbf{B}_2 c^2(h) + \mathbf{B}_3 c^3(h) \tag{21}$$

and

$$\mathbf{B} = \mathbf{B}_1 + \mathbf{B}_2 + \mathbf{B}_3. \tag{22}$$

Then $\mathbf{B}_3 = \mathbf{B} - \mathbf{B}_1 - \mathbf{B}_2$ and

$$\mathbf{C}(h) = \mathbf{B}_1 c^1(h) + \mathbf{B}_2 c^2(h) + (\mathbf{B} - \mathbf{B}_1 - \mathbf{B}_2) c^3(h). \tag{23}$$

Computing eigenvectors $\mathbf{Q}_1$ gives

$$\mathbf{Q}_1\mathbf{C}(h)\mathbf{Q}_1^{\mathrm{T}} = \mathbf{Q}_1\mathbf{B}_1\mathbf{Q}_1^{\mathrm{T}} c^1(h) + \mathbf{Q}_1\mathbf{B}_2\mathbf{Q}_1^{\mathrm{T}} c^2(h) + \mathbf{Q}_1(\mathbf{B} - \mathbf{B}_1 - \mathbf{B}_2)\mathbf{Q}_1^{\mathrm{T}} c^3(h). \tag{24}$$

Multiplying by the inverse of the diagonal matrix of eigenvalues this is the covariance for classic PCA factors

$$\mathbf{A}_1\mathbf{C}(h)\mathbf{A}_1^{\mathrm{T}} = \mathbf{A}_1\mathbf{B}_1\mathbf{A}_1^{\mathrm{T}} c^1(h) + \mathbf{A}_1\mathbf{B}_2\mathbf{A}_1^{\mathrm{T}} c^2(h) + \mathbf{A}_1(-\mathbf{B}_1 - \mathbf{B}_2)\mathbf{A}_1^{\mathrm{T}} c^3(h) + \mathbf{I}c^3(h). \tag{25}$$

Then, computing the matrix multivariate variogram from the average of the rotated matrices as before is

$$\mathbf{\Gamma}(h) = \mathbf{I} - \mathbf{M}_1 c^1(h) - \mathbf{M}_2 c^2(h) - (-\mathbf{M}_1 - \mathbf{M}_2) c^3(h) - \mathbf{I}c^3(h). \tag{26}$$

From the definition of the relationship between nested covariances and nested variograms, it is convenient to introduce a matrix

$$\mathbf{M}^{(3)} = \mathbf{M}_1 + \mathbf{M}_2 \tag{27}$$

then the variogram is also

$$\mathbf{\Gamma}(h) = \mathbf{I} - \mathbf{M}_1 c^1(h) - (\mathbf{M}^{(3)} - \mathbf{M}_1) c^2(h) + \mathbf{M}^{(3)} c^3(h) - \mathbf{I}c^3(h). \tag{28}$$

Making $h \to \infty$ gives an identity matrix because the elementary structures become zero. Thus, an additional rotation could or not improve the orthogonality. The lack of orthogonality in the factors matrix variogram is at short lag distances Δ. The extended MAF comes from choosing an existing non-diagonal matrix for computing new eigenvectors as

$$\mathbf{Q}_2\mathbf{M}^{(3)}\mathbf{Q}_2^{\mathrm{T}} = \mathbf{Q}_2[\mathbf{M}_1 + \mathbf{M}_2]\mathbf{Q}_2^{\mathrm{T}}. \tag{29}$$

The new factor scores have a variogram as

$$\mathbf{\Gamma}_{Y2}(h) = \mathbf{I} - \mathbf{P}_1 c^1(h) - (\mathbf{D}^{(3)} - \mathbf{P}_1) c^2(h) + \mathbf{D}^{(3)} c^3(h) - \mathbf{I}c^3(h), \tag{30}$$

where $\mathbf{P}_1 = \mathbf{Q}_2\mathbf{M}_1\mathbf{Q}_2^{\mathrm{T}}$ and $\mathbf{P}_2 = \mathbf{Q}_2\mathbf{M}_2\mathbf{Q}_2^{\mathrm{T}}$. Further orthogonalization using eigenvalues may imply the use of Eq. (12). This is to make $\mathbf{D}^{(3)}$ identity, it destroys existing identity matrices and

$$\mathbf{\Gamma}_{Y2}(h) = \mathbf{D}^{-1} - \mathbf{P}_1 c^1(h) - (\mathbf{I}^{(3)} - \mathbf{P}_2) c^2(h) + \mathbf{I}^{(3)} c^3(h) - \mathbf{D}^{-1} c^3(h). \tag{31}$$

A matrix of eigenvectors diagonalizes $\mathbf{Q}_3\mathbf{P}_1\mathbf{Q}_3^{\mathrm{T}}$ but at the cost of loosing previous diagonal matrices. This is

$$\mathbf{\Gamma}_{Y2}(h) = \mathbf{Q}_3\mathbf{D}^{-1}\mathbf{Q}_3^{\mathrm{T}} - \mathbf{D}c^1(h) - (\mathbf{I}^{(3)} - \mathbf{D}) \times (c^2(h) + \mathbf{I}^{(3)} c^3(h) - \mathbf{Q}_3\mathbf{D}^{-1}\mathbf{Q}_3 c^3(h). \tag{32}$$

Further attempts to diagonalize $\mathbf{Q}_3\mathbf{D}^{-1}\mathbf{Q}_3^{\mathrm{T}}$ matrices will only oscillate the approximate orthogonality of $\mathbf{\Gamma}_{Y2}(h)$.

3.2. Support effect on the computation of MAF

Usually, sampling and simulations of the Gaussian vector random function $\mathbf{Z}(x)$ are carried on at a quasi-point support. The problem is that factor scores may come from a small support simulation that may be spatially averaged by re-blocking of the realizations prior or after back rotation. This is common for simulation of blocks in mining, and up scaling for finite element flow simulation in petroleum reservoir modeling and hydrology.

Multivariate support effect on PCA is studied in Vargas-Guzmán et al. (1999b) who introduce the methodology of computing average spatial cross-covariances for up scaling using the LMC. The dispersion covariance matrix for attributes measured in elements of support υ within a region of support V is

$$\mathbf{D}^2(\upsilon|V) = \sum_{u=1}^{q} \mathbf{B}_u \left[\frac{1}{V^2} \int_V \mathrm{d}x \int_V g^u(x - x')\,\mathrm{d}x' - \frac{1}{\upsilon^2} \int_\upsilon \mathrm{d}x \int_\upsilon g^u(x - x')\,\mathrm{d}x' \right]. \tag{33}$$

The scalar quantities within brackets are elementary dispersion variances. Then,

$$\mathbf{D}^2(\upsilon|V) = \sum_{u=1}^{q} \mathbf{B}_u d^u(\upsilon|V). \tag{34}$$

The eigenvectors for spatial average multivariate covariances matrices may be independent of support only if matrix $\mathbf{B}_u$ can be factored out. This is the case of intrinsic coregionalization. On the other hand, the eigenvalues are the dispersion variances of the PCA factors.

The approach explained above can be applied to study support effect in MAF but instead of multivariate dispersion covariances one has to appeal to the regularized multivariate variogram. Vargas-Guzmán et al. (1999a) introduce a regularized cross-variogram that allows for a regularized LMC

$$\mathbf{\Gamma}_\upsilon(h) = \sum_{u=1}^{q} \mathbf{B}_u \left[g^u(h) - \frac{1}{\upsilon^2} \int_\upsilon \mathrm{d}x \int_\upsilon g^u(x - x')\,\mathrm{d}x' \right]. \tag{35}$$

Since the block support is constant, the within-block average elementary variogram r is also scalar constant, then

$$\mathbf{\Gamma}_\upsilon(h) = \sum_{u=1}^{q} \mathbf{B}_u [g^u(h) - r]. \tag{36}$$

From Eq. (35) and previous results in Eq. (19), it is evident that MAF eigenvectors are independent of h and the size of blocks, therefore covariance matrices can be applied regardless of support as far as the two nested structures regularized LMC is followed. More than two structures will not be orthogonalized properly and the scale effect will appear, this is also applicable for attributes at different support, which may not be used in MAF. If more than two nested structures are present there is no a unique single set of eigenvectors that can be chosen. For a given support each delta lag distance will provide different results. In these cases, corrections for the scale effect on MAF may be attempted using the same delta lag distances as in the MAF on point and regularized multivariate variograms. Thus, factors computed at point support are used for data at point support. After re-blocking, the data should be back rotated with the MAF coming from the regularized model.

3.3. Effect of anisotropy in the computation of MAF

Introducing anisotropy into MAF means the matrix of factors should simultaneously diagonalize the covariance matrix in the major directions of anisotropy. Consider the LMC for two nested structures along two principal directions of anisotropy is

$$\mathbf{C}_1(h) = \mathbf{B}_{11}c^{11}(h) + \mathbf{B}_{12}c^{12}(h), \tag{37}$$

$$\mathbf{C}_2(h) = \mathbf{B}_{21}c^{21}(h) + \mathbf{B}_{22}c^{22}(h),$$

where $\mathbf{B}_{11} + \mathbf{B}_{12} = \mathbf{B}_{21} + \mathbf{B}_{22}$. Thus, PCA or zero lag distance diagonalization is the same for both models. Following the Eq. (37), it is evident that complete diagonalization of both models by MAF may only be achieved if the coregionalization matrices are proportional. This is $\mathbf{B}_{11} = a\mathbf{B}_{21}$ and $\mathbf{B}_{12} = b\mathbf{B}_{22}$, in this case the MAF orthogonalization of one direction automatically diagonalizes the variogram on the other principal direction regardless of the range and the coregionalization matrices in the covariances. If the matrices of coregionalization are not proportional, the problem is one of simultaneous orthogonalization of more than two structures that apparently has no linear solution as was shown in Section 3.1. The effect of anisotropy is related to the amount of non-proportional coregionalization matrices present in the principal directions of anisotropy. In the case of three dimensions, the discussion above is still valid under the same restrictions.

3.4. Model versus data-based computation of MAF

From the analysis in previous sections, two possibilities for computation of MAF in geostatistics are available, one based on sample matrix covariance and the second based on a model matrix covariance. In the first approach, MAF is computed from geostatistical data, and does not require modeling of cross-variograms (Desbarats and Dimitrakopoulos, 2000). The numerical computation of sample cross-variograms for PCA factors is included as part of the algorithm for a set of lag distances that fall within specified interval of delta lag-distances. The final MAF factor scores are independent of each other for all lag distances. Therefore, each MAF factor is treated as a scalar random function and may be stochastically modeled separately. However, this approach is valid if the back rotation of modeled values does not include non-linear operations and the factor scores are Gaussian. It is shown that MAF is theoretically a sound orthogonalization only if two nested structures suffice for modeling the multivariate covariance. From this, it is apparent that ignoring modeling of the LMC might lead to unknown errors if two structures do not suffice for adequate modeling the multivariate covariance. The interesting part of this data-based approach is that the two nested structures may not necessarily be known models and has the advantage that it may allow for computations without restriction to known models. Computing MAF with this first approach is heavily dependent on the quality of the numerical sample cross-covariances for the PCA factors. MAF are supposed to be constant for the interval of lag distances, then, looking at the coefficient of variation of the factor loadings may help to see the quality of the estimate. Also note that at difference of remote sensing images, the limited number of samples in geostatistics may require vector random field concepts and models of covariances.

The second approach is model-based that is made on the vector random field. Note that the elementary covariances $c^u(h)$ may not be directly involved in MAF computation at all. This approach has the advantage that only numerical coregionalization matrices are required and reduce the computation of MAF to discriminant analysis. However, the disadvantage is that coregionalization matrices can only be well known after modeling with the LMC, which is considered a cumbersome task. This brings a question about what if the required models are not in the group of commonly known models. However, this is consistent with most geostatistical approaches that are performed under the random field concept and are restricted to combinations of known models.

The next example illustrates the computation of MAF using model-based approach with Mathematica software. It numerically shows that the approach works for two nested structures. In addition the maximization and minimization of autocorrelation occur as a consequence of the property in Eq. (12) for the coregionalization matrices of factors.

4. Computation of MAF using MATHEMATICA

The MATHEMATICA software is an excellent tool able to handle matrix computations involving eigenvectors and eigenvalues. The example computation of MAF presented in this section was made using MATHEMATICA and the commands are copied from the corresponding run. Two known coregionalization matrices for four attributes were obtained after modeling and are:

$$\mathrm{B1} := \begin{pmatrix} 0.70 & 0.25 & 0.20 & 0.15 \\ 0.25 & 0.30 & 0.35 & 0.30 \\ 0.20 & 0.35 & 0.60 & 0.09 \\ 0.15 & 0.30 & 0.09 & 0.90 \end{pmatrix},$$

$$\mathrm{B2} := \begin{pmatrix} 0.30 & 0.23 & 0.10 & 0.15 \\ 0.23 & 0.70 & 0.20 & 0.20 \\ 0.10 & 0.20 & 0.40 & 0.13 \\ 0.15 & 0.20 & 0.13 & 0.10 \end{pmatrix}.$$

The two elementary covariances are exponential and Gaussian as follows

$$\mathrm{g1[h\_]} := \mathrm{Exp}[-\mathrm{h} \div 100]$$

$$\mathrm{g2[h\_]} := \mathrm{Exp}[-(\mathrm{h} \div 25)^2].$$

The next commands plot the elementary structures

Plot[g1[h], {h, 0.1, 200}] (Fig. 1)

and

Plot[g2[h], {h, 0.1, 200}] (Fig. 2)

The total zero lag distance covariance is

$$\mathrm{B} := \mathrm{B1} + \mathrm{B2}$$

MatrixForm[B]

$$\begin{pmatrix} 1 & 0.48 & 0.30 & 0.30 \\ 0.48 & 1 & 0.55 & 0.50 \\ 0.30 & 0.55 & 1 & 0.22 \\ 0.30 & 0.50 & 0.22 & 1 \end{pmatrix}.$$

PCA is performed; eigenvectors and eigenvalues are obtained

Q1 := Eigenvectors[B]

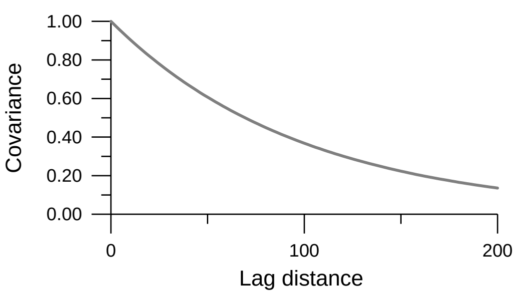

Fig. 1. Elementary exponential covariance.

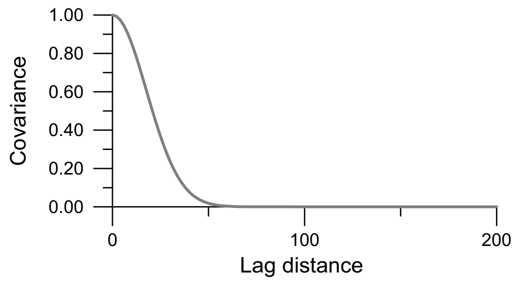

Fig. 2. Elementary Gaussian covariance.

MatrixForm[Q1]

$$\begin{pmatrix} 0.4691780 & 0.5934460 & 0.472777 & 0.451857 \\ 0.0588408 & -0.0474221 & -0.688363 & 0.721419 \\ 0.8550450 & -0.1247820 & -0.322922 & -0.386068 \\ 0.2128540 & -0.7937270 & 0.445375 & 0.355432 \end{pmatrix},$$

L1 := Q1.B.Transpose[Q1]

MatrixForm[L1]

$$\begin{pmatrix} 2.19836 & 0 & 0 & 0 \\ 0 & 0.781682 & 0 & 0 \\ 0 & 0 & 0.681196 & 0 \\ 0 & 0 & 0 & 0.338763 \end{pmatrix}.$$

The zero off-diagonal terms are left as from the original output, thus the exercise could be reproduced.

The coregionalization matrices are rotated yielding the coregionalization matrices for PCA factors as follows

V1 := Q1.B1.Transpose[Q1].Inverse[L1]
V2 := Q1.B2.Transpose[Q1].Inverse[L1]
V := Q1.B.Transpose[Q1].Inverse[L1]

MatrixForm[V1]

$$\begin{pmatrix} 0.5753820 & 0.1046220 & 0.0009108 & 0.5591050 \\ 0.0372009 & 0.8492960 & -0.1582630 & 0.2027650 \\ 0.0002822 & 0.1379180 & 0.7778690 & -0.0302086 \\ 0.0861569 & 0.0878775 & -0.0150229 & 0.1220390 \end{pmatrix}$$

MatrixForm[V2]

$$\begin{pmatrix} 0.4246180 & -0.1046220 & -0.0009108 & -0.5591050 \\ -0.0372009 & 0.1507040 & 0.1582630 & -0.2027650 \\ -0.0002822 & 0.1379180 & 0.2221310 & 0.0302086 \\ -0.0861569 & -0.0878775 & 0.0150229 & 0.8779610 \end{pmatrix}.$$

Note that both follow Eq. (12). The covariance for PCA factors is computed as

$$\mathrm{G[h\_]:=V1\times g1[h]+V2\times g2[h]}$$

which is diagonal only for $h=0$.

Since this covariance is asymmetric as seen from the model above, an average covariance is computed. The coregionalization matrices are made symmetric

$$\mathrm{S1:=(Transpose[V1]+V1)2^{-1}}$$

$$\mathrm{S2:=(Transpose[V2]+V2)2^{-1}}$$

and a symmetric covariance matrix for a single delta lag distance $h=50$ is

$$\mathrm{M:=(G[50]+Transpose[G[50]])/2}$$

MatrixForm[M]

$$\begin{pmatrix} 0.3567640 & 0.0417111 & 0.00035089 & 0.1897770 \\ 0.0417111 & 0.5178840 & -0.08710890 & 0.0854790 \\ 0.0003509 & -0.0871089 & 0.47587000 & -0.0133029 \\ 0.1897770 & 0.0854790 & -0.0133029 & 0.0910070 \end{pmatrix}.$$

Note that the same eigenvectors are obtained if the computation is made for the matrix S1 reducing MAF to classic discriminant analysis. Computing eigenvectors for this previous matrix is

$$\mathrm{Q2:=Eigenvectors[M]}$$

MatrixForm[Q2]

$$\begin{pmatrix} -0.302823 & -0.773975 & 0.498274 & -0.246951 \\ -0.643697 & -0.086164 & -0.686805 & -0.326388 \\ 0.545815 & -0.618079 & -0.529144 & 0.200177 \\ 0.442762 & 0.107317 & -0.005400 & -0.890177 \end{pmatrix}.$$

The PCA coregionalization matrices are rotated giving the min/max coregionalization matrices

$$\mathrm{U1:=Q2.S1.Transpose[Q2]}$$

$$\mathrm{U2:=Q2.S2.Transpose[Q2]}$$

$$\mathrm{U:=Q2.V.Transpose[Q2]}$$

These new matrices are symmetric and of course U is still the identity matrix. The covariance for the MAF factors is

$$\mathrm{G2[h\_]:=U1\times g1[h]+U2\times g2[h]}$$

where, the rounded results are

MatrixForm[U1]

$$\begin{pmatrix} 1.0 & 0 & 0 & 0 \\ 0 & 0.75 & 0 & 0 \\ 0 & 0 & 0.61 & 0 \\ 0 & 0 & 0 & 0.0 \end{pmatrix}$$

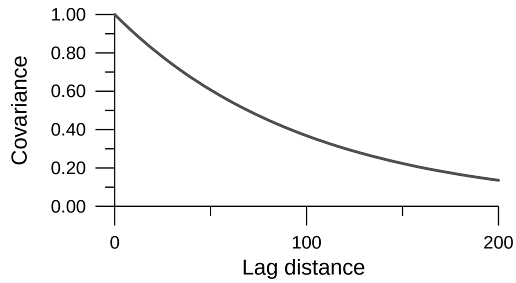

Fig. 3. Autocorrelation for first MAF factor.

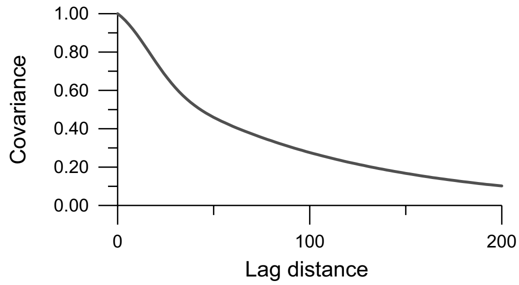

Fig. 4. Autocorrelation for second MAF factor.

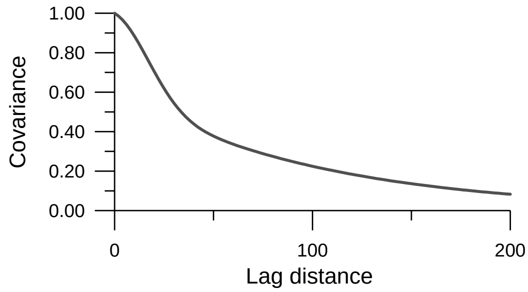

Fig. 5. Autocorrelation for third MAF factor.

MatrixForm[U2]

$$\begin{pmatrix} 0.0 & 0 & 0 & 0 \\ 0 & 0.25 & 0 & 0 \\ 0 & 0 & 0.39 & 0 \\ 0 & 0 & 0 & 1.0 \end{pmatrix}.$$

The diagonal terms show the discrimination of the two structures. The individual diagonal matrices may have negative terms. The first attribute is almost entirely modeled by the exponential, the fourth attribute is almost entirely the Gaussian model, and the other two attributes correspond to linear combinations. Plots in Figs. 3–6 show these results

$\mathrm{Plot[G2[x]_{[[1,1]]},\{x,0.1,200\}]}$ (Fig. 3)

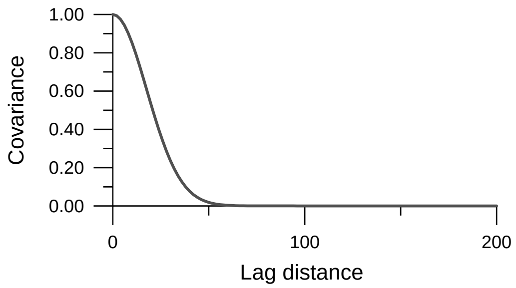

Fig. 6. Autocorrelation for fourth MAF factor.

$\mathrm{Plot}[\mathrm{G2}[\mathrm{x}]_{[[2,2]]}, \{\mathrm{x}, 0.1, 200\}]$ (Fig. 4)

$\mathrm{Plot}[\mathrm{G2}[\mathrm{x}]_{[[3,3]]}, \{\mathrm{x}, 0.1, 200\}]$ (Fig. 5)

$\mathrm{Plot}[\mathrm{G2}[\mathrm{x}]_{[[4,4]]}, \{\mathrm{x}, 0.1, 200\}]$ (Fig. 6)

The final matrix of factors is computed as

A : = Q2.Inverse[D1].Q1

MatrixForm[A]

$$\begin{pmatrix} 0.2785580 & 0.181747 & 0.122120 & -1.107710 \\ -1.014031 & 0.295917 & -0.119204 & -0.144531 \\ -0.343396 & 0.058629 & 1.015470 & 0.031766 \\ -0.183890 & 1.386220 & -0.621429 & -0.318580 \end{pmatrix}.$$

5. Discussion and conclusions

Modeling of the matrix covariance with the LMC reduces computation of MAF to classic discriminant analysis of the coregionalization matrices that may be easily solved with Mathematica software. This paper has shown that MAF computation with delta lag distances is analogous to discriminant analysis of the coregionalization matrices. The computation becomes very simple and other programs for computation of spectral decomposition can also handle MAF. If the modeling is avoided, a numerical computation of a set of delta lag matrix covariances for the PCA factors is required for computing MAF.

The discrimination of the nested structures is clearly illustrated by Figs. 3 and 6 from results obtained with Mathematica in the example. The result of this example is that individual elementary nested structures do not directly participate in the orthogonalization and MAF is reduced to discriminant analysis with the coregionalization matrices.

It has been shown here that PCA factors computed from the covariance at zero lag distance have the property that the coregionalization matrices for two nested structures in the multivariate covariance add to the identity matrix. This gives possibility of MAF orthogonalization because both matrices are diagonalized with the eigenvector matrix of any of the two nested components. This is due to linearity and supports that MAF is equivalent to discriminant analysis of the coregionalization matrices. The general problem of non-linearity and orthogonalization of more than three nested components calls for further research.

The support effects have been modeled and results can be obtained by the model-based MAF approach performed for a regularized multivariate covariance for the same delta lag distances utilized. If two nested structures are sufficient for modeling the Gaussian vector random field, the scale effect vanishes. The scale effect of MAF is indeed the scale effect on discriminant analysis. An analogous situation has been described for anisotropy, where the main directions of anisotropy need to respond to proportional coregionalization matrices (i.e., coplanar vectors) thus anisotropy can be handled, otherwise it becomes a problem of simultaneous orthogonalization of more than two nested structures. Note that anisotropy is not considered by classic discriminant analysis.

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