Modeling coregionalization

(Goovaerts, P. (1989), Geostatistics for Natural Resources Evaluation

Suppose there are \( k \) colocated random variables. Modeling coregionalization requires computing and fitting of \( k + \binom{k}{2} = \frac{k(k+1)}{2} \) auto and cross-semivariograms (or covariance functions).

Suppose \( Z_i(s_j), i = 1, \ldots, k \) are \( k \) intercorrelated random variables and \( s_1, s_2, \ldots, s_n \) are the spatial locations that we observe these variables. Consider a linear combination of the type 
\[
Y = \sum_{i=1}^{k} \sum_{j=1}^{n} w_{ij} Z_i(s_j).
\]
It’s variance must be nonnegative and therefore,
\[
\text{var}(Y) = k \sum_{i=1}^{k} \sum_{j=1}^{n} \sum_{a=1}^{n} \sum_{b=1}^{n} w_{ai} w_{bj} c(s_i, s_j).
\]

This variance can be expressed in terms of a matrix \( C \) which contains covariances and cross-covariances involving the \( k \) random variables. Therefore, the matrix \( C \) must be positive semidefinite, or equivalently, the matrix of semivariograms must be conditionally negative semidefinite. To achieve this, we express each random variable as a function of \( p \) independent random variables each one with mean zero and covariance function \( c_i(h) \):

\[
Z_i(s) = \sum_{l=1}^{p} a_{il} Y_l + \mu_i, \quad i = 1, \ldots, k.
\]

Here they are:
\[
\begin{align*}
Z_1(s) &= a_{11} Y_1 + a_{12} Y_2 + \ldots + a_{1p} Y_p + \mu_1 \\
Z_2(s) &= a_{21} Y_1 + a_{22} Y_2 + \ldots + a_{2p} Y_p + \mu_2 \\
\vdots &= \vdots \\
Z_k(s) &= a_{k1} Y_1 + a_{k2} Y_2 + \ldots + a_{kp} Y_p + \mu_k
\end{align*}
\]

with, \( E[Y_l(s)] = 0, l = 1, \ldots, p. \)
\( E[Z_i(s)] = \mu_i, i = 1, \ldots, k. \)
\( \text{cov}[(Y_l(s), Y_{l'}(s+h))] = c_l(h) \) if \( l = l' \), and 0 otherwise.

Using the above we can express the covariance between two random variables \( Z_i(s) \) and \( Z_i(s+h) \) as follows:
\[
c_{12}(h) = \text{cov}[Z_1(h), Z_2(s+h)] = \text{cov}(a_{11} Y_1 + a_{12} Y_2 + \ldots + a_{1p} Y_p + \mu_1, a_{21} Y_1 + a_{22} Y_2 + \ldots + a_{2p} Y_p + \mu_2,)
\]
\[
= a_{11}a_{21}c_1(h) + a_{12}a_{22}c_2(h) + \ldots + a_{1p}a_{2p}c_p(h).
\]

Similarly the expression of the cross-semivariogram is:
\[
\gamma_{12}(h) = a_{11}a_{21}\gamma_1(h) + a_{12}a_{22}\gamma_2(h) + \ldots + a_{1p}a_{2p}\gamma_p(h).
\]
Example:
Consider two random variables $Z_1(s)$ and $Z_2(s)$ and suppose we express them as linear combinations of $Y_1, Y_2, Y_3$.

\[
Z_1(s) = a_{11}Y_1(s) + a_{12}Y_2(s) + a_{13}Y_3(s) + \mu_1 \\
Z_2(s) = a_{21}Y_1(s) + a_{22}Y_2(s) + a_{23}Y_3(s) + \mu_2
\]

Then the auto and cross semivariograms can be expressed as follows:

\[
\begin{align*}
\gamma_{11}(h) &= a_{11}^2 \gamma_1(h) + a_{12}^2 \gamma_2(h) + a_{13}^2 \gamma_3(h) \\
\gamma_{22}(h) &= a_{21}^2 \gamma_1(h) + a_{22}^2 \gamma_2(h) + a_{23}^2 \gamma_3(h) \\
\gamma_{12}(h) &= a_{11}a_{21} \gamma_1(h) + a_{12}a_{22} \gamma_2(h) + a_{13}a_{23} \gamma_3(h)
\end{align*}
\]

Or using different notation:

\[
\begin{align*}
\gamma_{11}(h) &= u_1 \gamma_1(h) + u_2 \gamma_2(h) + u_3 \gamma_3(h) \\
\gamma_{22}(h) &= v_1 \gamma_1(h) + v_2 \gamma_2(h) + v_3 \gamma_3(h) \\
\gamma_{12}(h) &= w_1 \gamma_1(h) + w_2 \gamma_2(h) + w_3 \gamma_3(h)
\end{align*}
\]

The semivariograms $\gamma_1(h), \gamma_2(h), \gamma_3(h)$ are called the basic models and we express the previous system of equations for each basic model as follows:

Combinations of the first basic model $\gamma_1(h)$

\[
\begin{pmatrix}
\gamma_{11}(h) & \gamma_{12}(h) \\
\gamma_{21}(h) & \gamma_{22}(h)
\end{pmatrix}
= \begin{pmatrix} u_1 & w_1 \\ w_1 & v_1 \end{pmatrix}
\begin{pmatrix}
\gamma_1(h) \\
0
\end{pmatrix}
= \begin{pmatrix}
u_1 \gamma_1(h) + u_2 \gamma_2(h) + u_3 \gamma_3(h) \\
0
\end{pmatrix}.
\]

Combinations of the second basic model $\gamma_2(h)$

\[
\begin{pmatrix}
\gamma_{11}(h) & \gamma_{12}(h) \\
\gamma_{21}(h) & \gamma_{22}(h)
\end{pmatrix}
= \begin{pmatrix} u_2 & w_2 \\ w_2 & v_2 \end{pmatrix}
\begin{pmatrix}
\gamma_2(h) \\
0
\end{pmatrix}
= \begin{pmatrix}
u_2 \gamma_1(h) + v_2 \gamma_2(h) + v_3 \gamma_3(h) \\
0
\end{pmatrix}.
\]

Combinations of the third basic model $\gamma_3(h)$

\[
\begin{pmatrix}
\gamma_{11}(h) & \gamma_{12}(h) \\
\gamma_{21}(h) & \gamma_{22}(h)
\end{pmatrix}
= \begin{pmatrix} u_3 & w_3 \\ w_3 & v_3 \end{pmatrix}
\begin{pmatrix}
\gamma_3(h) \\
0
\end{pmatrix}
= \begin{pmatrix}
u_3 \gamma_1(h) + v_3 \gamma_2(h) + w_3 \gamma_3(h) \\
0
\end{pmatrix}.
\]

The system will be positive definite if all the matrices of the coefficients $u, v, w$ are positive definite, i.e. $u_j, v_j > 0$ and $u_j v_j > w_j^2$ (determinant is larger than zero).