Multivariate Geostatistics

D. Renard

N. Desassis

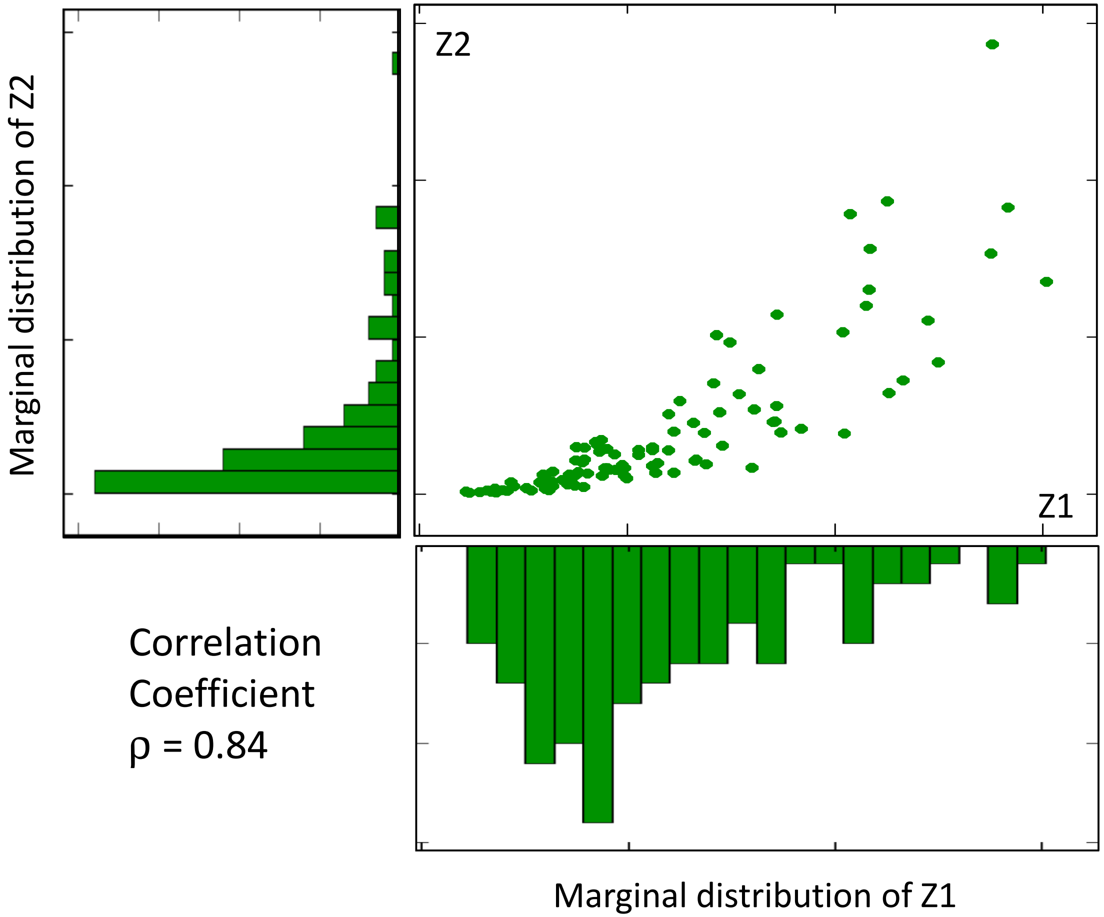
o Why multivariate geostatistics

- Highlight structural relationship between variables
- Improve the estimation of one variable using auxiliary variables :
  - sampled at the same locations : “isotopic” case
  - not all sampled at the same points : “heterotopic” case
- Estimate several variables consistently
- Must be extended to any set of variables

- Examples:
  - Top and bottom of a layer
  - Depth of a horizon and gradient (slope) information
  - Thickness and accumulation (2-D orebody)
  - Indicator of various facies

o Point Statistics

- Covariance: $$C_{12} = Cov(Z_1, Z_2) = E\left[(Z_1 - m_1)(Z_2 - m_2)\right]$$
- Scatter plots



Correlation Coefficient
$\rho = 0.84$

o Linear Regression

- Regressions

Linear regression of Z_2 over Z_1: $Z_2^* = aZ_1 + b$

Committed error: $R = Z_2 - Z_2^* = Z_2 - aZ_1 - b$

Non bias: $E(R) = m_2 - am_1 - b = 0 \Leftrightarrow b = m_2 - am_1$

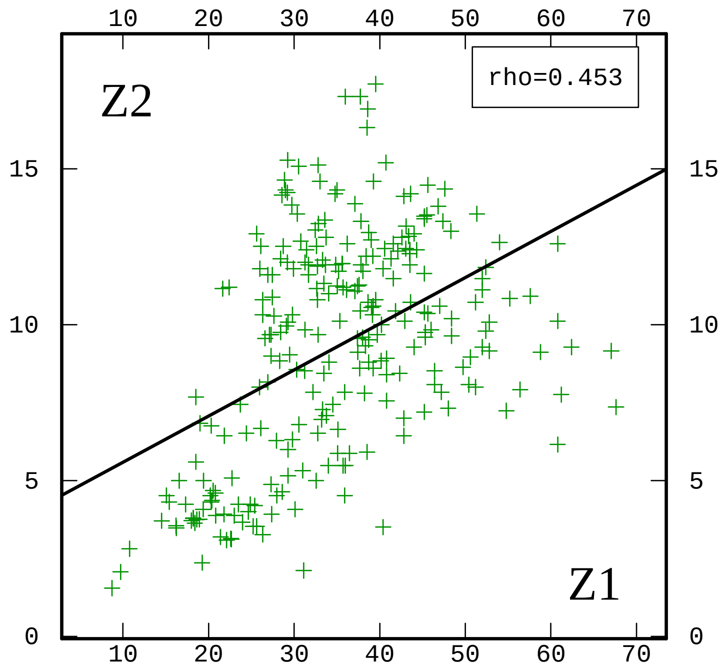
Optimality:

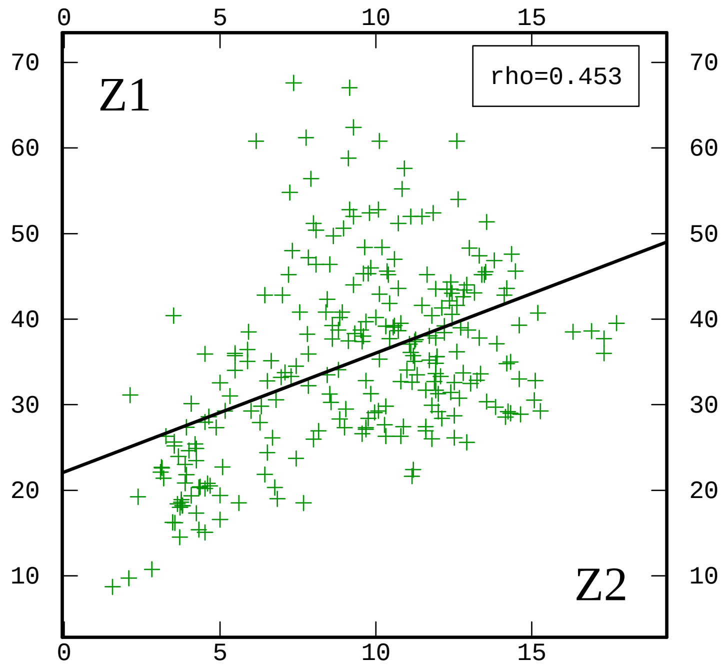
$$\begin{aligned} Var(R) &= Var(Z_2) + a^2 Var(Z_1) - 2aCov(Z_1, Z_2) \\ &= \sigma_2^2 + a^2\sigma_1^2 - 2aC_{12} \quad \text{minimum} \end{aligned}$$

$$\Rightarrow a = \frac{C_{12}}{\sigma_1^2} = \frac{Cov(Z_1, Z_2)}{Var(Z_1)} = \rho \frac{\sigma_2}{\sigma_1}$$

- Hence the linear regression: $\dfrac{Z_2^* - m_2}{\sigma_2} = \rho \dfrac{Z_1 - m_1}{\sigma_1}$

o Linear Regression





regression Z2|Z1 $\neq$ regression Z1|Z2

$$Z_2^* = \rho \frac{\sigma_2}{\sigma_1}(Z_1 - m_1) + m_2$$

$$Z_1^* = \rho \frac{\sigma_1}{\sigma_2}(Z_2 - m_2) + m_1$$

o Spatial Statistics

Monovariate case (reminders)

- Stationary:

$$m = E\left[Z(x)\right]$$

$$C(h) = Cov\left(Z(x), Z(x+h)\right) = E\left[\left(Z(x)-m\right)\left(Z(x+h)-m\right)\right]$$

$$Var\left[Z(x)\right] = C(0)$$

- Intrinsic:

$$E\left[Z(x+h)-Z(x)\right] = 0$$

$$\gamma(h) = \frac{1}{2}E\left[Z(x)-Z(x+h)\right]^2$$

o Spatial Statistics

Multivariate case:

- Stationary:

$$m_1 = E\left[Z_1(x)\right]$$

$$m_2 = E\left[Z_2(x)\right]$$

$$C_{12}(h) = Cov\left(Z_1(x), Z_2(x+h)\right) = E\left[\left(Z_1(x)-m_1\right)\left(Z_2(x+h)-m_2\right)\right]$$

- Intrinsic:

$$\gamma_{12}(h) = \frac{1}{2} E\left[Z_1(x+h)-Z_1(x)\right]\left[Z_2(x+h)-Z_2(x)\right]$$

o Model

- In order to ensure the positivity of the variances of all linear combinations, we must fit an authorized multivariate model simultaneously to all the simple and cross structures

- **Linear Model of Coregionalization.**
- All simple and cross-variograms are modeled using the same set of basic structures:

$$\gamma_{ij}(h) = \sum_k b_{ij}^k \gamma^k(h)$$

- Each sill matrix must be definite positive. In particular: $\left|b_{ij}^k\right| \leq \sqrt{b_{ii}^k b_{jj}^k}$
  - a structure can be present in 1 and/or 2 simple variograms and be absent from the cross-variogram
  - a structure which figures in a cross-variogram must also be present in the two simple variograms
  - the cross-variogram must remain within an “envelop”

o Cokriging

- Considering two variables Z_1 and Z_2, informed on two sets of samples S_1 and S_2 identical (isotopic) or not (heterotopic).

- **Cokriging** is an estimation technique which produces an estimation of Z_1 (or Z_2) at the target point x_0 so that the estimation error:

$$\varepsilon = Z_1(x_0) - Z_1^*(x_0)$$

  - is unbiased (zero mean)
  - is minimum variance (optimality)

Simple Cokriging

o Principle

- Z_1 and Z_2 are **stationary** with **constant known means**

$$m_1 = E\left[Z_1\right] \quad \text{and} \quad m_2 = E\left[Z_2\right]$$

- The estimation is obtained as a linear combination of all data

$$Z_1^*\left(x_0\right) = \sum_{S_1} \lambda_\alpha^1 Z_1(x_\alpha) + \sum_{S_2} \lambda_\beta^2 Z_2(x_\beta) + m_1\left(1 - \sum_{S_1} \lambda_\alpha^1\right) - m_2 \sum_{S_2} \lambda_\beta^2$$

- where the weights are obtained as the solution of the Cokriging system:

$$\begin{cases} \sum_{\alpha' \in S_1} \lambda_\alpha^1 C_{\alpha\alpha'}^{11} + \sum_{\beta \in S_2} \lambda_\beta^2 C_{\alpha\beta}^{12} = C_{\alpha 0}^{11} & \forall \alpha \in S_1 \\ \sum_{\alpha \in S_1} \lambda_\alpha^1 C_{\alpha\beta}^{12} + \sum_{\beta' \in S_2} \lambda_\beta^2 C_{\beta\beta'}^{22} = C_{\beta 0}^{12} & \forall \beta \in S_2 \end{cases}$$

- and the estimation variance: $Var(\varepsilon) = C_{00}^{11} - \sum_{\alpha \in S_1} \lambda_\alpha^1 C_{\alpha 0}^{11} + \sum_{\beta \in S_2} \lambda_\beta^2 C_{\beta 0}^{12}$

o In matrix notation

- Cokriging system (regular if no duplicate):

$$\begin{bmatrix} C_{\alpha\beta}^{11} & C_{\alpha\beta}^{12} \\ C_{\alpha\beta}^{21} & C_{\alpha\beta}^{22} \end{bmatrix} \times \begin{bmatrix} \lambda_{\alpha}^{1} \\ \lambda_{\beta}^{2} \end{bmatrix} = \begin{bmatrix} C_{\alpha 0}^{11} \\ C_{\beta 0}^{12} \end{bmatrix}$$

- Estimation:

$$Z_1^*(x_0) = \begin{bmatrix} Z_1(x_\alpha) \\ Z_2(x_\beta) \end{bmatrix}^t \times \begin{bmatrix} \lambda_{\alpha}^{1} \\ \lambda_{\beta}^{2} \end{bmatrix} + m_1\left(1 - \sum_{S_1} \lambda_{\alpha}^{1}\right) - m_2 \sum_{S_2} \lambda_{\beta}^{2}$$

- Variance of the estimation error:

$$Var(\varepsilon) = C_{00}^{11} - \begin{bmatrix} \lambda_{\alpha}^{1} \\ \lambda_{\beta}^{2} \end{bmatrix}^t \times \begin{bmatrix} C_{\alpha 0}^{11} \\ C_{\beta 0}^{12} \end{bmatrix}$$

o Principle

- Z_1 and Z_2 are **stationary** with **constant unknown means**:
- The estimation is obtained as a linear combination of data :

$$Z_1^*(x_0) = \sum_{S_1} \lambda_\alpha^1 Z_1(x_\alpha) + \sum_{S_2} \lambda_\beta^2 Z_2(x_\beta)$$

- where the Kriging weights are obtained as solution of the Kriging system:

$$\sum_{\alpha' \in S_1} \lambda_\alpha^1 C_{\alpha\alpha'}^{11} + \sum_{\beta \in S_2} \lambda_\beta^2 C_{\alpha\beta}^{12} + \mu_1 = C_{\alpha 0}^{11} \quad \forall \alpha \in S_1$$

$$\sum_{\alpha \in S_1} \lambda_\alpha^1 C_{\alpha\beta}^{12} + \sum_{\beta' \in S_2} \lambda_\beta^2 C_{\beta\beta'}^{22} + \mu_2 = C_{\beta 0}^{12} \quad \forall \beta \in S_2$$

$$\sum_{\alpha \in S_1} \lambda_\alpha^1 = 1$$

$$\sum_{\beta \in S_1} \lambda_\beta^2 = 0$$

o In matrix notation

- Cokriging system (regular if no duplicate):

$$\begin{bmatrix} C_{\alpha\beta}^{11} & C_{\alpha\beta}^{12} & 1 & 0 \\ C_{\alpha\beta}^{21} & C_{\alpha\beta}^{22} & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} \lambda_\alpha^1 \\ \lambda_\beta^2 \\ \mu_1 \\ \mu_2 \end{bmatrix} = \begin{bmatrix} C_{\alpha 0}^{11} \\ C_{\beta 0}^{12} \\ 1 \\ 0 \end{bmatrix}$$

- Variance of the estimation error:

$$Var(\varepsilon) = C_{00}^{11} - \begin{bmatrix} \lambda_\alpha^1 \\ \lambda_\beta^2 \\ \mu_1 \\ \mu_2 \end{bmatrix}^t \times \begin{bmatrix} C_{\alpha 0}^{11} \\ C_{\beta 0}^{12} \\ 1 \\ 0 \end{bmatrix}$$

- Ordinary cokriging can be written in variogram

Cokriging weights

o Remarks

- Pay attention to the order of magnitude of the weights:
  - The weights of Z_1 have no unit
  - The weights of Z_2 have the unit: $\dfrac{Z_1}{Z_2}$
- In Ordinary Cokriging: $\sum_{\beta \in S_1} \lambda_\beta^2 = 0$
  - The negative weights of Z_2 when associated to large values, can lead to a negative cokriged estimation.

o Generalities

- Cokriging can be simplified if:
  - Variables are spatially independent:

$$C_{ij}(h) = Cov\left[Z_i(x), Z_j(x+h)\right] = 0 \quad \forall h$$

  - Variables are intrinsically correlated

$$\frac{C_{ij}(h)}{C_{ii}(h)} = cste \quad \forall i, j$$

- Then Cokriging of each variable coincides with Kriging (in isotropic case)

Cokriging simplifications

o Generalities

- Cokriging can be simplified in the **model with residuals** (Markov):

$$C_{12}(h) = a\ C_{11}(h)$$

$$C_{22}(h) = a^2 C_{11}(h) + C_R(h)$$

- This corresponds to the following decomposition:

$$Z_2(x) = a\ Z_1(x) + b + R(x)$$

with R and Z1 not correlated

- Then Cokriging is equivalent to 2 Kriging

$$\begin{cases} Z_1^{\ CK} = Z_1^{\ K} \\ Z_2^{\ CK} = a\ Z_1^{\ K} + b + R^K \end{cases}$$

o General definition

- If the variable Z_1 is known exhaustively and when cokriging a target, we use:
  - The two variables measured at sample points
  - The value of Z_1 collocated on the target sample
- Collocated (simple) Cokriging system for estimating Z_2 at target:

$$\begin{bmatrix} C^{11}_{\alpha\beta} & C^{12}_{\alpha\beta} & C^{11}_{\alpha 0} \\ C^{21}_{\alpha\beta} & C^{22}_{\alpha\beta} & C^{12}_{\alpha 0} \\ C^{11}_{\alpha 0} & C^{12}_{\alpha 0} & C^{11}_{00} \end{bmatrix} \times \begin{bmatrix} \lambda^1_\alpha \\ \lambda^2_\beta \\ \lambda^1_0 \end{bmatrix} = \begin{bmatrix} C^{12}_{\alpha 0} \\ C^{22}_{\beta 0} \\ C^{12}_{00} \end{bmatrix}$$

- Note that the last column-line of the system changes for each target: this does not allow optimization in the Unique neighborhood (unless using some algebraic trick)

o Extension of the Markov Model

- We start from the same decomposition:

$$Z_2(x) = a\ Z_1(x) + b + R(x)$$

- Consider that Z_1 is known exhaustively:

$$\begin{aligned} Z_2^{CK}(x_0) &= a\ Z_{1,0} + b + R^K(x_0) \\ &= a\ Z_{1,0} + b + \sum_\alpha \lambda_\alpha \left[Z_{2,\alpha} - aZ_{1,\alpha} - b \right] \\ &= \sum_\alpha \lambda_\alpha Z_{2,\alpha} + a\left(Z_{1,0} - \sum_\alpha \lambda_\alpha Z_{1,\alpha} \right) + b\left(1 - \sum_\alpha \lambda_\alpha \right) \end{aligned}$$

- Non bias implies that:

$$\sum_\alpha \lambda_\alpha = 1$$

$$\sum_\alpha \lambda_\alpha Z_{1,\alpha} = Z_{1,0}$$

o Extension of the Markov Model

- Collocated Cokriging system (with 2 variables) corresponds to kriging of the residuals under unbiasedness constraints:

$$\begin{bmatrix} C_{\alpha\beta} & 1 & Z_{1,\alpha} \\ 1 & 0 & 0 \\ Z_{1,\alpha} & 0 & 0 \end{bmatrix} \times \begin{bmatrix} \lambda_\alpha \\ \mu_1 \\ \mu_2 \end{bmatrix} = \begin{bmatrix} C_{\alpha 0} \\ 1 \\ Z_{1,0} \end{bmatrix}$$

- This corresponds to the well-known **external drift kriging** method

o Variable extraction

- When the variable Z is modeled using a nested variogram

$$C(h) = C_1(h) + C_2(h)$$

- We can imagine the following decomposition:

$$Z(x) = Z_1(x) + Z_2(x) + m$$

assuming that:

$$Cov\left(Z_1(x), Z_1(x+h)\right) = C_1(h)$$

$$Cov\left(Z_2(x), Z_2(x+h)\right) = C_2(h)$$

$$Cov\left(Z_1(x), Z_2(x+h)\right) = 0$$

- Starting from Z measurements, we estimate $Z_1^*(x) = \sum_\alpha \lambda_\alpha Z_\alpha(x)$

- Factorial Cokriging system: $\left[C_{\alpha\beta}\right] \times \left[\lambda_\alpha\right] = \left[C_{\alpha 0}^1\right]$

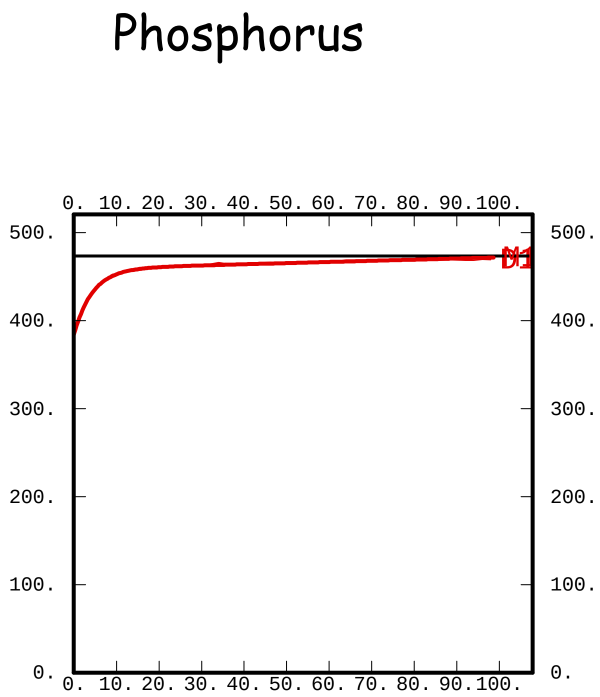
o Application

- In metallography, trace elements are usually masked by instrumental noise linked to several hours of exposure

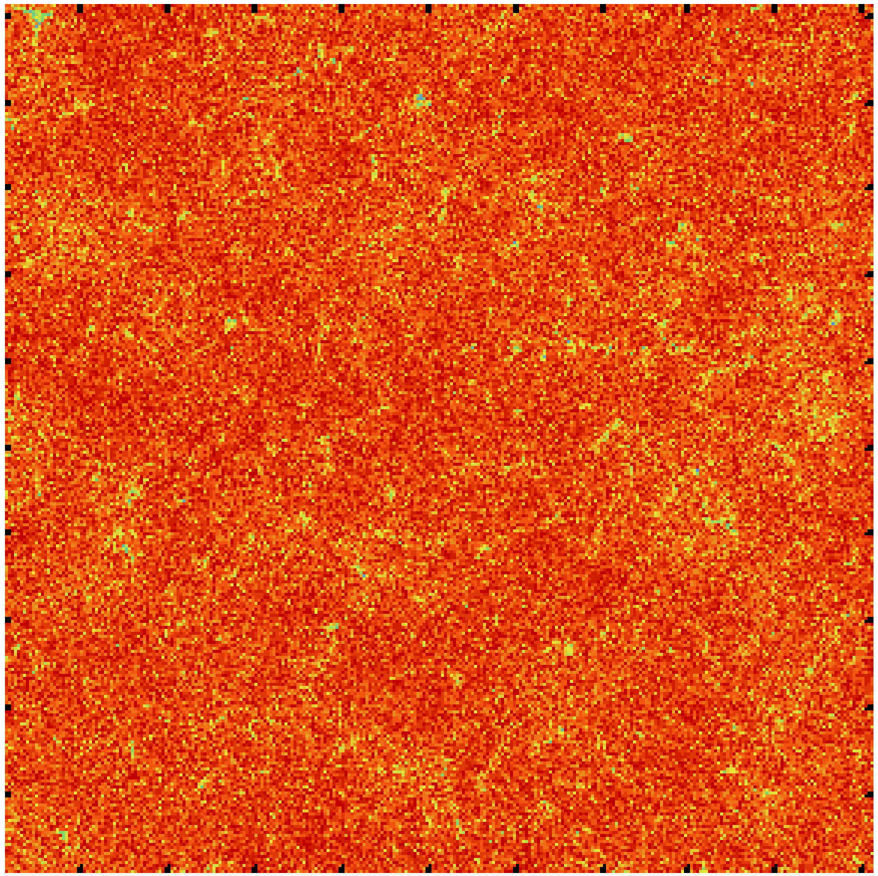
- In this application, the treated sample represents an image of 512*512 pixels where the P trace elements is measured.
  Factorial Kriging Analysis is used to filter the noise out.

- Moreover, several additional elements can be used to enhance the noise filtering: this is the case with Cr and Ni.

o Monovariate



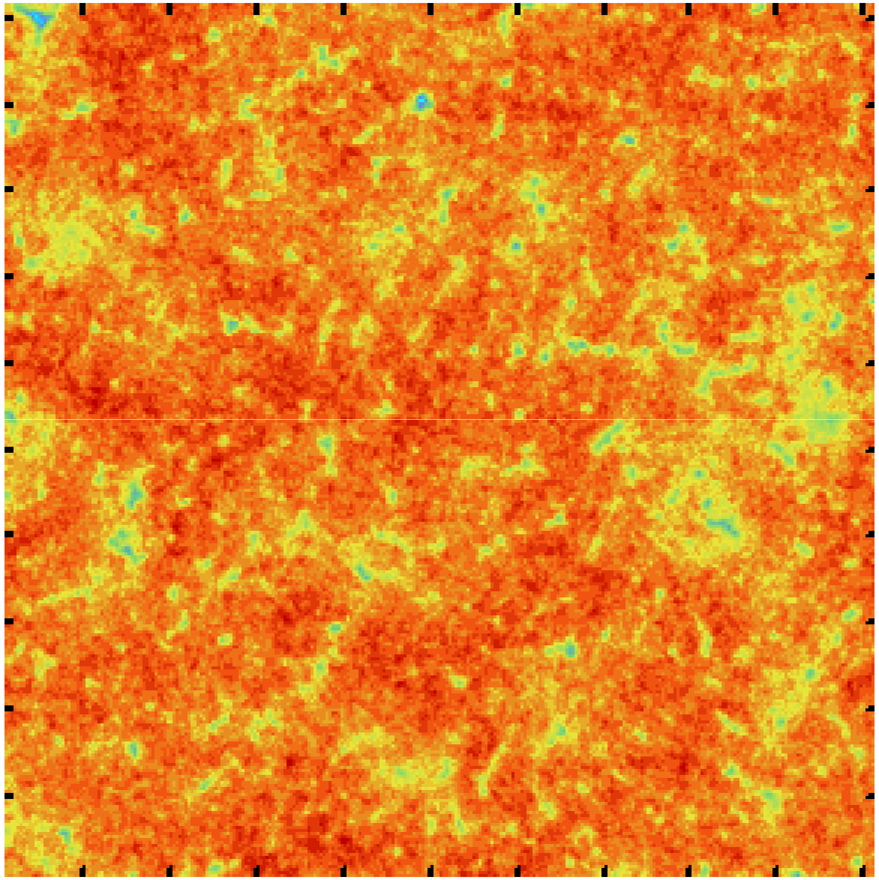
$$\gamma(h) = 384\ Nugget + 75\ Exp(h/13) + 13\ |h|$$



o Monovariate

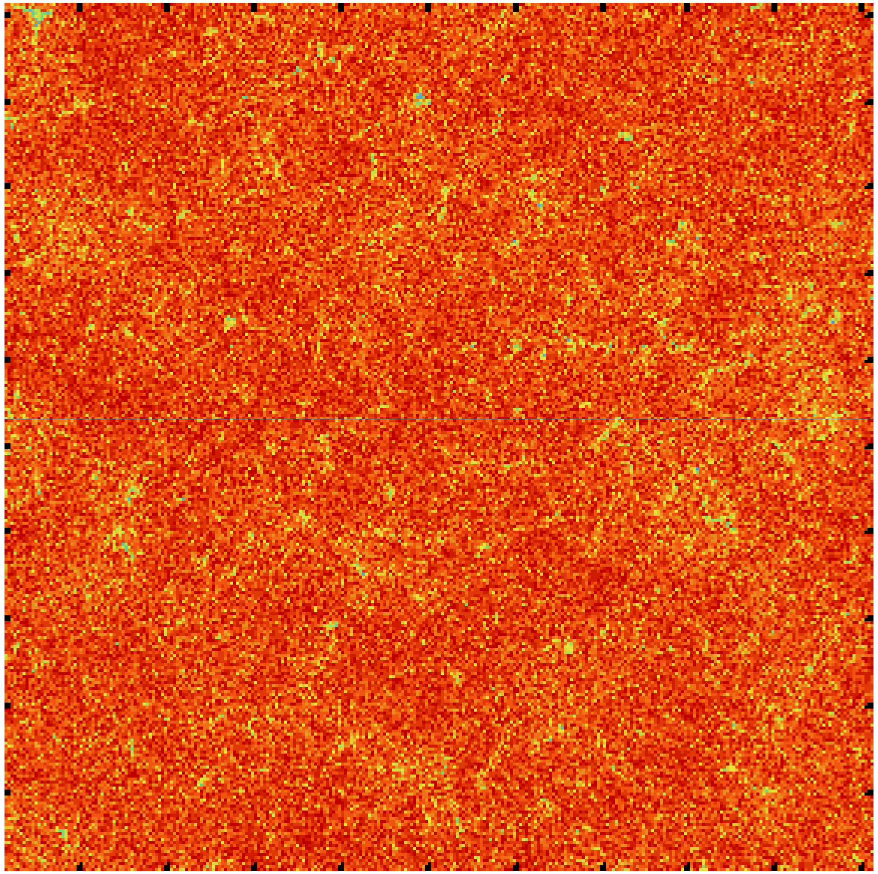
De-noised Phosphorus

monovariate
nugget effect filtering



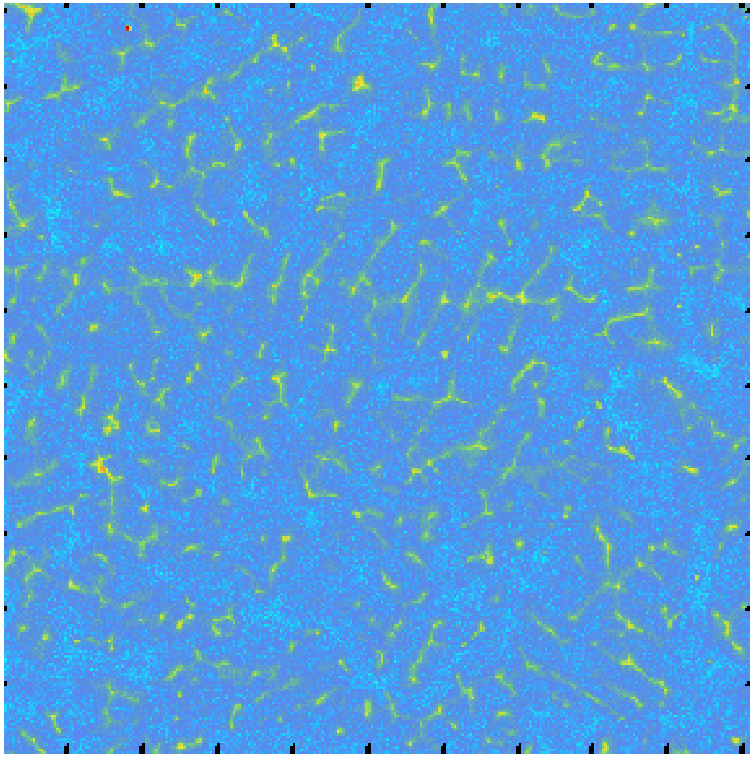
o Multivariate

Phosphorus

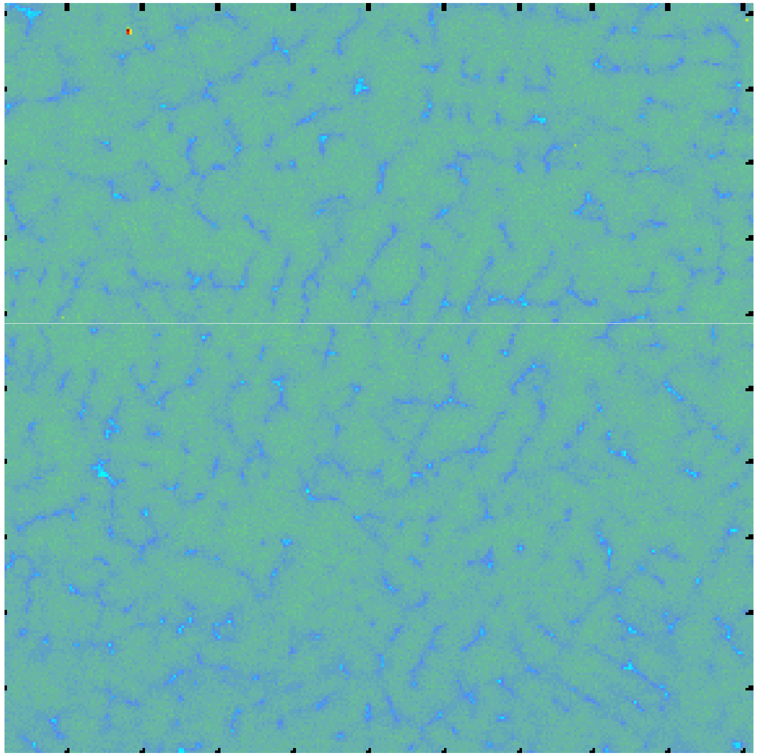


o Multivariate

Auxiliary variables



Nickel

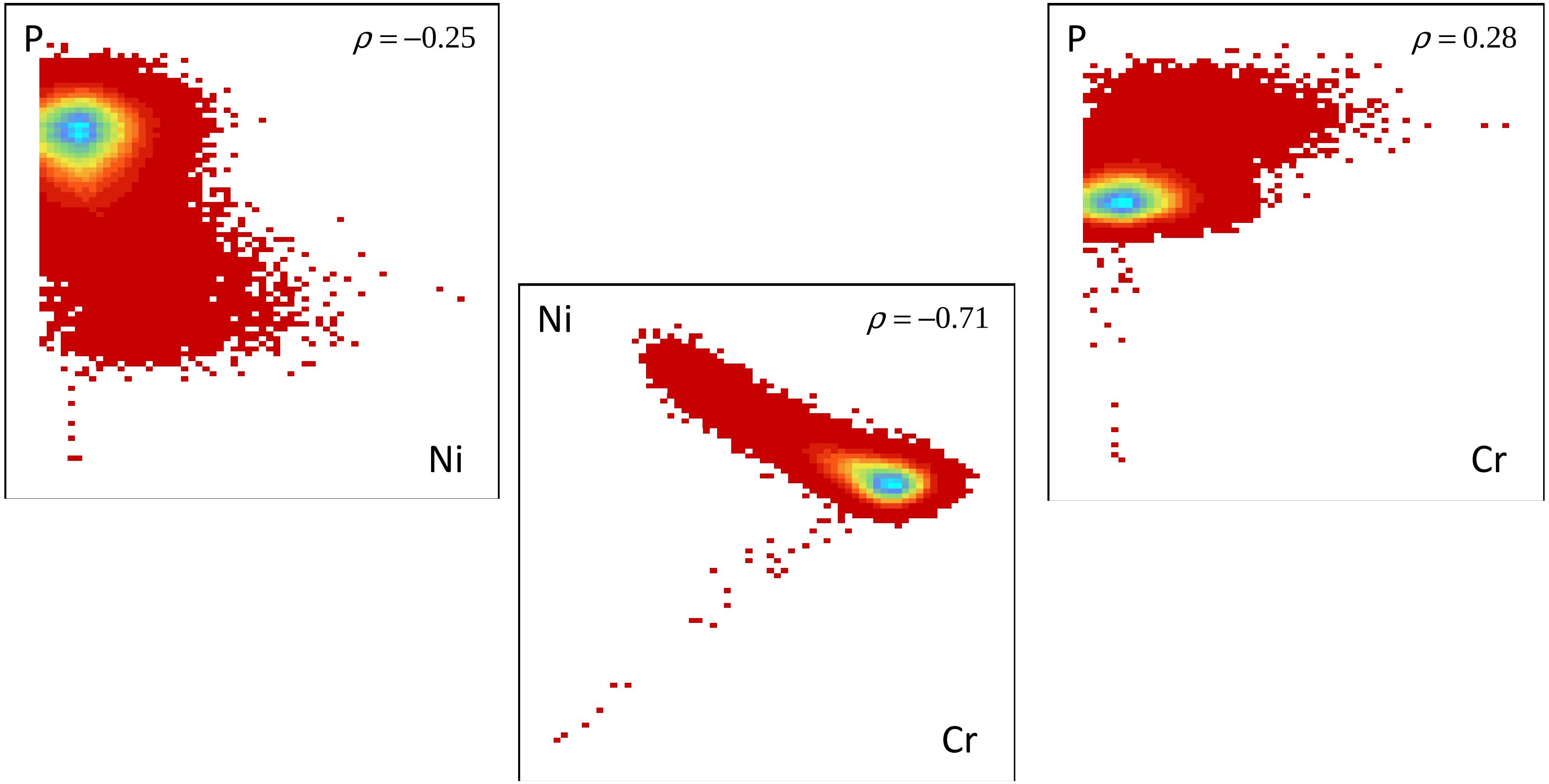


Chromium

Factorial Cokriging Analysis

o Multivariate

Correlations between variables

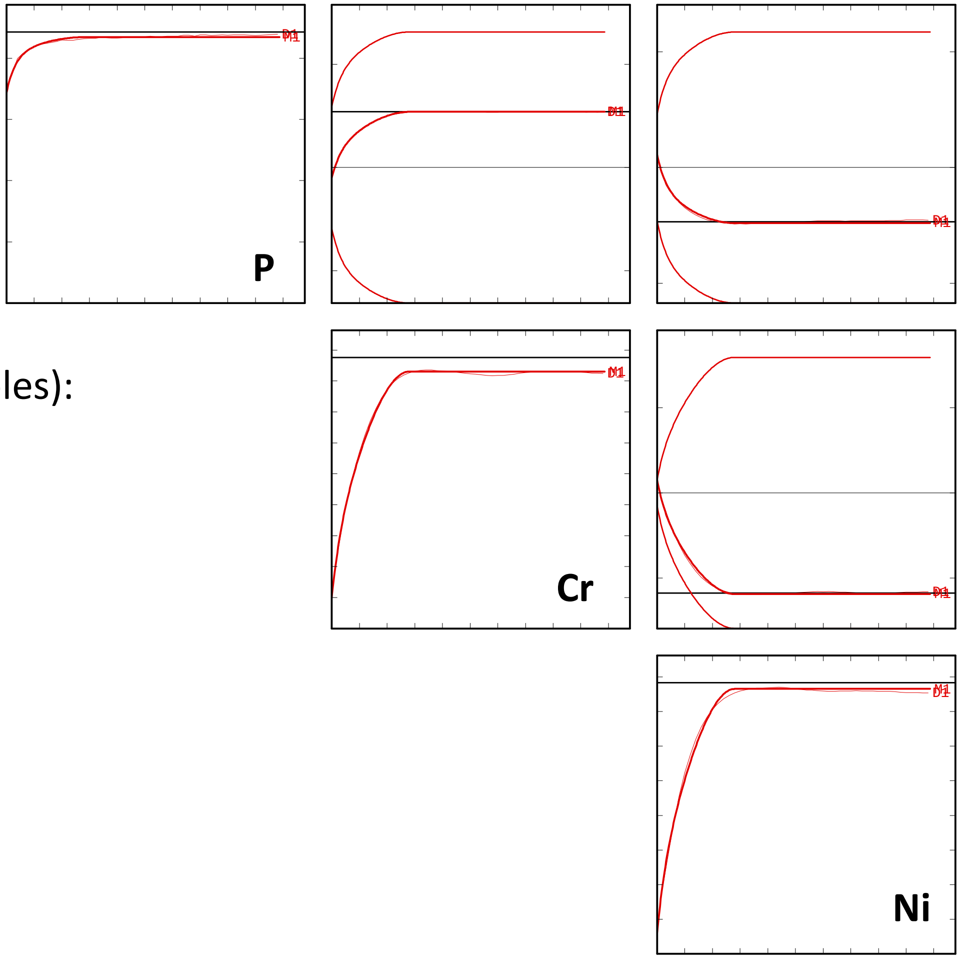


o Multivariate

Multivariate Model

Variances

P	443
Cr	876096
Ni	781456



Correlation matrices (normalized variables):

$$Nugget \begin{pmatrix} 77.4 & -5.0 & 5.8 \\ -5.0 & 11.6 & 8.8 \\ 5.8 & 8.8 & 8.0 \end{pmatrix}$$

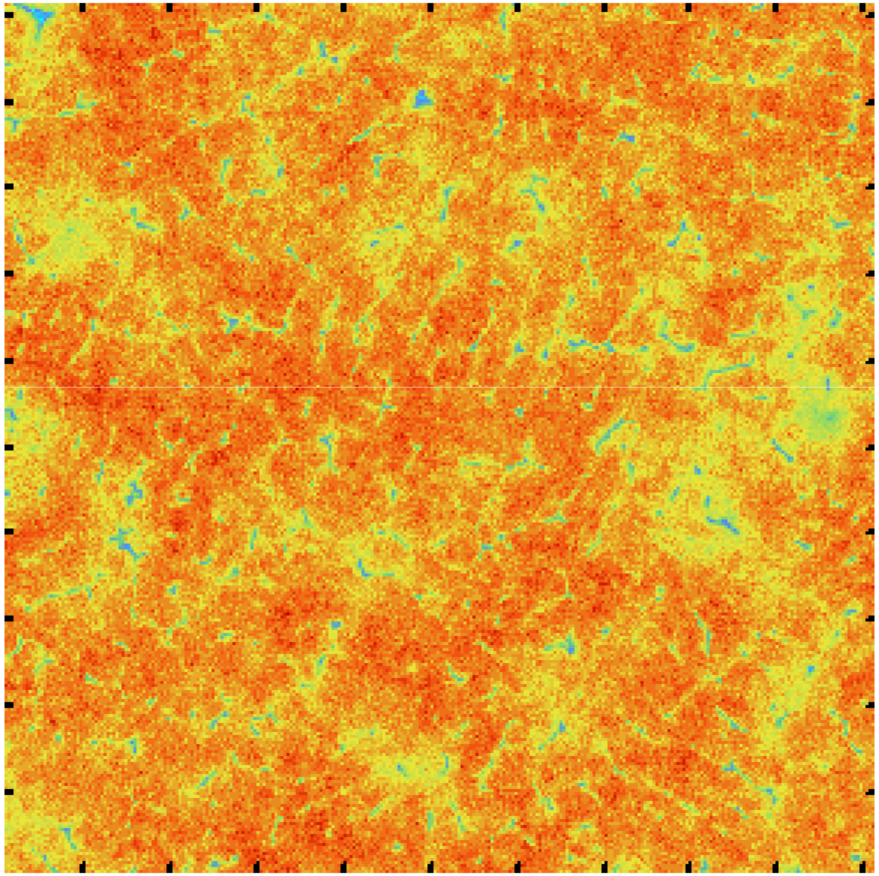
$$+Exp(h/10) \begin{pmatrix} 14.7 & 14.8 & -17.2 \\ 14.8 & 22.2 & -22.3 \\ -17.2 & -22.3 & 23.4 \end{pmatrix}$$

$$+Sph(h/28) \begin{pmatrix} 5.6 & 0 & 0 \\ 0 & 61.0 & -58.0 \\ 0 & -58.0 & 66.6 \end{pmatrix}$$

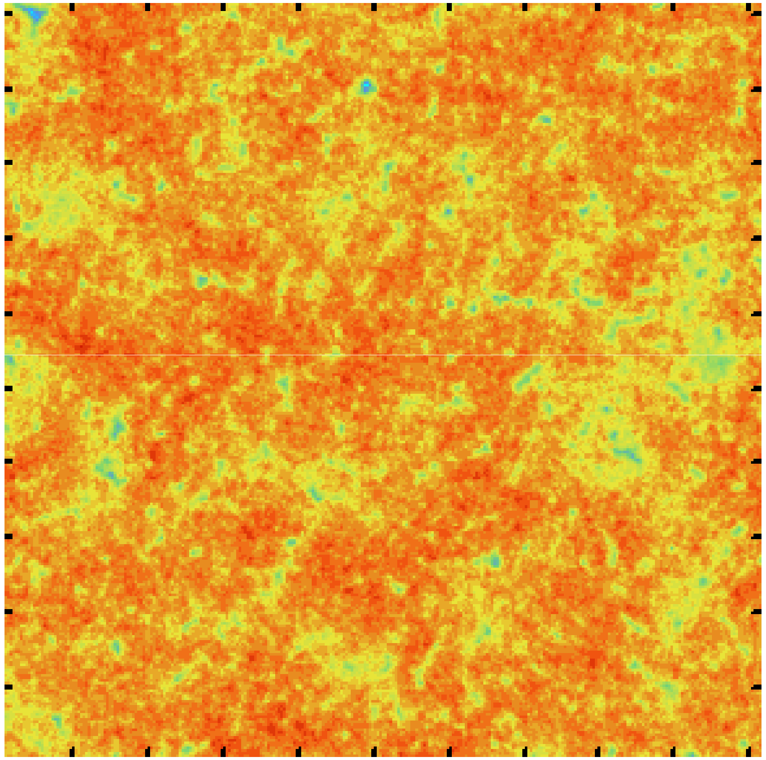
o Multivariate

De-noised Phosphorus

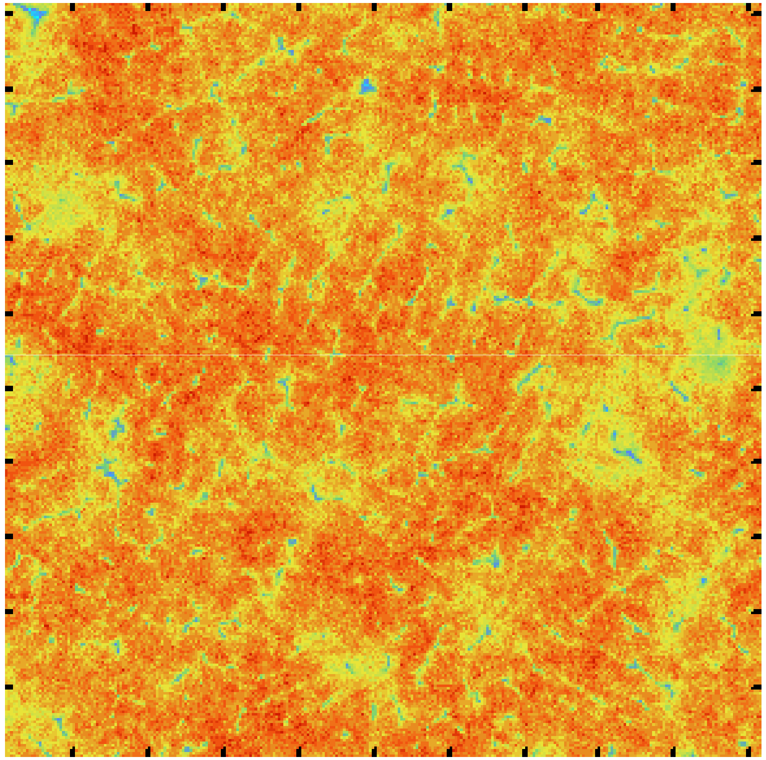
multivariate
nugget effect filtering



o Comparisons



Monovariate



Multivariate

o Comparisons