

Plug-ins for spatial continuity analysis

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1. Definition

These plugins are a set of tools to help definition of continuity and modeling permissible functions in geostatistical analysis. There are 4 plugins, 3 related with experimental values and 1 with automatic fitting of variogram models. They are all based on gamV of GSLib. The first plugin is an automated form to generate h-scatterplots of samples in a defined direction. The second plugin is a variogram/covariance map. The third is related with experimental continuity function calculations and the forth is an automatic fitting of variograms in a LMC model.

Hscatterplot is a scatterplot of two set of samples separated by a vector distance. This plugin can help the modeler to understand outlier values along a direction. The algorithm output generates a matplotlib image with scatters of experimental pairs given an orientation.

Variomap is an algorithm to create maps of variogram and covariogram over a plane to determine directions of maximum, secondary and vertical continuity trough a set of samples. The algorithm has as an output a matplotlib image with interpolated experimental continuity functions given a plane orientation. The orientation is the attitude of the line of maximum decline.

Variograms is an algorithm to calculate several spatial continuity functions. There are the common experimental values as variogram and covariogram and robust models as pairwise and relative variograms. Variograms plugin have an output list for calculations in automatic fitting plugin.

Automatic fitting plugin is an algorithm to automate modeling of experimental variograms in a LMC (Linear model of correlogionalization) and LMR(Linear model of regionalization). It uses the output file of Variograms plugin. This plugin generates as output a matplotlib image with experimental values of maximum, secondary and vertical directions plotted and their models. The variogram parameters are printed in command prompt.

2. Variography theory

First step of geostatistical analysis is calculate the degree of continuity between random variables. This can be due with statistical functions of spatial data. As considered a stationary hypothesis this functions can be prior determined only by the vector direction and are not related with spatial Cartesian of samples. Spatial continuity functions can be described by the propriety measure as statistics to calculate similarity or dissimilarity[Han95]. Dissimilarity function can be describe as differences between two variables separated by a vector h , as demonstrated in Figure 1. The most common function of dissimilarity is variogram.

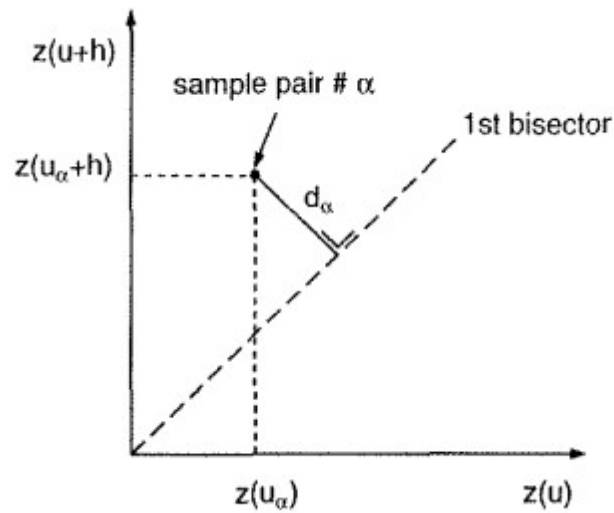


Figure 1 – Dissimilarity function demonstrated in h-scatterplot[Pie97]

The experimental variogram function can be calculated by the Equation 1:

$$\gamma(h) = \frac{1}{2n} \sum_{i=1}^n (z_i - z_{i+h})^2 \quad (1)$$

As z_i is the sample value in a support i , z_{i+h} is the sample value for a vector distance h and n is the total number of variables.

Another important experimental value is the covariogram and can be related with Equation 2. Covariogram is a measure of similarity of spatial variables:

$$C(h) = \frac{1}{n} \sum_{i=1}^n (z_i - m_i)(z_{i+h} - m_{i+h}) \quad (2)$$

As m_i the average value in the tail of the vector and m_{i+h} the average value in the head of the vector. There are several spatial continuity functions for calculating similarity or dissimilarity of random variables, some of them are more affected by outlier values and other have much more mathematical mean than others. Table 1 demonstrates different spatial continuity functions

Table 1 – Different spatial continuity functions

Experimental function	Propertie measured	Equation
Variogram	Data dissimilarity	$\sum_{i=1}^n \frac{(z_i - z_{i+h})^2}{n}$
Covariogram	Data similarity	$\frac{1}{n} \sum_{i=1}^n (z_i - m_i)(z_{i+h} - m_{i+h})$

Correlogram	Data similarity	$\frac{1}{n} \sum_{i=1}^n \frac{(z_i - m_h)(z_{i+h} - m_h)}{\sigma_h^2 \sigma_t^2}$
Pair-Wise	Data dissimilarity	$\frac{1}{n} \sum_{i=1}^n \frac{(z_i - z_{i+h})^2}{\left[\frac{z_i - z_{i+h}}{2} \right]^2}$
Madogram	Data dissimilarity	$\frac{1}{n} \sum_{i=1}^n z_i - z_{i+h} $
Relative variogram	Data dissimilarity	$\frac{1}{n} \sum_{i=1}^n \frac{(z_i - z_{i+h})^2}{\left[\frac{m_i + m_{i+h}}{2} \right]^2}$

For a regular spatial location of data, variogram and covariograms can be calculated only by regular spatial distances and multiple of lag distance. Figure 2 demonstrates the variogram calculation for a west-east direction.

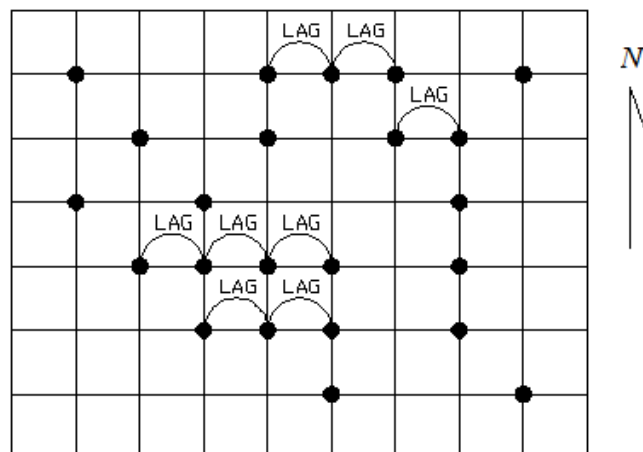


Figure 2 – variogram calculations in a regular grid

In a case of irregular grid, variograms and covariograms can be calculated using tolerances in geometrical parameters. This can rely on lag tolerance, angular tolerance and band tolerance. Figure 3 demonstrates the tolerances in a direction for calculating variograms.

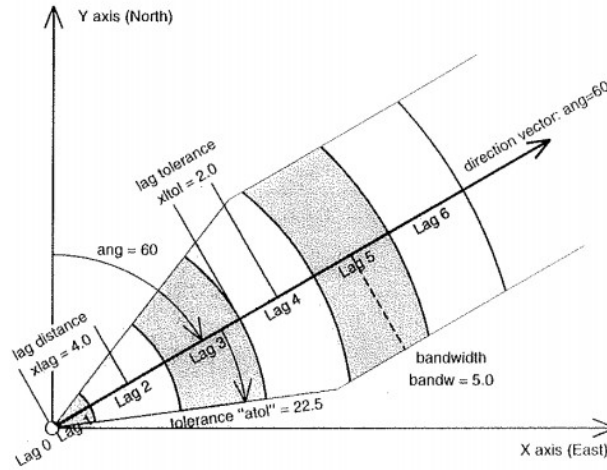


Figure 3 – Variogram tolerances[Cla981]

Different programs will use different aspects related with direction tolerances. Sgems use a cylindrical bandwidth despite GSlib that use different tolerances for horizontal and vertical directions.

Experimental variograms are the base for using variogram models. A permissible variogram model can create conditions for resolution of kriging matrices. A permissible model must be:

- (i) The model must be a pair function $\gamma(h) = \gamma(-h)$
- (ii) The model must be a positive definite function and all combinations of their values must be greater or equal to zero as demonstrates in Equation 3:

$$\sum_{i=1}^n \sum_{j=1}^n \lambda_i \lambda_j \gamma(x_i - x_j) \geq 0 \quad (3)$$

As λ_i a proportional constant and x_i e x_j are the differences of the variables in a support i and j .

- (iii) The model must be limited by a value, generally characterized as a prior variance of phenomena.

Three models are the most common used in geostatistical analysis: the spherical model, the Gaussian model and the exponential model. All of them are called transitive models and have a sill value that function reaches. Figure 4 demonstrated the mean models for spatial analysis.

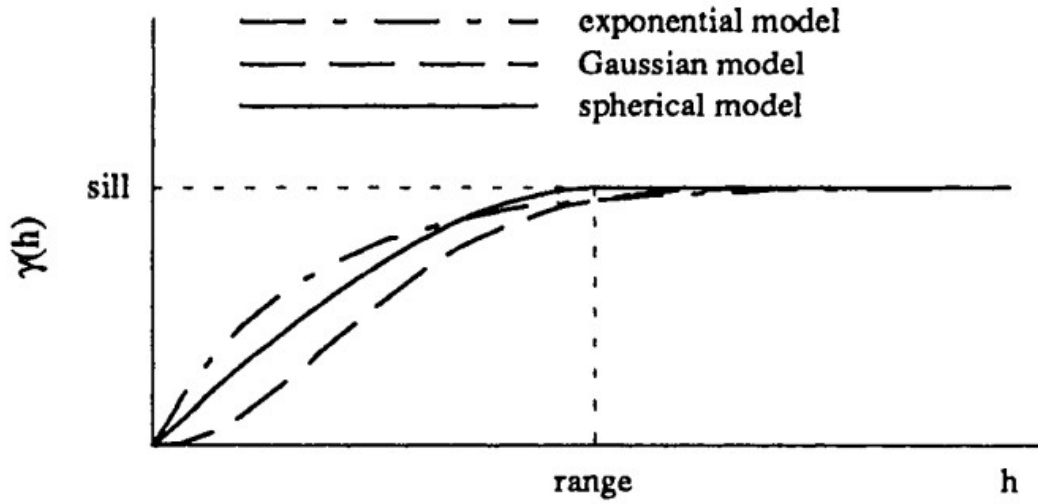


Figure 4 – Variogram models, Spherical, Gaussian and Exponential.[Iss89]

The equations of exponential model, gaussian model and spherical model are demonstrated in Equations 4,5 and 6

$$C_{\text{exp}}(h) = b e^{-\frac{|h|}{a}} \quad (4)$$

$$C_{\text{gauss}}(h) = b e^{-\left(\frac{h}{a}\right)^2} \quad (5)$$

$$C_{\text{sph}}(h) = \begin{cases} \frac{3}{4a^3} (ah - h^2) & 0 \leq h \leq a \\ b & h > a \end{cases} \quad (6)$$

As **b** a sill value, **a** a range value and **h** a distance vector. A nugget effect can be incorporated in these models to represent the variance in short scale and the errors associated with sampling. Different directions can have different ranges and sills. This phenomena called anisotropy and can be understand as differences in parameters along rotation of variograms.

Two are the most common anisotropies: The geometrical form and the zonal form. The geometrical form can be represented as different ranges troughs different directions. Figure 5 demonstrates a geometrical

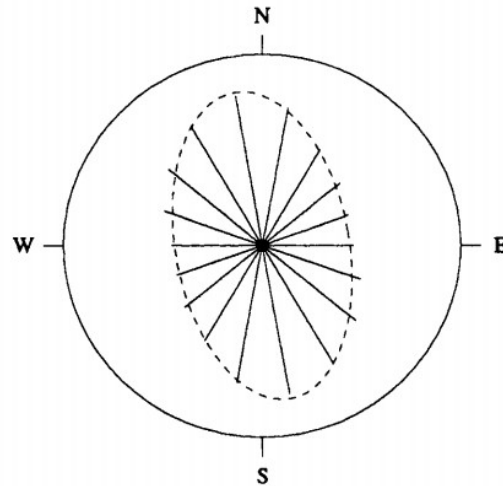


Figure 5 - Geometrical anisotropy [Iss89]

The zonal form can be describe as differences in sill values thought the rotation of variograms. Figure 6 demonstrates a zonal and geometric anisotropy in the same variogram plane. The variogram which have different patamar in different direction is considered a case of zonal anisotropy. The variograms which have the same patamar but different ranges can be considered a case of geometric anisotropy.

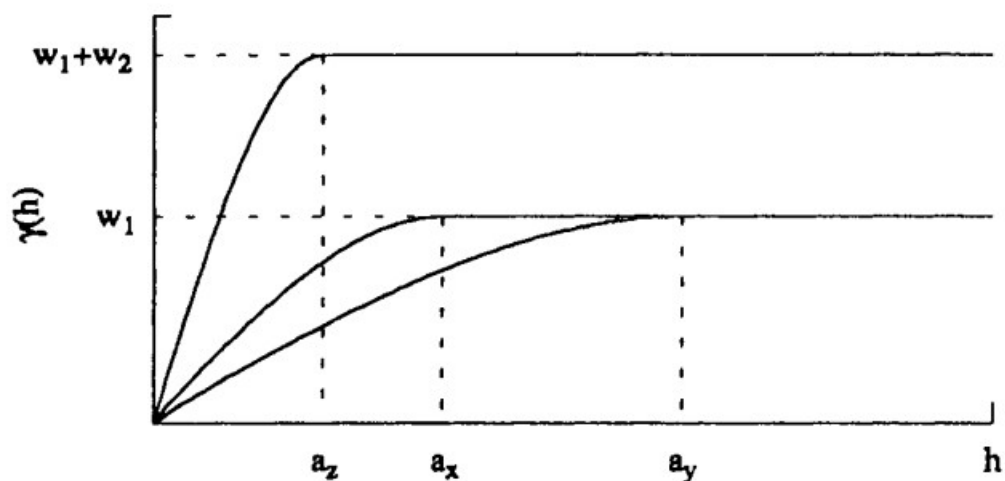


Figure 6 - Zonal and geometric anisotropy[Iss89]

Variogram models can be adjusted automatically using mathematical criteria. For not creating artifacts variogram models can be adjusted in previous directions of maximum, secondary and vertical continuity. These methods are called semi-automatic adjustment and are more reliable than free mathematical adjustment.

Variograms can be modeling using least squares methodology as demonstrated in Equation 7:

$$\sum_{i=1}^n \delta_d^i \delta_p^i (\gamma_{\text{exp}} - \gamma_{\text{mod}})^2 \quad (7)$$

As δ_d^i the weights of lag distance, δ_p^i is the weights of experimental variogram pairs, γ_{exp} are the experimental variogram values and γ_{mod} is the function modeled. For different variogram models, the one with lower residual value demonstrated in equation 7 is the best adjustment. Using Monte Carlo methodology and interating all possible parameters and models, we can find a model that minimizes the residual values of variogram. Figure 7 demonstrates a model adjusted by experimental values.

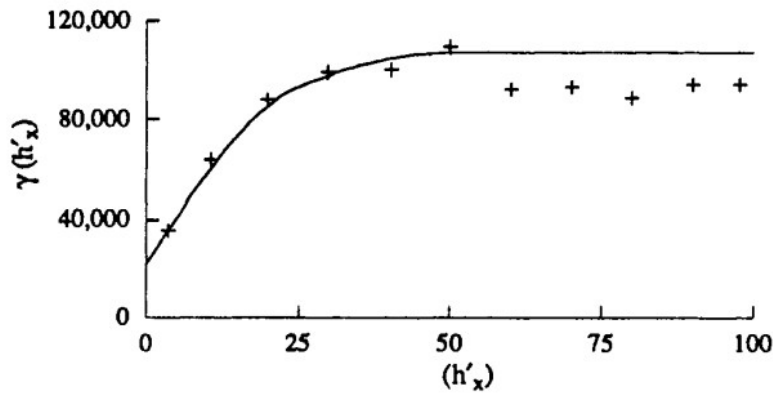


Figure 7 - Model adjusted

3. Plugins for variogram analysis

3.1 Hscatterplot

3.1.1 Algorithm

The algorithm of hscatterplot proceeds in three steps

- 1) Calculate all Cartesian values between points
- 2) Define a permissible point value despite tolerances
- 3) Plot a graph with permissible values along

3.1.2 Plug-in interface

The inputs of hscatterplot is defined as relation above:

- I. Box of head properties of samples
- II. Box of tail properties of samples
- III. Define azimuth and dip for this scatter
- IV. Define variogram parameters
 - a. Number of lags
 - b. Lag distance

- c. Linear tolerance
- d. Horizontal angular tolerance
- e. Vertical angular tolerance
- f. Horizontal bandwidth
- g. Vertical bandwidth

Head Property

i

<- None ->

Tail Property

ii

<- None ->

Azimuth

iii

Dip

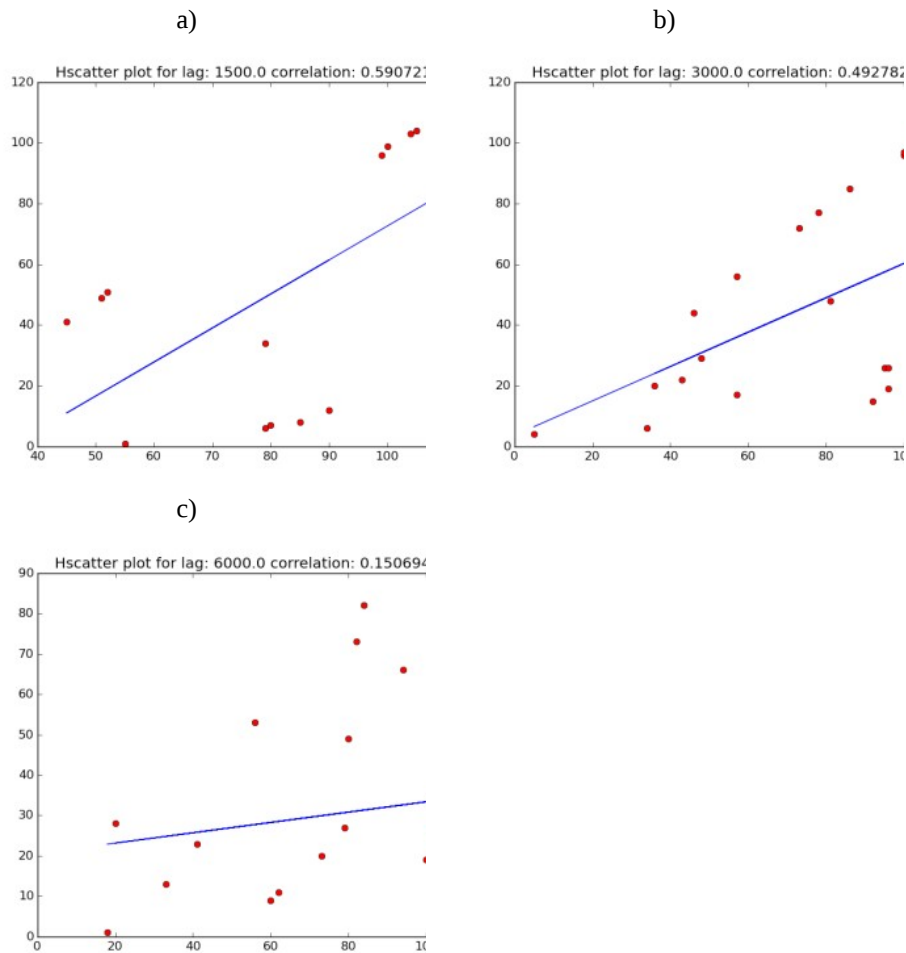
Varlogram Parameters

iv

Number of lags	
Lag Distance	0,01
Linear tolerance	0,01
Horizontal angular tolerance	
Vertical angular tolerance	
Horizontal bandwidth	0,01
Vertical bandwidth	0,01

3.1.3 Results

The results of h-scatterplot is a list of h-scatterplots for a direction as demonstrated below



3.2 Variogram Map

3.2.1 Algorithm

The algorithm of variogram map proceeds in 4 steps

- 1) Calculate all Cartesian values between points
- 2) Define a permissible point value despite tolerances
- 3) Calculate experimental values and interpolated them
- 4) Plot a graph with permissible values along

3.2.2 Plug-in interface

The inputs of variomap are defined as relation above:

- I. Box of head properties of samples
- II. Box of tail properties of samples
- III. Define covariogram map or variogram map
- IV. Define the direction of the line of maximum declive of the plane
- V. Define variogram tolerances
 - a. Number of lags

- b. Lag distance
- c. Linear tolerance
- d. Horizontal angular tolerance
- e. Vertical angular tolerance
- f. Horizontal bandwidth
- g. Vertical bandwidth

Head Property*i*

<- None ->

Tail Property*ii*

<- None ->

Spatial function

☐ Covariance

☒ Variogram*iii*

Direction*iv*

Dip

Azimuth

Variogram Parameters*v*

Number of lags

Lag Distance

0,01

Linear tolerance

0,01

Horizontal angular tolerance

Vertical angular tolerance

Horizontal bandwidth

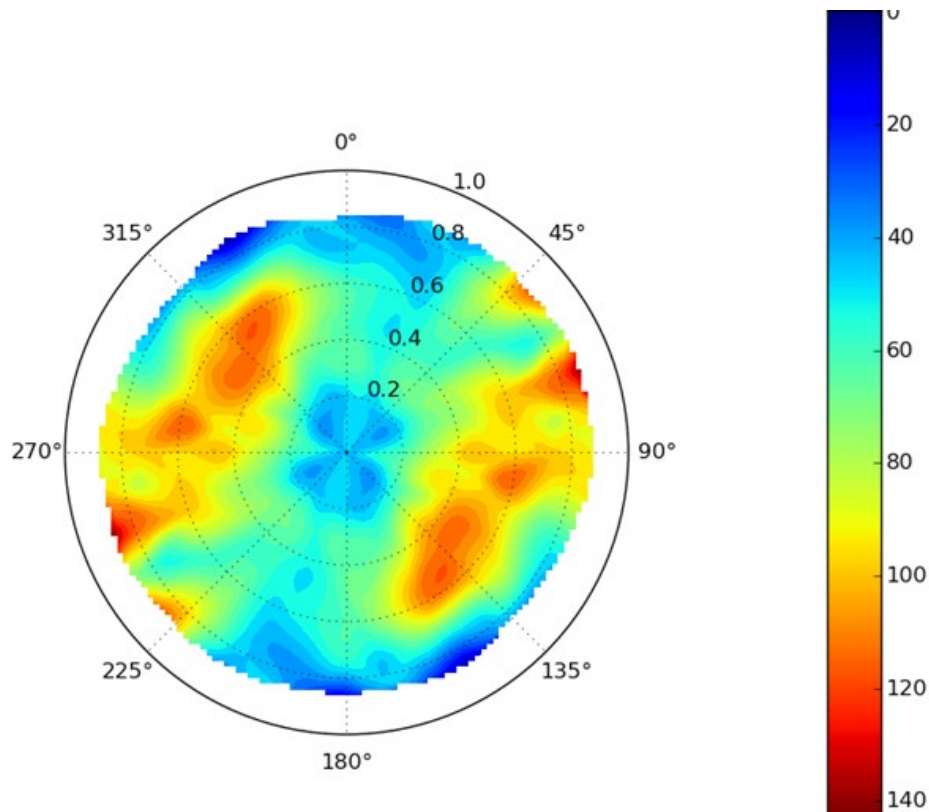
0,01

Vertical bandwidth

0,01

3.1.3 Results

The results of variogram map are demonstrated as a matplotlib image:



3.3 Experimental values calculation

3.3.1 Algorithm

This plugin follows 5 steps:

- 1) Calculate all Cartesian values between points
- 2) Define a permissible point value despite tolerances
- 3) Calculate experimental values
- 4) Generate a hml file for SGems use
- 5) Generate a report file for Automatic fitting calculations

3.3.2 Plug-in interface

The inputs of variomap are defined as relation above:

- I. Box for head property
- II. Box for tail property
- III. Save file report parameters
 - a. File address
 - b. Number related to head property (use for matrixes in automatic fitting)
 - c. Number related to tail property (use for matrixes in automatic fitting)
- IV. File address for SGems file
- V. Select spatial function calculation
 - a. Variogram

- b. Relative Variogram
 - c. Madogram
 - d. Correlogram
 - e. Covariogram
 - f. PairWise
- VI. Select direction parameters
 - a. Number of azimuths to calculate
 - b. Number of dips to calculate
 - c. Angular difference between azimuths
 - d. Angular difference between dips
 - e. Start azimuth
 - f. Start dip
- VII. Variogram parameters
 - a. Number of lags
 - b. Lag distance
 - c. Linear tolerance
 - d. Horizontal angular tolerance
 - e. Vertical angular tolerance
 - f. Horizontal bandwidth
 - g. Vertical bandwidth
- VIII. Option to invert correlogram axis

Head Property*i*

<- None ->

Tail Property*ii*

<- None ->

Save File report*iii*

File adress

Number of head

Number of tail

Save File SGems export*iv***Spatial function**☐ Variogram☐ Correlogram☐ Relative variogram☐ Covariogram☐ Madogram☒ PairWise*v***Direction***vi*

Number of Azimuths

Number of Dips

Azimuths angular difference

Dips angular difference

Start azimuth

Start dip

Variogram Parameters*vii*

Number of lags

Lag Distance

Linear tolerance

Horizontal angular tolerance

Vertical angular tolerance

Horizontal bandwidth

Vertical bandwidth

Options☐ Invert correlogram axis*viii*

3.3.3 Results

Plugin results in two .txt files. One with report of values used in automatic fitting demonstrated in Figure 8:

1	1					
2	1					
3	Azimuth	Dip	lag	variogram	pairs	
4	52.0	52.0	58.1545705606	9.24916637421	6	
5	52.0	52.0	116.57300937	21.2179040047	513	
6	52.0	52.0	145.511340995	29.554942594	1319	
7	52.0	52.0	197.025336662	35.7603360267	521	
8	52.0	52.0	256.302051659	50.1442324991	228	
9	52.0	52.0	296.095852557	34.6298718414	391	
10	52.0	52.0	343.511222479	48.8499528159	112	
11	52.0	52.0	391.829489694	31.8268508629	27	
12	52.0	52.0	451.015852412	36.0015474806	29	
13	52.0	52.0	494.202696064	6.06060007324	25	
14	142.0	0.0	26.9986893685	16.0213040128	46	
15	142.0	0.0	52.4256353591	20.997214893	88	
16	142.0	0.0	77.4004372674	26.61251121	221	
17	142.0	0.0	100.385019609	27.2642445317	1038	
18	142.0	0.0	123.674675849	27.7086215269	156	
19	142.0	0.0	143.618582892	21.7021290419	54	
20	142.0	0.0	176.775139503	19.0453477993	43	
21	142.0	0.0	193.450466109	55.0124522048	51	
22	142.0	0.0	225.774319131	72.8389951986	15	
23	142.0	0.0	244.069037124	32.7760599957	33	
24	52.0	142.0	97.4838048941	28.7166246092	311	
25	52.0	142.0	133.044757122	36.1656242728	3067	
26	52.0	142.0	218.894304164	35.3455600894	2537	
27	52.0	142.0	273.036004923	39.4407207622	2711	
28	52.0	142.0	354.154508621	36.8044364919	2044	

Figure 8 - Report file of experimental variograms

Other file is used for SGems variogram input, as demonstrated in Figure 9:

```
<experimental_variograms>
  <variogram>
    <title>variogram - azth=0, dip=0</title>
    <direction>6.12323e-017 1 0 </direction>
    <x>10 20 30 40 50 60 70 80 90 100 110 120 130 </x>
    <y>47269.6 58396.9 76246 76557.6 87014.7 85063.8 94962 84258.7 91352.9 88263.9 91812.1 88913.1 95804.9 </y>
    <pairs>378 606 569 755 771 1057 948 1167 945 1112 967 1082 973 </pairs>
  </variogram>
  <variogram>
    <title>variogram - azth=45, dip=0</title>
    <direction>0.707107 0.707107 0 </direction>
    <x>10 20 30 40 50 60 70 80 90 100 110 120 130 </x>
    <y>61165 90325.2 90205.1 100184 97945.8 89053.7 85506.5 83763.8 78781.6 79745.6 89975.6 93041.4 87755.7 </y>
    <pairs>347 520 605 725 695 651 875 687 849 822 711 689 796 </pairs>
  </variogram>
</experimental_variograms>
```

Figure 9 – Hml file to use in SGems program

3.4 Automatic fitting

3.4.1 Algorithm

This plugin follows 4 steps:

- 1) Import experimental values generated in plugin 3
- 2) Get principal directions of variogram
- 3) Automate variogram fitting in each direction
- 4) Approve variogram model if it is a LMC

3.4.2 Plug-in interface

The inputs of variomap are defined as relation above:

- I. Insert report file address generated in plugin 3.3
- II. Insert number of iterations used in Monte Carlo methodology
- III. Insert number of variograms for each variable
- IV. Insert the number of variables (direct + cross)
- V. Insert the number of lags for variograms
- VI. Insert the number of structures to model
- VII. Insert the minimum experimental variograms pairs to use
- VIII. Select each direction of maximum, secondary and vertical continuity
- IX. Insert restrictions of variogram parameters
 - a. Minimum and maximum contribution
 - b. Minimum and maximum nugget effect
 - c. Minimum and maximum range for each continuity direction

Insert open file adress

i

Insert number of iterations

ii

Insert number of variograms in file content

iii

Insert number of variables

iv

Insert number of lags

v

Insert number of modeled structures

vi

Minimum number of pairs

vii

☐ Select

viii

Max range direction box

Azimuth

Dip

☐ Select

Min range direction box

Azimuth

Dip

☐ Select

Vertical range direction box

Azimuth

Dip

☐ Restrictions

ix

Max range restrictions

Min contr

Max contr

Min nugget

Max nuggert

Max range

Min range

Max range

Min range

Min range

Max range

Vertical range

Min range

Max range

5. References

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Wackernagel, H. (1995). *Multivariate Geostatistics*. Fontainebleu: Springer.