# Example application of the Cologne Protocol for the Early Neolithic of Central Europe using QGIS and SAGA

R. Peters 14. April 2020

#### **Notation conventions:**

Name of file, folder or directory
Column- or row heading
/Menu / 1st submenu / 2. submenu / etc.; button
Option, value entries
(exemplification)
<default value/>

#### **Programs / Program Version:**

- QGIS 3.10
- SAGA 2.3.1
- (R 3.6.2.)

This manual presents an example application of the **Cologne Protocol** using QGIS and SAGA. You can either execute the task stepwise by hand (chapter A "Manual") or use the semi-automatic QGIS Python/R scripts (\*.py/\*.rsx) available at the GitHub Repository [https://github.com/C-C-A-A/CologneProtocol-QGIS] and described in chapter B ("Scripts"). The scripts are however experimental and manual and scripts come without any kind of guarantee, so please make sure to double-check your results. Regardless of what approach you choose, please read the manual and consult the publication and supplement (*Schmidt et al. 2020*).

The manual describes the first two parts of the Cologne Protocol, which are a GIS-analysis of site distribution and the identifying of so-called Core Areas. The construction of Voronoi diagrams and "Largest Empty Circles" are conducted in QGIS. Kriging and converting the kriging results into isolines is done in SAGA. The step of selecting the Optimally Describing Isoline is not explained in this manual and can be found in the R or the MapInfo manual. The aim of this manual is neither to explain the theoretical background nor the further steps of the Cologne Protocol. For these points please refer to the associated publication including the supplementary information.

Step 1-5 of the Cologne Protocol can be performed in QGIS (Pre-Processing.py), building the semivariogram is either done in SAGA or using an QGIS R-script

(Variogram.rsx). For kriging we use a SAGA function or call this function from QGIS (Kriging.py). Post-processing, e.g. creating contour lines and calculating the area and number of sites per isoline (Step 8-11) should be performed in SAGA as well or by using the Post-Processing.py from within QGIS. In short, the manual approach requires using QGIS and SAGA, is more flexible but can be tiring while the models and scripts can all be run from QGIS, do save time but require R to be installed as well.

#### Steps:

A) Manual	2
1) Shape-Layer with sites as points	2
2) Creating Voronoi polygons	5
3) Extraction of vertices	7
4) Aggregation of vertices	8
5) Defining the radius of the "Largest Empty Circle"	10
6) Kriging - Preparations and Grid	16
7) Kriging - Semivariogram	19
8) Kriging - inspect and export raster output	21
9) Creating contour lines (isolines)	22
10) Calculating the area and the number of sites per isoline	25
11) Data export	28
12) Selecting the "Optimally Describing Isoline"	29
B) Scrips	29

# A) Manual

### 1) Shape-Layer with sites as points

As case study we use part of a distribution map of Early Neolithic sites in Central Europe. The map is based on *Preuss* (1998, Karte 1) and available from the CRC 806 database (<a href="https://crc806db.uni-koeln.de/start/">https://crc806db.uni-koeln.de/start/</a>). Besides point symbols representing single sites the original map also included symbols for an agglomeration of five sites. The digital data set has been processed to resolve this issue.

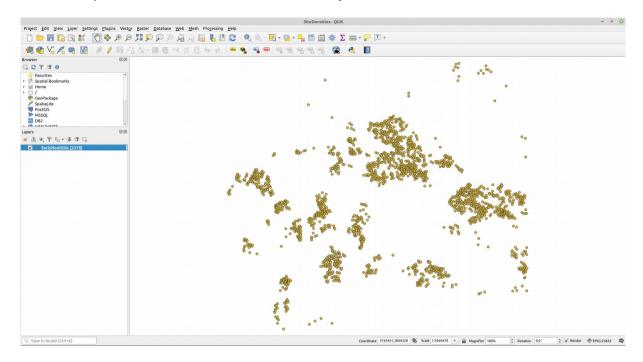
Make sure to download the files in Gauss-Krüger projection not the WGS84 (Latitude/Longitude) files.

Start QGIS and load your or the example data set:

Layer / Add Layer / Add Vector Layer...

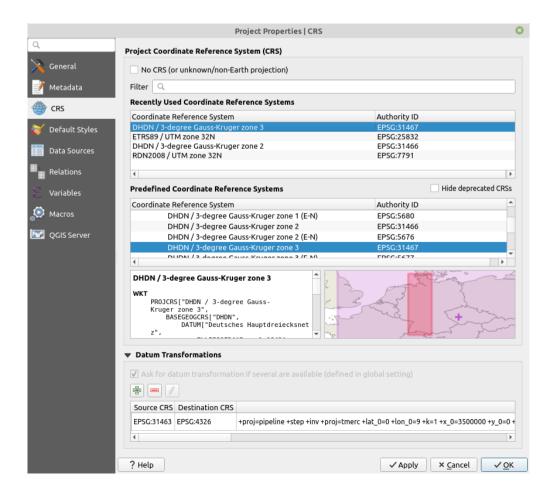
13\_earlyNeolithic\_FRG\_sites\_GK3.shp

Our example data set consists of 2378 early Neolithic sites.

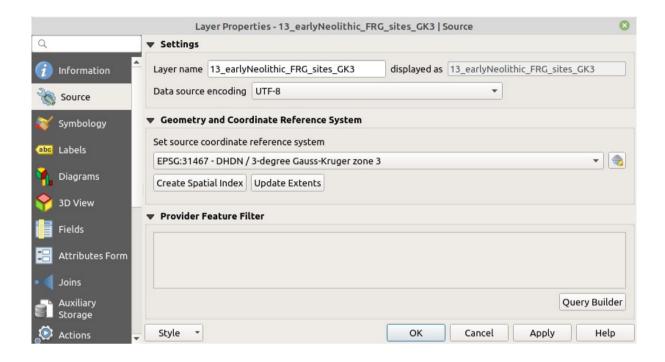


Check the projection system of your QGIS project and of the sites layer. Both should be EPSG 31467 (DHDN / 3-degree Gauss-Krüger zone 3). If they are not, change them accordingly.

Project / Properties / CRS...



#### Right Click on Layer / Properties / Source...



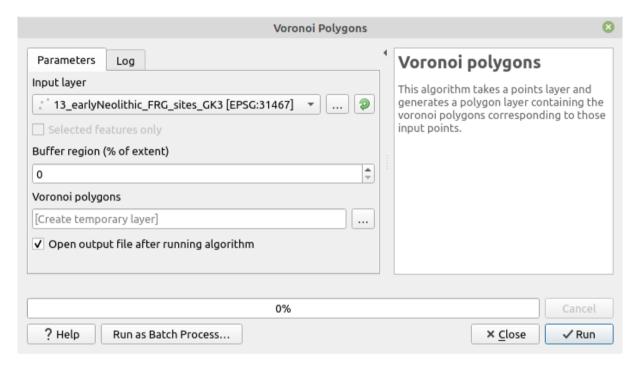
#### 2) Creating Voronoi polygons

The Cologne Protocol uses the Largest Empty Circle (LEC) or more precisely the LEC radii to measure site distances. To locate the central points of the largest empty circles, voronoi diagrams are constructed and the voronoi vertices are extracted.

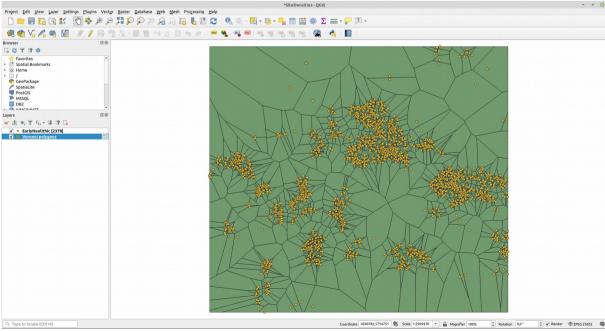
Vector / Geometry Tools / Voronoi Polygons...

<u>Input Layer:</u> 13\_earlyNeolithic\_FRG\_sites\_GK3.shp

Buffer region (% of extent): 0



#### Result: Voronoi polygons.shp

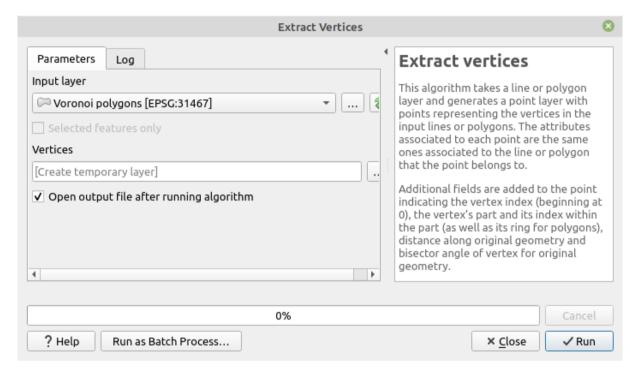


#### 3) Extraction of vertices

Extract nodes/vertices of the voronoi diagrams.

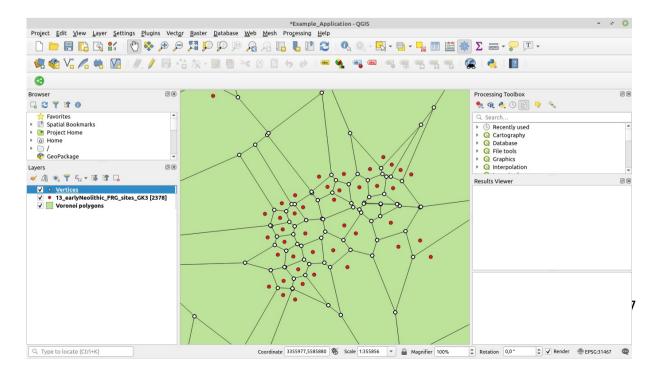
Vector / Geometry Tools / Extract Vertices

<u>Input layer:</u> Voronoi polygons



Result: Vertices.shp

Close-up with sites as red dots, voronoi diagrams as black lines and nodes/vertices as white dots. Exactly three sites are located on every circumference of a LEC.

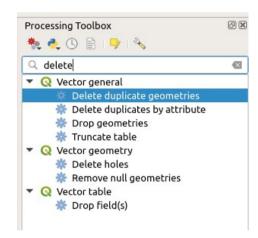


# 4) Aggregation of vertices

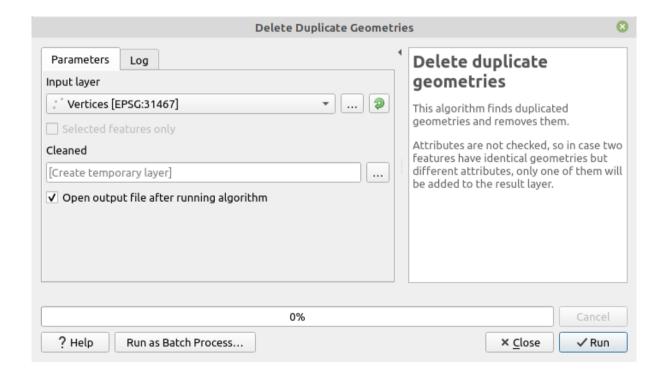
At the vertices/nodes several polygons meet, therefore extracting the nodes has led to duplicate vertices. Those have to be deleted. One possibility for deleting duplicates in QGIS is:

Open Processing Toolbox (Ctrl+Alt+T):

/Processing Toolbox / Vector general / Delete duplicate geometries... Search for: Delete duplicate geometries

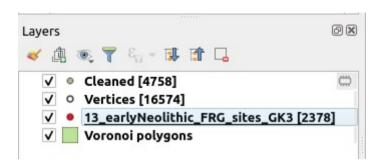


<u>Input layer:</u> Vertices



Result: Cleaned.shp

Using the example data you should end up with about 4758 vertices (duplicates deleted). You can add the number of features to the Layers panel by right clicking on the layer and selecting "Show feature count".



#### 5) Defining the radius of the "Largest Empty Circle"

The distance between vertex/node and the nearest measurement (site) is equal to the radius of the Largest Empty Circle (LEC). We will now measure the distance between vertices and sites (measurements/observations).

/ Processing Toolbox / Vector analysis / Distance to nearest hub (points)...

Source points layer: Shape-File with Vertices (Cleaned)

<u>Destination hubs layer:</u> Shape-File with sites (13\_earlyNeolithic...)

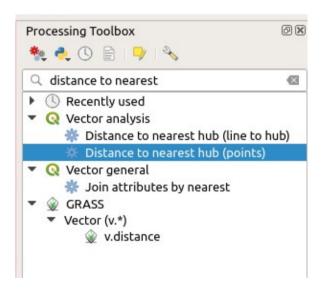
<u>Hub layer name attribute:</u> ID Column ( ID)

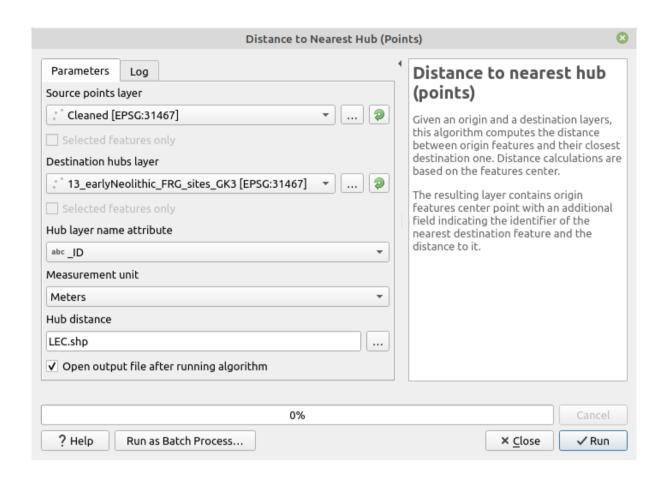
Measurement unit: Meters

Important: the unit of measurement has to be equal to the project unit of measurement (in our case meter).

This time it is vital to export the results, a temporary layer won't do because we will be using the LEC shp-File in SAGA. Save results as:

#### LEC.shp



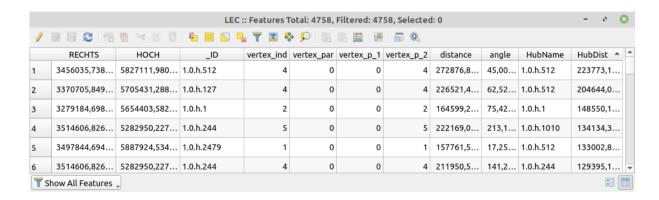


Have a look at the resulting Shape-File:

Choose Layer / Layer / Open Attribute Table...

Among others, you should find following columns:

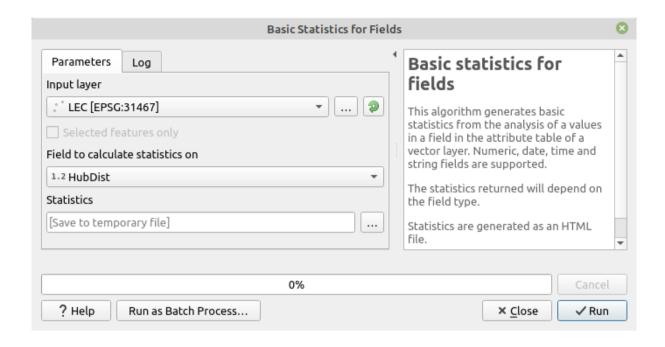
HubName HubDist ID of the nearest measurement (site) distance between node and measurement (LEC radius)



The maximum "HubDist" (LEC radius) for our dataset is ca. 223773 m.

To get basic Statistics for LEC-radii:

Vector / Analysis Tools / Basic Statistics for Fields...



#### 5a Calculate Statistics

The Kriging procedure requires the variables lag distance and maximum search distance. We will calculate these parameters in QGIS and then move on to SAGA to build a semivariogram and compute the interpolation. For the maximum search distance (MaxSearchDist) the diagonal of the LEC bounding box is divided by two. To estimate lag distance (LagDist) we divide the bounding box diagonal by 250. Both values will be used later in SAGA.

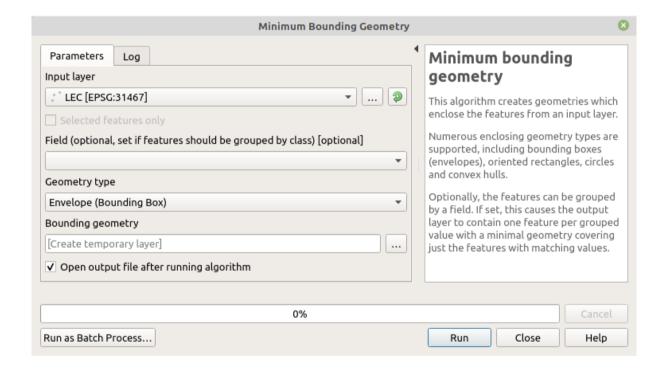
First, create the bounding box for the LEC/vertices:

Processing Toolbox / Vector Geometry / Minimum bounding geometry...

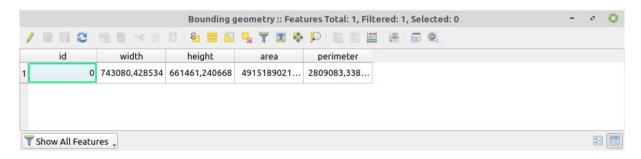
<u>Input Layer:</u> LEC.shp

Field: "

Geometry Type: Envelope (Bounding Box)



Open Attribute Table of new layer "Bounding geometry" (Right Click on Layer / Open Attribute Table) and open Field Calculator (Ctrl +1)



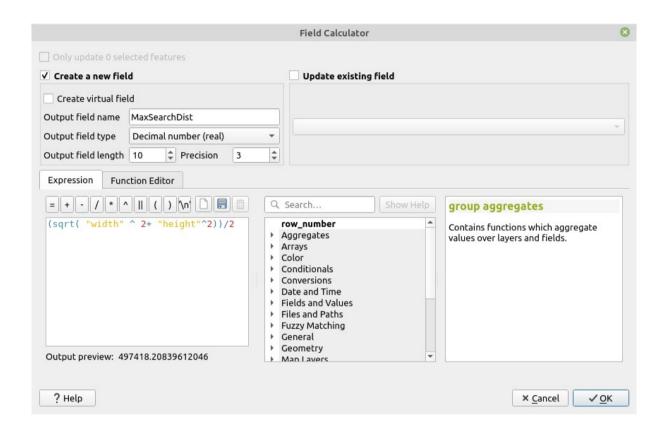
Check "Create a new field"

Output field name: MaxSearchDist

Output field type: Decimal number (real)

Output field length: 10
Precision: 3

Formula: sqrt( "width" ^ 2+ "height" ^ 2)/2



And you should also calculate the Lag Distance to be used in the Semivariogram:

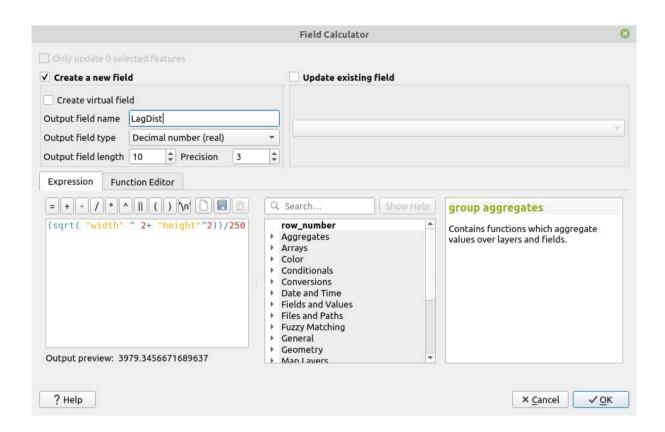
#### Check "Create a new field"

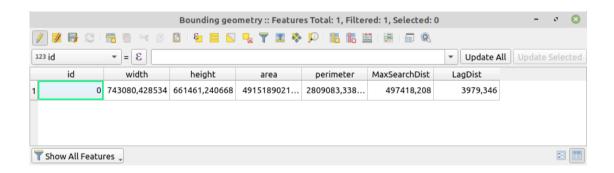
Output field name: LagDist

Output field type: Decimal number (real)

Output field length: 10 Precision: 3

Formula: sgrt( "width" ^ 2+ "height" ^ 2)/250





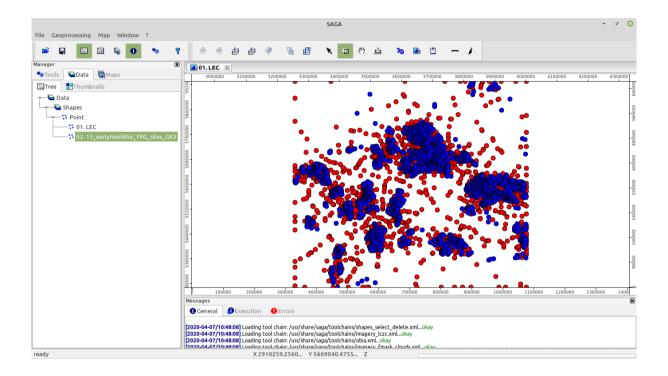
#### 6) Kriging - Preparations and Grid

Save your results, close QGIS and start SAGA. Open the layers with the LEC-Radii and layer with initial measurements (sites):

File / Open...

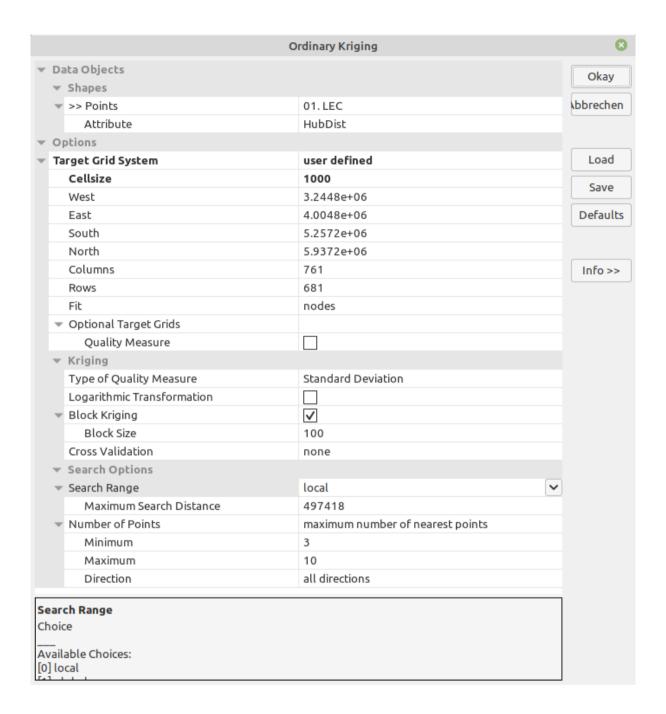
13\_earlyNeolithic\_FRG\_sites\_GK3.shp LEC.shp

Double-clicking on the layer will add the points to a map.



For interpolation, we will be using the Ordinary Kriging Module from SAGA. The parameters for building the semivariogram and for Kriging have to be entered first. For kriging we need a grid of evenly distributed points. The interpolation algorithm will estimate the site distance (radius of LEC) at every point of the grid, based upon the available vertices and their values for the radius of the LEC. For the current example we will create a grid with a spacing of 1000 m between each point. That means a raster file with  $1 \times 1$  km pixels is created.

Geoprocessing / Spatial and Geostatistics / Kriging / Ordinary Kriging...



Points: Layer we want to krige (LEC.shp)

Attribute: HubDist

<u>Target Grid system:</u> user defined

Cellsize: 1000

<u>Search Range:</u> local <u>Maximum Search Distance:</u> 497418

Number of Points Minimum: 3
Maximum: 10

<u>Direction:</u> all directions

Check "Quality Measure" to get plot of the variance for checking the quality of the interpolation. You can also activate "Block Kriging" (Block Size: 100) for smoothing. Changing blocksize or not using block kriging won't alter the results dramatically.

Press Okay to compute the sample semivariogram.

#### 7) Kriging - Semivariogram

The kriging procedure requires a theoretical semivariogram, which is used to estimate the radii of the LEC at every point of the grid. To compute this theoretical semivariogram, we need to explore the experimental semivariogram first. The Semivariogram displays the ratio of distance between pairs of points to the similarity (difference) of points in distance classes (lags).

To adjust lag distance and enter a theoretical model (formula) click:

Settings / Variogram Settings...

Choose one of the following functions, either a

linear regression/exponential model:

$$a + b * x + c * x ^2$$

or as an alternative, the power model:

$$a + b * x ^c$$

Variables explained:

a= nugget

b = sill

c = range

The spherical model doesn't seem to work, at least using our data set. Make sure to set nugget to zero (a=0). For example in the exponential model:

" $0 + b * x + c * x^2$ " or using the power model " $0 + b * x ^c$ ". Or simply:

Linear regression/exponential model:

$$b * x + c * x ^2$$

or as an alternative, the power model:

<u>Skip:</u> 1

<u>Lag Distance:</u> 3979 (calculated in QGIS)

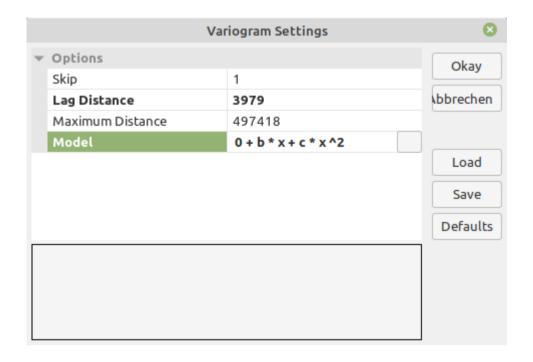
<u>Maximum Distance:</u> 497418 (= MaxSearchDist, calculated in QGIS)

Model:  $b * x ^c$ 

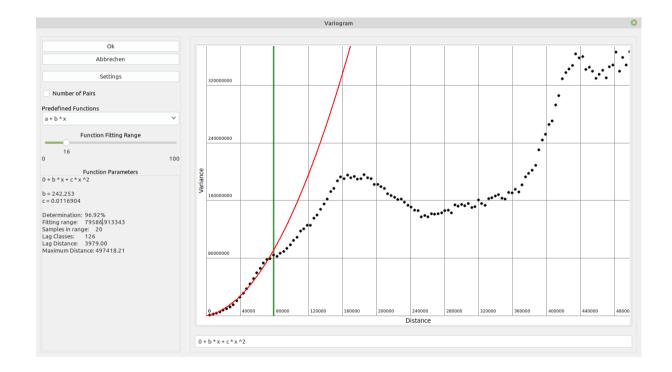
or

 $b * x + c * x ^2$ 

Enter the model of your choice in "Model" and click "Okay" to return to the semivariogram.



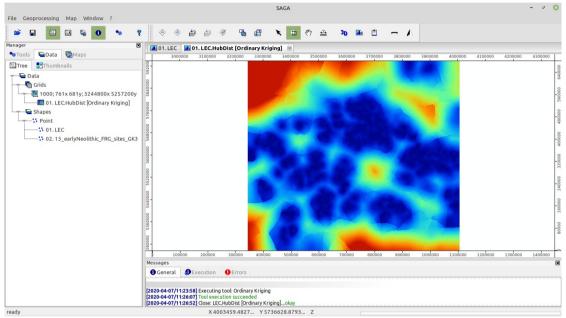
Adjust the fitting range to the first peak or plateau of the distribution by using the slider "Function Fitting Range" on the left side of the panel. In our case study it is at ca. 79586 on the x-axis (Fitting range = 79586.9). Of course, a decision has to be made on a case-by-case basis.



Click OK to start the Kriging process. Computing will take some while depending on your computer (processor, ram, hard disk).

# 8) Kriging - inspect and export raster output

The result of the kriging interpolation is a raster map of the prediction and, if you checked "Quality Measure", the variance or standard deviation of the results. Double-click on the new grid to add it to a map.



You can export the raster as Surfer Grid so you can import it in QGIS later.

Geoprocessing / File / Grid / Export / Export Surfer Grid ...

#### 9) Creating contour lines (isolines)

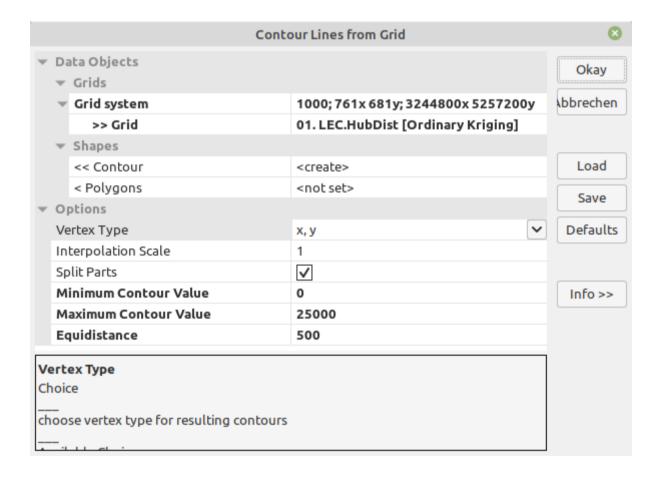
Using the kriging raster we will create isolines, convert them to polygons and compute the area and number of sites per isoline. Number of sites and isoline area are important for selecting the "Optimally Describing Isoline" (*Zimmermann et al. (2004, 53-55)*).

First we will extract the isolines or contour lines from the raster. The easiest way to find functions in SAGA is to search for them:

Geoprocessing / Find and run tool / Contour Lines from Grid...

or

Geoprocessing / Shapes / Grid / Vectorization / Contour Lines from Grid...



In our case study we need contour lines starting at 0 and ending at 25000 m with an equidistance of 500 m. It is advised to calculate as few isolines as possible.

Grid: our new Kriging grid (the original not the export)

<u>Contour:</u> <create>

<u>Polygons:</u> <not set> (we want lines not polygons yet)

<u>Vertex Type:</u> x, y

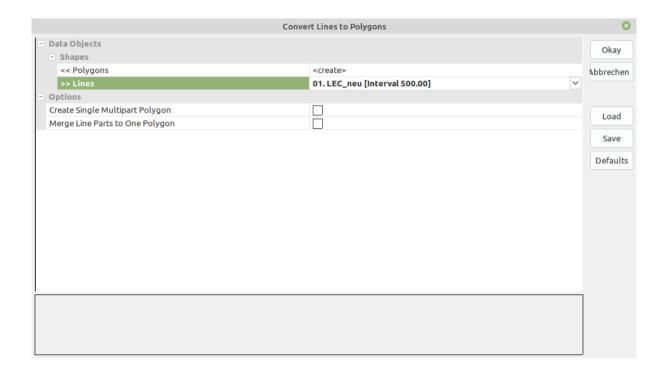
<u>Interpolation Scale:</u> 1

<u>Split Parts:</u> checked

Minimum Contour Value: 0

<u>Maximum Contour Value:</u> 25000 <u>Equidistance:</u> 500

Geoprocessing / Shapes / Conversion / Convert Lines to Polygons...



Polygons: <create>

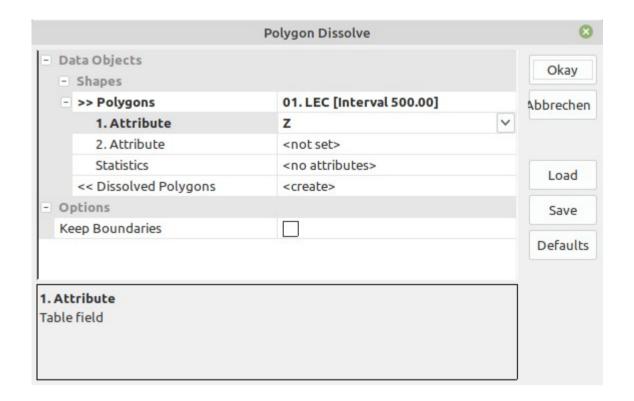
<u>Lines:</u> the contour line layer created above

<u>Create Single Multipart Polygon:</u> unchecked

Merge Line Parts to One Polygon: unchecked

Dissolve Polygons using the iso-value (Z):

Geoprocessing / Shapes / Polygons / Polygon Dissolve...



Polygons:

1. Attribute:

2. Attribute:

<u>Statistics:</u> << <u>Dissolved Polygons:</u>

Keep Boundaries:

Polygon layer created above

Ζ

<not set>

<no attributes>

<create>

unchecked

# 10) Calculating the area and the number of sites per isoline

Use the newly created dissolved isoline polygon layer and check the box "Area" and "Number of Parts"

Geoprocessing / Shapes / Polygons / Polygon Properties...

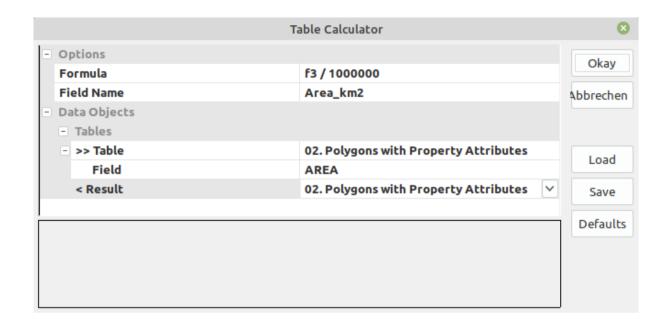
	Pol	ygon Properties	8
ts			Okay
		02. LEC [Interval 500.00] [Dissolved: Z]	Abbrechen
ns with Property Attributes		02. LEC [Interval 500.00] [Dissolved: Z]	
			Load
vertices			Save
		✓	Defaults
9	gons pons with Property Attributes  Parts  Vertices	gons ons with Property Attributes Parts Vertices	ons 02. LEC [Interval 500.00] [Dissolved: Z]  ons with Property Attributes 02. LEC [Interval 500.00] [Dissolved: Z]   Parts  Vertices

Polygons:
Polygons with Property Attributes:
Number of Parts:
Number of Vertices:
Perimeter:
Area:

Dissolved polygon layer created above Dissolved polygon layer created above checked unchecked unchecked checked

The calculated areas will be in your map unit (in our case study: m²). If we want km² we have to:

Processing / Table / Calculus / Table Calculator...

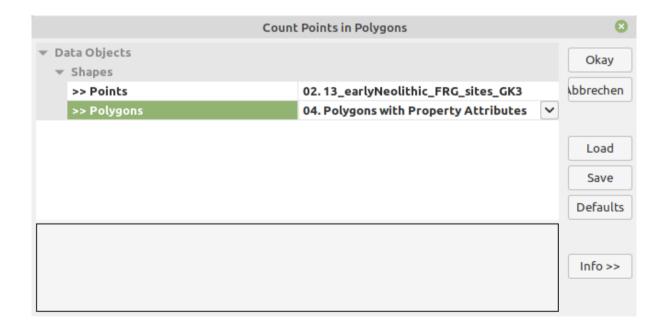


Formula:
Field Name:
>>Table:
Field:
<Result:
layer)

f3 / 1000000 (third field of the table) Area\_km2 (name of field to be created) Polygon layer with attributes AREA (field to be divided) Polygon layer with attributes (update

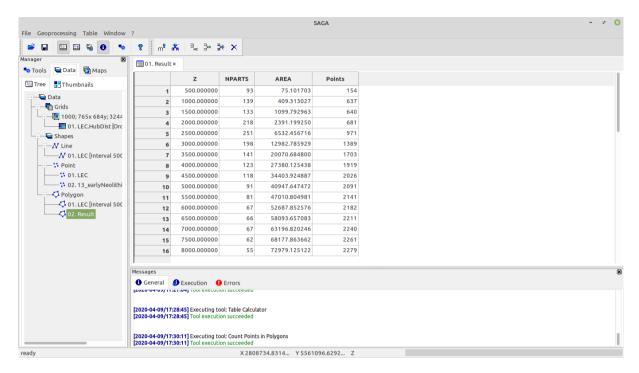
#### Geoprocessing / Shapes / Points / Points Count Points in Polygons

Now we count the number of sites within each isoline. "Points" is the original layer with measurements (sites) and "Polygons" is the dissolved Isoline polygon layer (might be called "Polygons with Property Attributes" or "Result").



#### Have a look at the attributes

#### Right Click on Layer > Attributes > Show

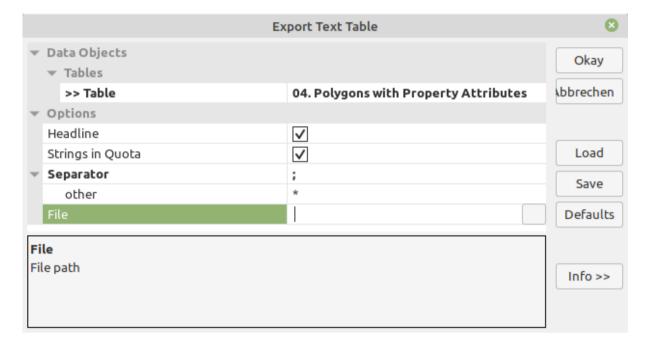


You should end up with a shp-file of polygons and columns for each isoline value (Z), the number of part the isolines consist of (NPARTS), the area per isoline and the number of sites (Points) within each isoline. The figure above shows the results using the first formula (linear regression/exponential model).

#### 11) Data export

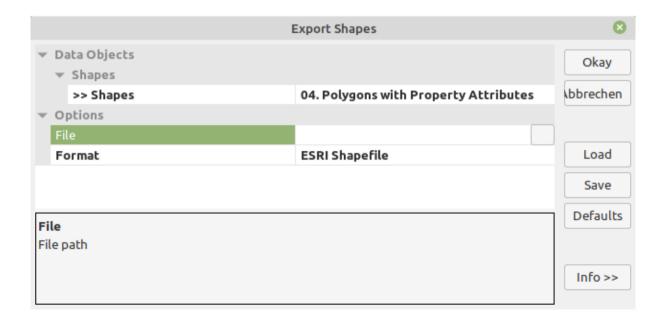
Export the results (might be called "Polygons with Property Attributes" or "Result") as comma-separated values (\*.csv):

Geoprocessing / File / Tables / Export / Export Text Table...



and as shape-File:

Geoprocessing / File / Shapes / Export / Export Shapes



# 12) Selecting the "Optimally Describing Isoline"

The step of selecting the Optimally Describing Isoline is not described in this manual. You can do this in a spreadsheet program (e.g. excel). Please refer to the R or the MapInfo manual.

# B) Scripts

#### 0. Preconditions

Precondition for using the Python and R scripts is having QGIS 3.10, SAGA 2.3.1 and R 3.6.2 installed. SAGA is usually installed as default during the QGIS setup, if you are working with Linux you might have to download and install SAGA on your own.

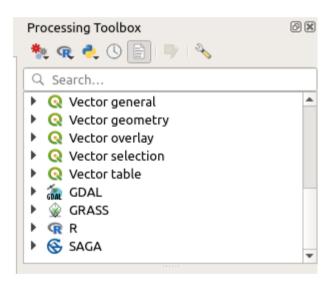
Download the four scripts from the GitHub Repository and unzip in a directory of your choice:

https://github.com/C-C-A-A/CologneProtocol-QGIS

Start QGIS and have a look at the Processing Toolbox:

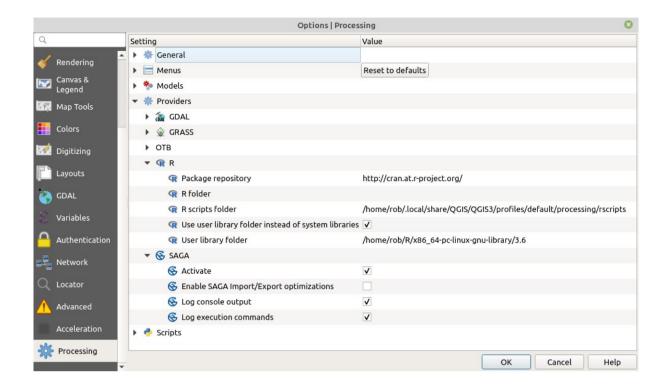
Processing / Toolbox...

There should be a R and SAGA icon in the box as well as a R and Python icon at the top of the panel:



If one of the icons is missing or a R or SAGA script or function cannot be run, check if R and SAGA is activated and if the program paths are right in :

Settings / Options / Processing / Providers....

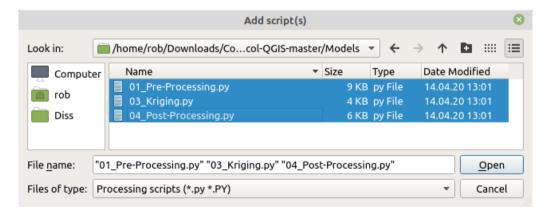


If it is still not working consult the QGIS User Guide:

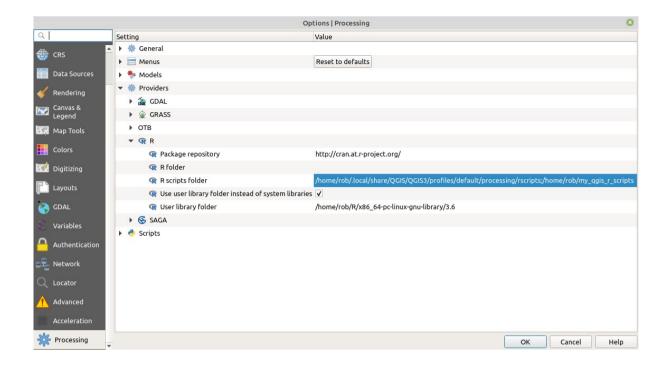
https://docs.ggis.org/3.10/en/docs/user\_manual/processing/3rdParty.html

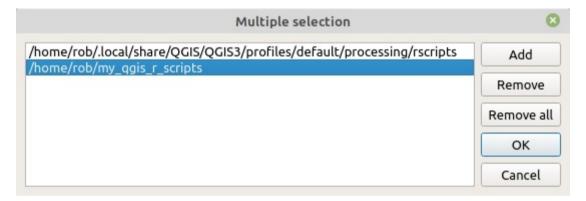
After configuring the external applications you can open the scripts. Click the Python icon at the head of the Processing Toolbox and choose "Add Script to Toolbox". Add the three Python scripts ("01\_Pre-Processing.py"; "04\_Post-Processing.py")

Processing Toolbox / Python Icon / Add Script to Toolbox...

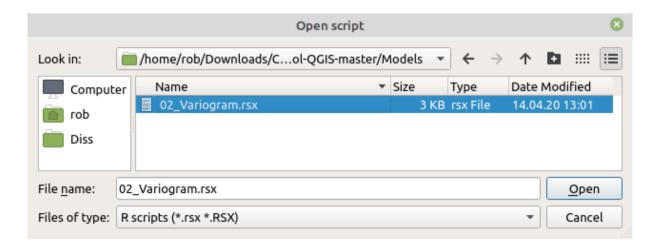


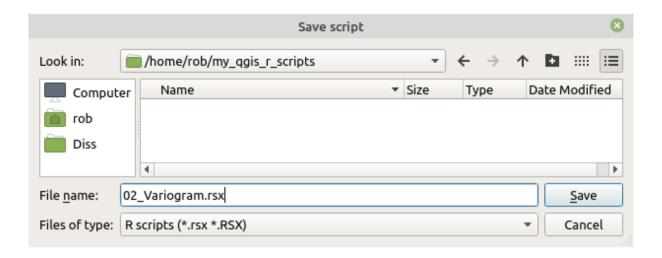
To open the R-script add your own or a new R scripts folder path to the processing options:



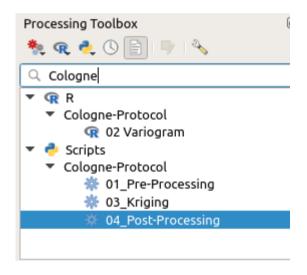


Then click the R icon in the Processing Toolbox header and choose "Create new R scrip" to add the\*.rsx file. Open "02\_Variogram.rsx" and save to the R scripts folder you just specified.



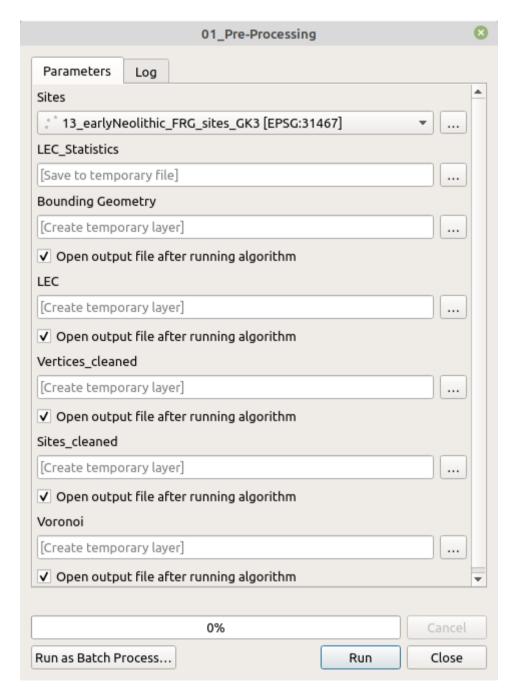


If you type "Cologne-Protocol" in the Processing Toolbox Search box you should be able to find all four scripts:



#### 1. Pre-Processing

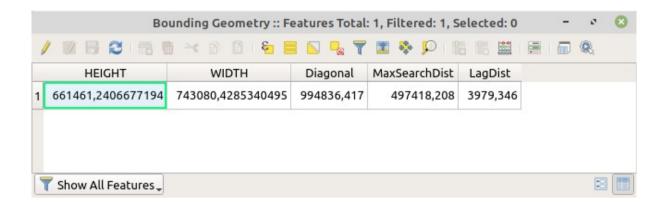
Double Click the "01\_Pre-Processing"-Script and enter the sites layer you want to use.



Running the script will create the following layers:

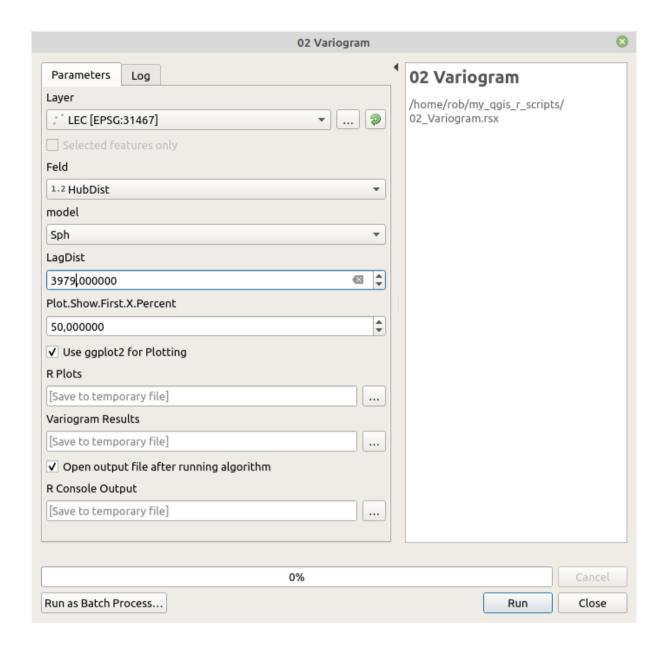
Sites_clean	Input sites without duplicates	
Voronoi	Voronoi diagrams	
Vertices_cleaned	Vertices of the voronoi diagrams without duplicates	
Bounding Geometry	Minimum Bounding Geometry of the vertices/LECs with	

	Fields "Diagonal" (Bounding Box Diagonal), "MaxSearchDist" (Half of the Bounding Box Diagonal), "LagDist" (Lag Distance = Bounding Box Diagonal / 250)
LEC	Largest Empty Circles Centroids with Radius in the Field "HubDist"

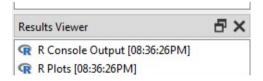


#### 2. Variogram

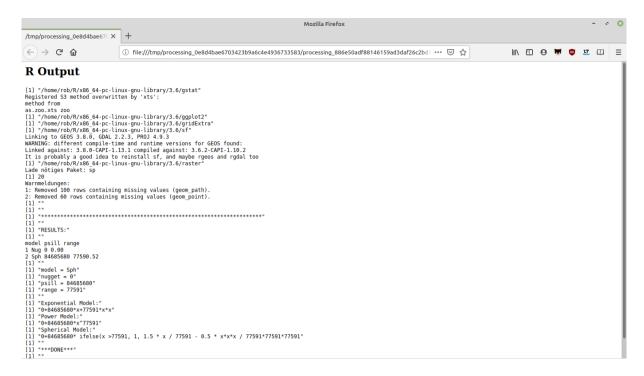
The R (\*.rsx) Variogram script requires an input layer, the layer containing the LEC-Radii (LEC.shp) and the field with the LEC-Radii to be specified. You should also choose the theoretical model (spherical, exponential, Gaussian or Mat). Independent from your choice of model the script will compute a spherical, exponential and power model for your data. In the field LagDist you should enter the value calculated above (Layer "Bounding Geometry", Field "LagDist"). The last two options specify if the frame of the plot should be zoomed to a certain percentage and whether the R base plot or ggplot2 is used for plotting.



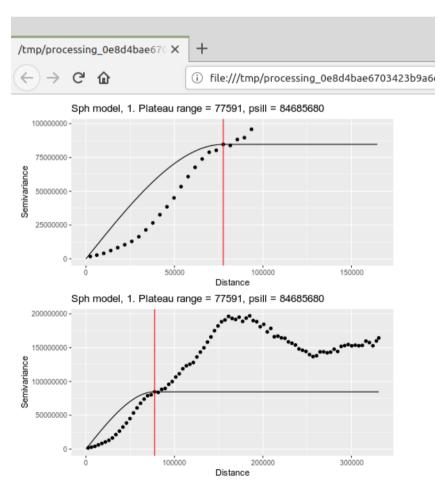
The Variogram-Script will produce two html results in the "Results Viewer". The "R Console Output" which is a text based log and "R plots" with the semi-variogram.



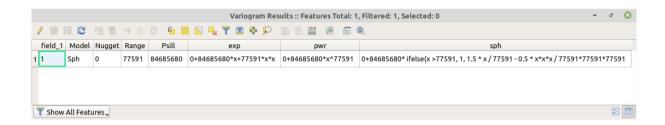
In the "R Console Output" you can look up the the nugget, psill and range of the computed variogram as well as the formulas of the different models you can use later on.



"R Plots" consist of a overall plot (bottom) and the zoomed in version (top). The sample variogram is plotted as black points, the theoretical model as black line and the range at the 1st plateau signified as vertical red line.

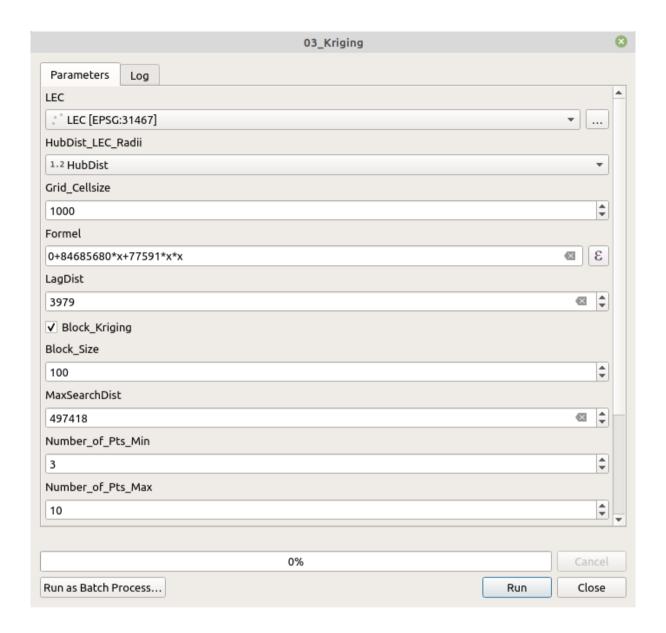


All variogram results can be found in newly created "Variogram Results" table:



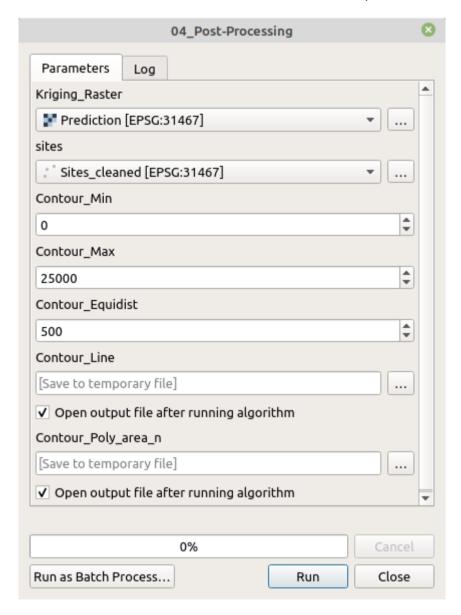
#### 3. Kriging

The Kriging script requires again the layer and field with the LEC-radii (Layer: LEC.shp; Field: "HubDist"). You should also enter the cell size of the raster layer to be created, the formula of the theoretical variogram model you want to choose (look up in "Variogram Results" table), the Lag Distance and Maximum Search Distance (look up in "Bounding Geometry" layer). For testing try to use a coarse grid.



#### 4. Post-Processing

Choose the just created Kriging raster and the "Sites\_clean" layer (important, not your original layer) and enter minimum and maximum of the contour lines to be extracted as well as the distance between contour lines (equidistance) in meter.



The most important results are saved in the Layer "Contour\_Poly\_Area\_n" with Fields containing the contour line value ("Z", e.g. 1000 = 1 km contour line), the number of polygon parts ("NPARTS"), the area enclosed by the contour line ("AREA") and the number of sites within each contour line ("NUM").

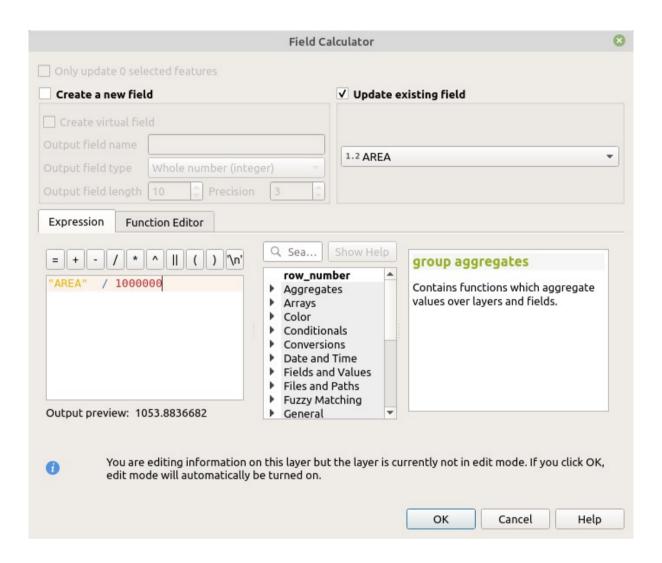
The Area of Contour-Polygons is in m<sup>2</sup> and should be converted to km<sup>2</sup>:

Open Attribute Table of new layer (*Right Click on Layer / Open Attribute Table*) and open Field Calculator (Ctrl + I):

#### Check "Update existing field"

Output field name: AREA

Formula: "AREA" / 1000000



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