



User manual - GisSOM

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1 INTRODUCTION

The purpose of this document is to explain how to install, use and read the results of the *GisSOM* software developed in the European Union funded H2020 project NEXT. GisSOM is developed for performing self-organizing maps and k-means clustering for multivariate data. The software provides means to do simple preprocessing to the input data and select variables for clustering. In addition to generation of SOMs from the input data, the SOM and k-means results for the spatial datasets can be visualized in the original geospace as well. GisSOM saves the SOM space-to-Geospace mapping results for spatial datasets as csv tables. The calculation and results use 32-bit floating point numbers, so the results have around 7 digits of significance. Detailed information on the software design and algorithms used is provided in D 4.11 Appendix 2.

1.1 Self-organizing maps and k-means

Self-organizing maps (SOM) is an unsupervised artificial neural network that arranges a set of n-dimensional vectors to a usually two-dimensional SOM lattice (Kohonen, 2001). The usability of SOM comes from its topology preserving nature, i.e., similar data vectors are assigned to SOM cells that are close together.

Although SOM can be considered as a clustering method itself, the number of cells in a SOM is generally too large for practical data classification, for instance. To reduce the number of clusters, GisSOM applies k-means clustering to the SOM result. K-means is a very basic clustering method where each data point is assigned to the cluster that best represents the data point, without considering the relation between or similarity of different clusters.

SOM and k-means computations are carried out using the somoclu package (Wittek et al., 2017). After the initialization of the SOM neuron weights, the training of SOM utilizes competitive learning (Kohonen, 2001): For a given data point, the neuron with the smallest Euclidean distance is found; this neuron is called the best matching unit (BMU). The weights of the BMU and the neurons close to it are updated to be closer to the data point. The formula for updating the weights is

$$w(t+1) = w(t) + \alpha(t)h(t)(x(t) - w(t))$$

where w(t+1) is the new weight for a given neuron, w(t) is the old weight, $\alpha(t)$ is monotonically decreasing coefficient (learning rate), h(t) is a neighborhood function, and x(t) is the input data value. The learning rate ensures that the area in which the weights are updated shrinks over time and the neighborhood function ensures that the update is smaller the farther away the neuron is from the BMU in SOM space. Also the neighborhood size may decrease as a function of time.

The quality of SOM is usually measured using two quantities. The *topological error* describes how closely similar data vectors are located on SOM and the *quantization error* is a measure of the goodness of clustering of data vectors in each SOM cell. In GisSOM, computation of only quantization error is implemented so far. Quantization error represents the deviation of each data vector from its corresponding BMU vector.

After SOM calculation, k-means clustering can be applied to its neurons. K-means is a clustering method that tries to minimize variances within clusters. The algorithm is iterative; it assigns

observations to the closest cluster centroid and recalculates the centroids. This is repeated until no updating happens.

The user provides the minimum and maximum number of clusters for which k-means clustering is tested. As the initial random assignment of clusters affects the results of the algorithm, k-means is run multiple times (user provides the number of initializations) for each number of clusters in the given range. The best clustering result for each number of clusters is saved. The goodness of clustering is measured using the Davies-Bouldin index (Davies & Bouldin, 1979).

2 INSTALLATION

The software comes with an installer. Double-click the installer to start the installation wizard and install the software.

2.1 Installation requirements

GisSOM requires Windows operating system (7, 8 or 10).

3 USING THE SOFTWARE

Open the software using the GisSOM icon that is created on your desktop, or by running the executable SomUI.exe, which is in the root of the installation directory .../GisSOM. This will open a wizard-style window (Figure 1) where you can load and study input data, perform simple transformations, provide SOM and k-means parameters, and study the results in SOM space, geospace, boxplots and scatterplots.

3.1 Load the data

In the first step of the wizard, you need to select the input data format (Figure 1) and locate the data file(s) from your computer. When you click an item in the data format dropdown menu, a file browser window opens where you can select your input data file(s). CSV format uses a single input file that contains all the input data variables, but in the case of GeoTIFF files, multiple files can be given, each containing a single data variable. When opening a CSV file, make sure the file is not open in Excel or any other spreadsheet-editing application, because then it can't be accessed.

Input data options are

- CSV Grid: A comma-delimited text file with comma (,) as the column separator and point (.) as the decimal separator. The file must have one header line containing the column names , and all columns must have a non-empty header . Also, spaces (), percentage signs (%) and double quotation marks (") are removed from headers. If whole columns and rows are missing (NoData), CSV scatter format is needed. See also the example testdata file in .../GisSOM/TestData.
- CSV Scatter: Use this when the data is not evenly spaced in a grid. If there are only individual missing values or missing values in the sides and center, CSV grid can be used (Figure 2a), but if whole columns and rows are missing, CSV scatter is needed (Figure 2b). CSV scatter is useful, for instance, for geochemical data, where the samples are collected at irregular spatial intervals (Figure 2c). The main drawback of the CSV Scatter input is that it makes it slower to produce the geospace result images than the SCV Grid input.
- TIF: A georeferenced single-band raster data format. In case of multi-band GeoTIFF files, each band within the raster should either be saved as individual single-band raster file or all the band values should be sampled and saved in CSV Grid format. Note that when using raster data, the alignment and size of the pixels and the NoData-value need to be the same in each GeoTIFF file. Also, as the file names are used as headers for the data, spaces (), percentage signs (%) and double quotation marks (") are removed. If entire rows or columns are NoData, CSV Scatter input format must be used. If whole columns and rows are missing (NoData), CSV scatter format is needed.
- Old results: Use this option if you want to visualize existing SOM results from GisSOM software. Navigate to the output folder GisSom and select the result subfolder (Out_*). Make sure you haven't changed the file names or paths of the results. Refer to section 3.5 for more information.

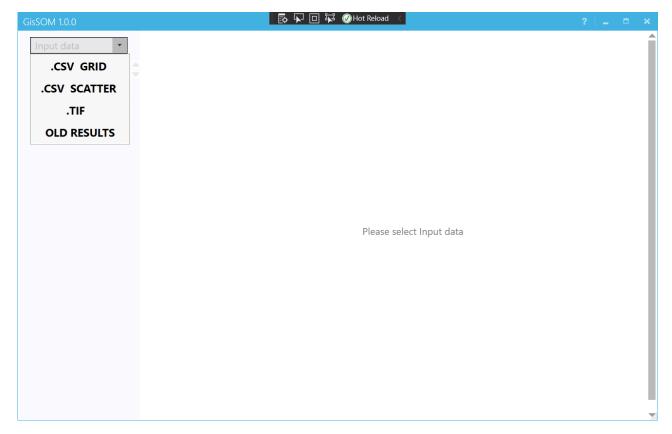
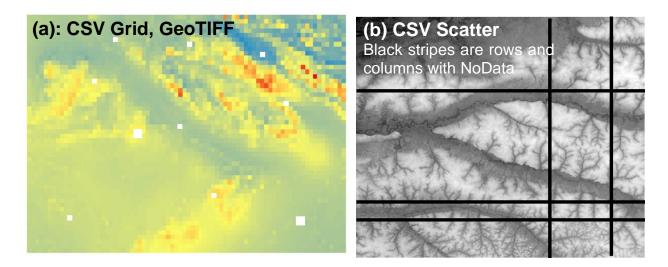


Figure 1. Selecting the data format. The data processing options will be visible only after the input data is loaded (see Figure 3).



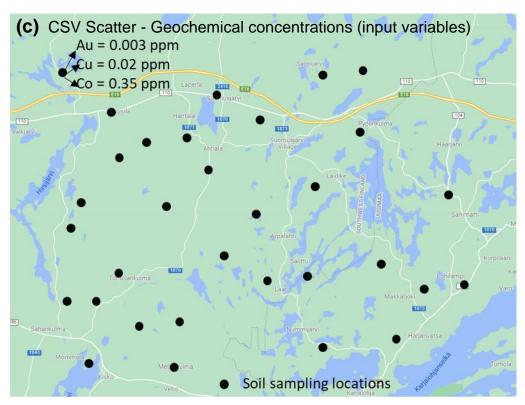
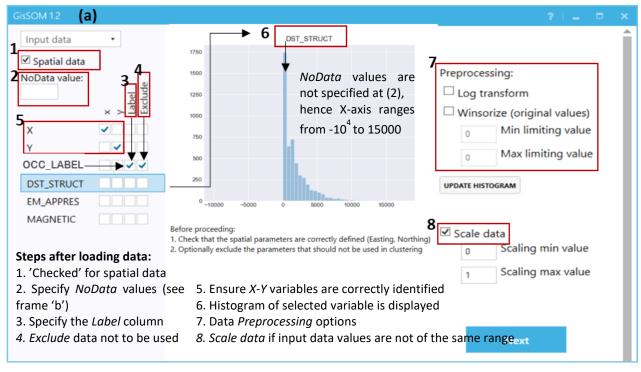


Figure 2. Example of grid type and scattered data points. The data in (a) can be used as grid data, as there are no missing columns or rows; except a few pixels (white pixels) where it is NoData. The data in (b) has several rows and columns missing (black stripes), e.g.: satellite imagery, so CSV scatter needs to be used, otherwise the result plots will misrepresent the data. CSV scatter can also be used in case of data collected from scattered locations as shown in (c) typical for, e.g., geochemical data.

3.2 Data preprocessing

Once you have selected the input data file(s), the GisSOM window shows you all the relevant data variables, including the possible spatial variables (Figure 3). In the next step, you need to study the data before it can be used in SOM. You need to select the correct North and East coordinates in the case of CSV files, exclude any data you don't want to use, and possibly transform data. The number of datapoints represented in the histogram is capped at 5000 to speed up performance, if the number of data points in a variable exceed this number, a random sample of 5000 is taken for plotting.



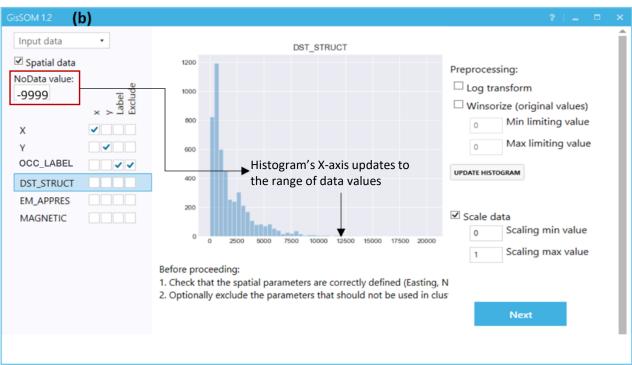


Figure 3. GisSOM interface after data is loaded and Data preprocessing menu

The following steps are required (Figure 3):

- Select the North and East coordinates by checking the "x" and "y" checkboxes for the correct variable from the left. This is not required for georeferenced raster data (GeoTIFF). If you are not using spatial data, untick the box "Spatial data?" on the right side. If you have labels in your data, i.e. a variable that represents true values, mark them using "Label" checkbox.
- Exclude the data variables that you don't want to be used in SOM by choosing "Exclude" for the correct variables on the left side. Note that geographic coordinates are automatically excluded if you define them as "x" and "y", as you normally do not want to use them in the SOM as variables. Also the variable marked as "label" is automatically excluded.
- As it is important to scale the data variables into a comparable range of values for SOM computation, each variable is normalized by default to the range of [0,1]. If the user wants to weigh data variables differently, they can provide variable specific ranges. Scaling is done using a simple shift and scale function:

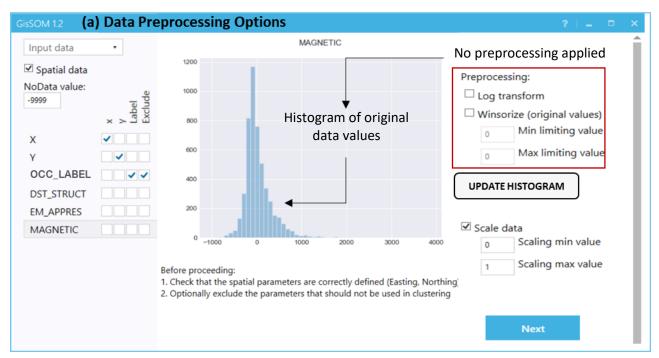
$$r = \frac{(r_{max} - r_{min}) * (x - x_{min})}{x_{max} - x_{min}} + r_{min}$$

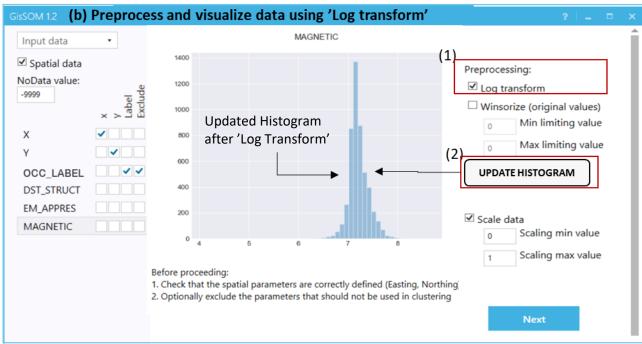
where r is the rescaled value, x is the original value, x_{min} and x_{max} are the minimum and maximum original data values, and r_{min} and r_{max} are the rescaled values defined by the user. Before visualization of the results, the values are transformed back using inverse of the formula. If you do not wish to apply any kind of rescaling, uncheck the checkbox.

- The histogram for the selected variable is displayed in the center. This helps to analyze the distribution of the selected variable's data values. Study the distribution of the variables that you want to use in SOM computation using their respective histograms. If the displayed histogram has a long tail in the high end, you can apply logarithmic transformation ("Log transform") or if both tails are long, limit extreme values ("Winsorize", Error! Reference source not found.) to emphasize differences near the peak of the distribution. Click "Update histogram" to see the changes in the histogram.
 - Logarithmic transform is carried out by first shifting all the variable values to the positive range. Then, a natural logarithm is applied to the values and SOM computation is performed using the transformed values. After the SOM computation, the values are inverted back using exponential function. This option can be used when the distribution of data is right-tailed and logarithmic transformation results in values that are closer to normal distribution.
 - Winsorizing means assigning a limiting value to variable values below and above the given limiting value. This can be used, if it is known that it is enough to classify very large values as only "large" and very small values as only "small", without consideration of how big or how small. Note that winsorizing will be applied to the original data values, irrespective of the values shown in the histogram, i.e., even if you apply logarithmic transformation first, the original data values (and not the log-transformed data values) will be winsorized.

Either of the two preprocessing options can be applied to the selected variable, not both. If in case the user wishes to undo the logarithmic transformation or winsorization, then

- uncheck the corresponding option and then click "Update histogram" to refresh and visualize the original data distribution.
- If dataset contains a numeric value signifying NoData values, provide it in the NoData value textbox. Not doing so can lead to erroneous results, or to the functions failing altogether in case of infinite or extreme null values (Figure 3a and b). GisSOM automatically screens for non-numeric values, so those do not have to be provided.
- Click "Next" to proceed to the next step





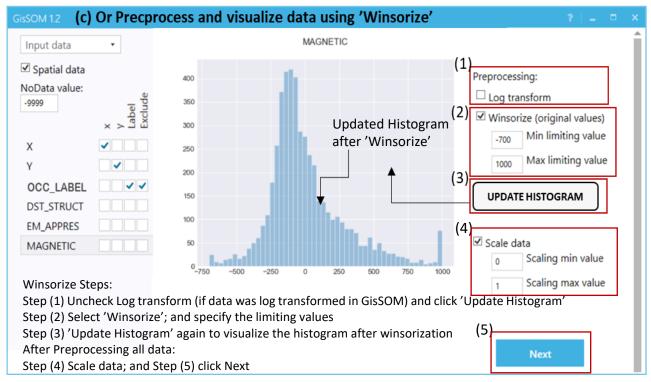
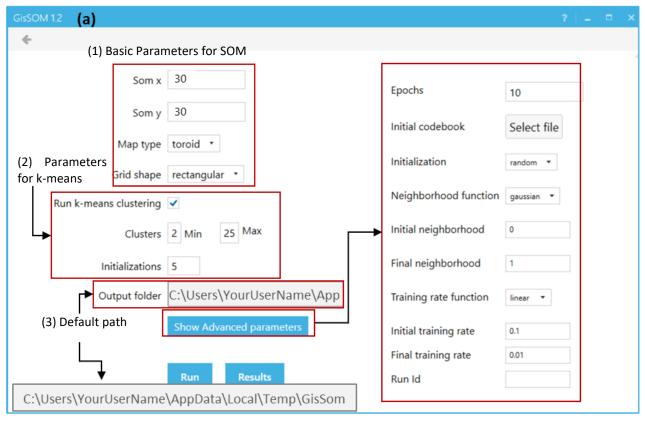


Figure 4. Data Preprocessing and visualization: (a) No preprocessing, the histogram displays original data values (b) Log transform of original data values, and (c) Winsorize the original data values. N.B.: Either of the two options can be used, but not both.

3.3 Choose SOM and k-means parameters

In the next step, you need to choose the parameters used in SOM and k-means clustering (Error! Reference source not found.). The input parameters are separated into two sections, basic parameters and advanced parameters. By default only the basic parameters are visible on screen, but you can view the advanced parameters by clicking on the "Advanced Parameters" -button.



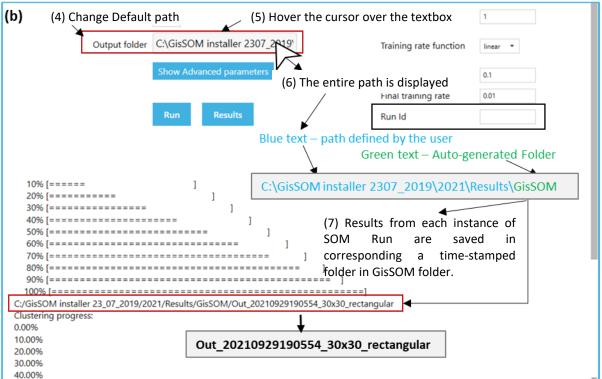


Figure 5 (a) Choosing parameters for SOM and k-means; (b) Saving the results

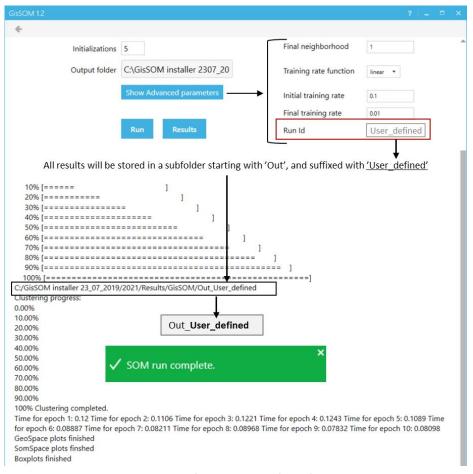


Figure 6. Run Id - Advanced Parameter to specify the name of the folder containing the results

3.3.1 Basic Parameters for SOM

- Choose the size of the SOM using "Som x" and "Som y". These refer to the number of SOM cells in horizontal and vertical direction. The default values are calculated using one rule of thumb for a square shaped map: the total number of cells is $5 * \sqrt{number\ of\ data\ points}$ so both "Som x" and "Som y" are square root of that value. Large SOM size causes SOM cells to be closer to the input data and thus more accurate with the cost of computing time. Higher accuracy also means that quantization errors are smaller.
- Map type: topology of the map, accepted values are "toroid" or "sheet". Sheet type SOM works in the same manner as SOM is visualized: the sides of the SOM map have an edge next to them and neighbors only on the other side. Toroid type SOM continues from one edge to the opposite, so that each SOM cell has the same number of neighbors. This is visualized in Figure 6Error! Reference source not found.

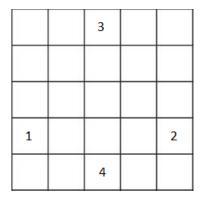


Figure 6. Neighbours in sheet and toroid type maps. For toroid 1 and 2 as well as 3 and 4 are neighbours; for sheet they are not.

Using sheet type often causes large and small values to be clustered near an edge whereas toroid doesn't have this issue. Using toroid type often causes a single cluster to be split in multiple parts as the clusters continue from on side to the other. These cases are visualized in Figure 7.

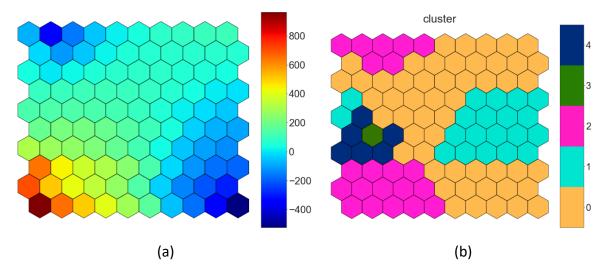


Figure 7. Sheet type causing values to be piled near an edge (a) and toroid type causing a cluster to appear on the other side (b).

 Grid shape: The shape of the grid that connects the nodes of the map. Accepted values: hexagonal or square. The software regards 4 closest SOM cells as neighbors in rectangular grid shape and 6 closest in hexagonal. The hexagonal grid starts from upper left corner and the top row is not indented.

3.3.2 Parameters for k-means

- You can choose to skip k-means clustering and run only SOM by removing the tick in Run k-means clustering.
- If you run k-means, you need to select the minimum and maximum number of clusters. The default for minimum is 2 and maximum is 25. This software applies k-means to the results

- of SOM using all values between these for the number of clusters and the most optimal number is chosen based on the smallest the Davies-Bouldin index.
- Choose the number of random *Initializations*. The default is 5. K-means is sensitive to the initialization, so multiple different initializations should be used. The software runs k-means using these different initializations and chooses the most optimal based on the smallest Davies-Bouldin index.

3.3.3 Output Folder

- The default output folder location where all the results will be saved is "C:\Users\YourUserName\AppData\Local\Temp\GisSom\".
- The default output folder can be changed using the *Output folder* textbox.
- A new folder "GisSOM" is created in the path defined by the user. The results for each instance are saved within this "GisSOM" directory, in a subdirectory, the name of which starts by "Out_" followed by the Run Id. Run Id is by default the date and time and SOM size-shape parameters unless the it is provided in the Advanced Parameters (see section 3.3.4). The timestamp is in the format "YYYYMMDDHHMMSS" (year-month-day-hour-minute-second).
- The final structure is *Outputfolder*\GisSOM\Out_Run Id where the text in blue is user-defined and the text in green represent the auto-generated folders (Figure 5b).

3.3.4 Advanced Parameters

- *Epochs* is the number of times that the data set will be used when training the SOM. The default is 10. Small values result in faster computation, but possibly also in an inaccurate SOM. Larger values increase computation time, but might also improve the quality of the SOM. Usually the quality will not increase after certain amount of epochs.
- Initial codebook: It is possible to provide a previously run SOM calculation codebook vectors as an initialization for the SOM. Codebook vectors are provided in the form of the "som.dictionary" file that the SOM calculation of GisSOM creates in the project output folder. The "som.dictionary" file is located in the result subfolder, under the main "GisSom" output directory. The initial codebook vector matrix must have the same number of elements as the input dataset and have the same "Som x" and "Som y" parameters. If initial codebooks are provided, the value provided for the Initialization parameter will be skipped altogether.
- Initialization: Initialization of the codebook vectors. Accepted values: "random" or "pca". If you provide initial codebook vectors, this value will be skipped. With random initialization, the initial codebook will be filled with random numbers ranging from 0 to 1. "pca" initializes the weights from the first two eigenvectors of the correlation matrix. "pca" method also includes a random component, so the resulting maps might show small variation.
- Neighbourhood function, Initial neighbourhood, Final neighbourhood: The Initial neighbourhood is the initial radius on the map where the update happens around a best matching unit, and the Final neighborhood is the radius where the update happens in the

final epoch. For the *Initial neighbourhood*, the default value of 0 will trigger a value of min(n_columns, n_rows)/2. Type of possible neighbourhood functions include "gaussian" and "bubble". "gaussian" function utilizes a decreasing Gaussian function away from the BMU when the weights of SOM are updated. The software utilizes a cut off that ensures that weights beyond the training radius are not updated. "bubble" function is a simple constant function resulting in all neurons around the BMU getting the same proportional update.

- Training rate function, Initial training rate, Final training rate: Initial training rate is the training rate in the first epoch, and Final training rate is the training rate for the last epoch. The Training rate function determines the cooling strategy between the initial and final learning rate, and possible values are "linear" or "exponential".
- Run Id: Use Run Id to change and define the name of the output directory within the "GisSom" folder. The results will be saved in the new directory with the name specifies in Run Id prefixed by "Out_". (See Figure 6)

3.3.5 Run and visualize results

- Click "Run" to run the software
- The log is generated and after successful run, "Som run complete" notification is displayed (Figure 6).
- Click "Results" (Figure 6) to visualize and analyse the results.

3.4 Results

In the last step, you can see the results. These are: "Somspace results", "Geospace results", "K-means clustering", "Boxplots", "Scatterplots" and "Interactive" (Figure 10. SOM space resultsFigure 10). You can access these using the buttons on top of the results window.

The result folder includes the SOM space and geospace results ("result_som.txt" and "result_geo.txt") and information on the run ("RunStats.txt") as text files and dictionary files ("som.dictionary", "cluster.dictionary"). The "result_som.txt" file contains the SOM codebook vectors. The SOM codebook vectors represent the values of each SOM cell in the input data variables.

Subfolders in the main results folder contain figures and/or data for geospace and SOM space results, boxplots, scatterplots, data preparation, original data, and the interactive plot. If input data is given in geoTIFF format, results in geospacer are also given in geoTIFF format. The folder structure is visualized in Figure 9. These subfolders can be accessed using the "Show results in filesystem" option in each of the results windows of the GisSOM interface (Figures 10, 11, 13, 14, 15).

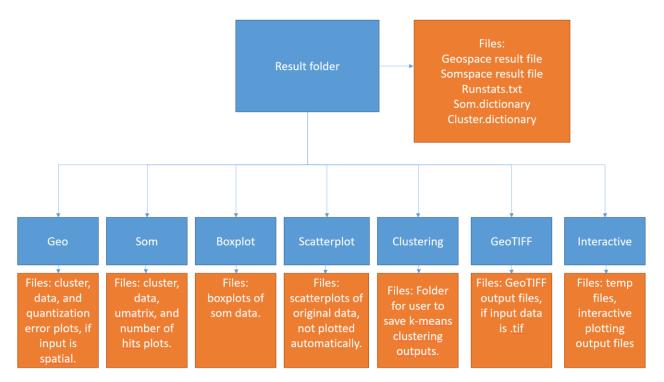


Figure 9. Structure of the result folders. Blue boxes represent folders and orange boxes represent files. For labelled input data in the csv format, a 'labels.csv' file is also generated in the main Result folder

3.4.1 Results in SOM space

These images (Figure 10) show the resulting SOM, color coded using various parameters:

- K-means cluster (Figure 10a). The left-most numbers on the legend represent the number of the cluster, and the numbers on the right represent number of data points per cluster (Figure 10b).
 - a. If labels are provided in the input data, the k-means cluster image (Figure 10a) shows the labels on the SOM cell. The labelled SOM nodes are indexed (Figure 9c) so that each combination of labels assigned to a SOM node gets a unique index. For instance, SOM cells with label index '1' in Figure 9a, contain the one data point with label '1'. SOM cells with label index '2' in Figure 10a contain two labelled data points each with label 1 (Figure 10c).
- 2. Value of each codebook vector element (corresponding to data variables), Figures 10d-f
- 3. U-matrix (the magnitude of the difference of the codebook vectors in neighboring SOM nodes), Figure 10g
- 4. Number of data points clustered in each SOM nodes, Figure 10h.

The "Add label data" (Figure 10i) button can be used to insert new datapoints with labels, and the data will be visualized in a new plot. The data must be provided in CSV format, and the number and order of columns must match the columns of the somspace results file ("result_som.txt" or "result_som.csv").

All results can be viewed in the containing folder using the "Show results in filesystem" option (Figure 10j)

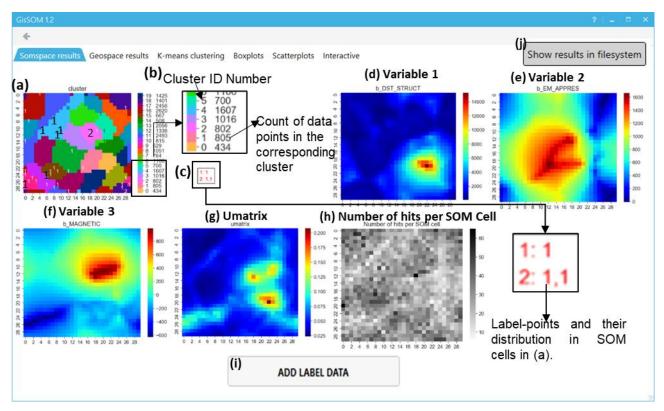


Figure 10. SOM space results. The frames (a) – (j) are described in Section 3.4.1.

3.4.2 Results in geospace

These images show the k-means clusters, the codebook vector elements (input variables) of the best-matching units and quantization error in geographical space (Figure 8 a; b-d; and e, respectively). Quantization error is the difference between the original data variable values and the SOM codebook vector elements of the SOM node where the data point has been projected to. High quantization error values show outliers in the data.

For non-spatial input data, the "Geospace results" window remains empty. The quantization error cannot be visualized, and it is reported only in the "RunStats.txt" -text file.

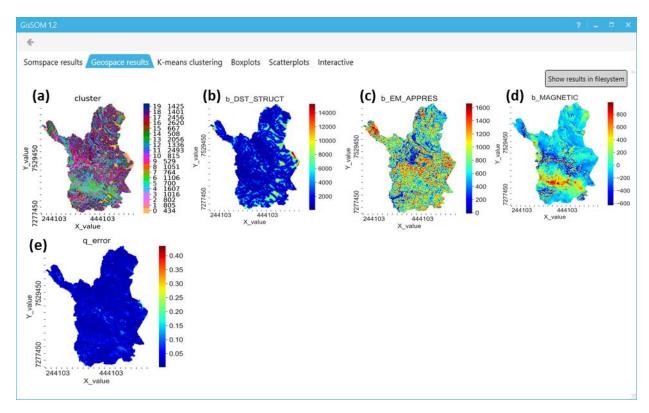
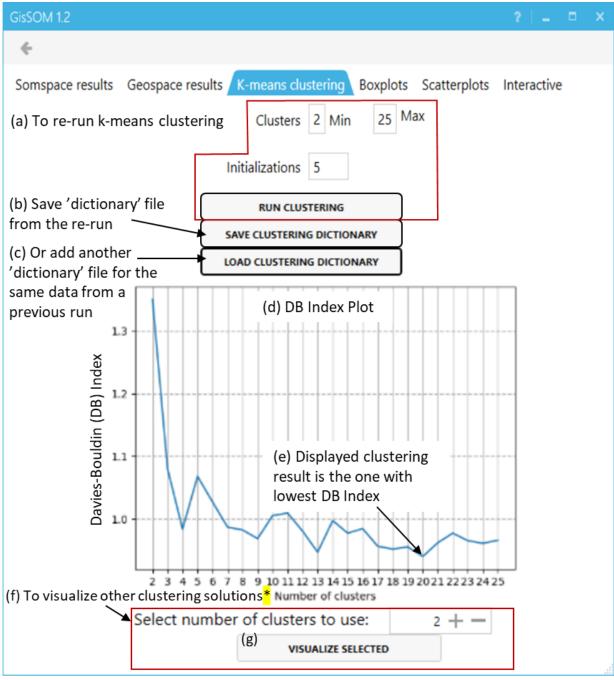


Figure 8. Geospace results.

3.4.3 K-means clustering

If you are not satisfied with the current clustering, or want to explore different clustering variants, it can be done in the K-means clustering tab (Figure 9). You can run the clustering again with different minimum and maximum number of clusters or initializations (Figure 12 a). It is advised to save the current clustering solution as a cluster dictionary file using the "Save Clustering Dictionary" option (Figure 12 b). This dictionary file can be reloaded using the "Load Clustering Dictionary" option (Figure 12c). The plot in Figure 12 (d) shows the Davies-Bouldin index for each number of clusters. Use "Select number of clusters to use" and click the "Use selected" button to get results for a different number of clusters (Figure 12f). This updates the results in the other tabs and the images will be redrawn with the selected number of clusters. These images will overwrite the previous images in the output folder.



*The updated results can be visualized in the tabs, and these will also overwrite the old results in the Output Folders

Figure 9. Clustering results.

3.4.4 **Boxplots**

These images show the boxplots for the SOM codebook vectors for each data variable. If the SOM result represents the data, the boxplots describe the distribution of original data values as well. The values are grouped by the k-means clusters (Figure 10). Color coding is the same as in the geospace and somspace images.

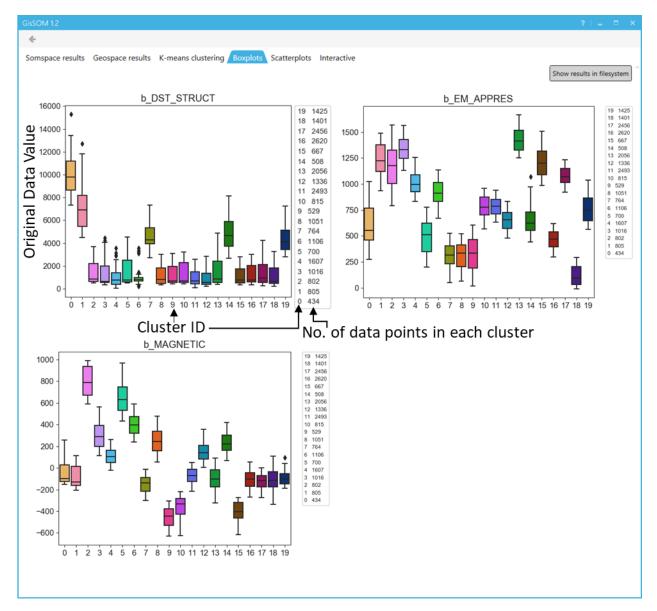


Figure 10. Boxplot results

The window includes one image for each data variable. In an image, there is one boxplot for each cluster. The line in the middle of the box is the median value and the borders of the box are the first (25 %) and third (75 %) quartiles. The lines extend from the box borders to reach the minimum and maximum values, but no more than 1.5 times the size of the box. If there are any points outside the box and lines, they are visualized using discrete points.

3.4.5 Scatterplots

Scatterplots are plotted for SOM codebook vectors. The initial Scatterplots tab is without any images (Figure 14). Scatterplots are not plotted or saved by default in the output folder. Because their number increases exponentially with the number of columns in the input data and depending on the dataset this can lead to a very large number of plots. Select the variables you want to plot and click "Draw Selected" to draw the scatterplot pairs you want. This also saves the drawn scatterplots

in the "Scatterplot" folder. Each image shows one pair of variables as a scatterplot (Figure 15) and each point in the scatterplot represents one SOM codebook vector. The dots are colored based on the cluster that the data point belongs to.

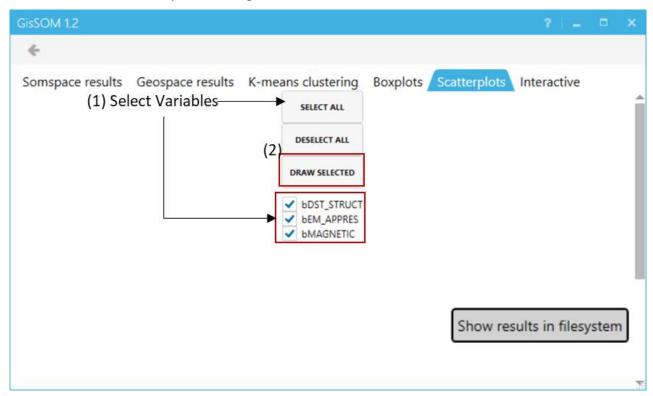


Figure 11. Scatterplot page after SOM calculation. No scatterplots have been drawn.



Figure 12. Scatterplots of selected variables

3.4.6 *Interactive* plotting

Hovering the mouse over the SOM grid plot will display the SOM x and y coordinates and the index of the cluster (Figure 13). There are two selection modes: "Cluster", which highlights data points assigned to an entire cluster on the geospace map, and "Som cell", which highlights data points assigned to one SOM node. By left-clicking on any cell on SOM, the data points assigned to the corresponding cluster or SOM node will be highlighted on the geospace plot on the right side (Error! Reference source not found.). For the output, you can choose between clusters or any of the original data variables.

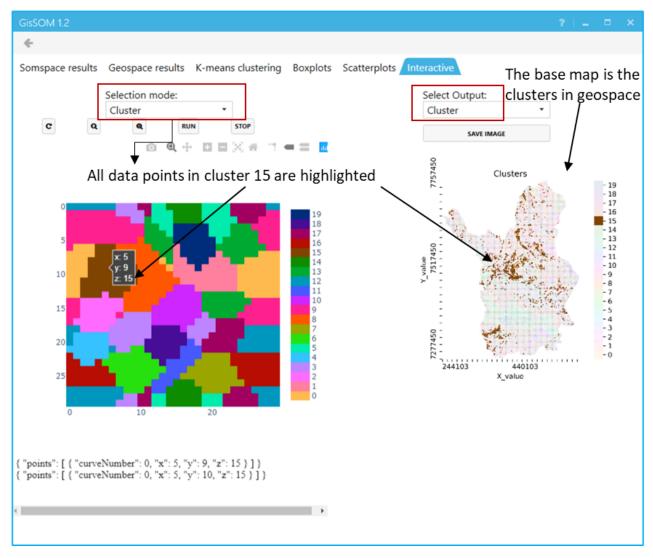


Figure 13. Interactive plot, selected cluster is drawn on the right-side image

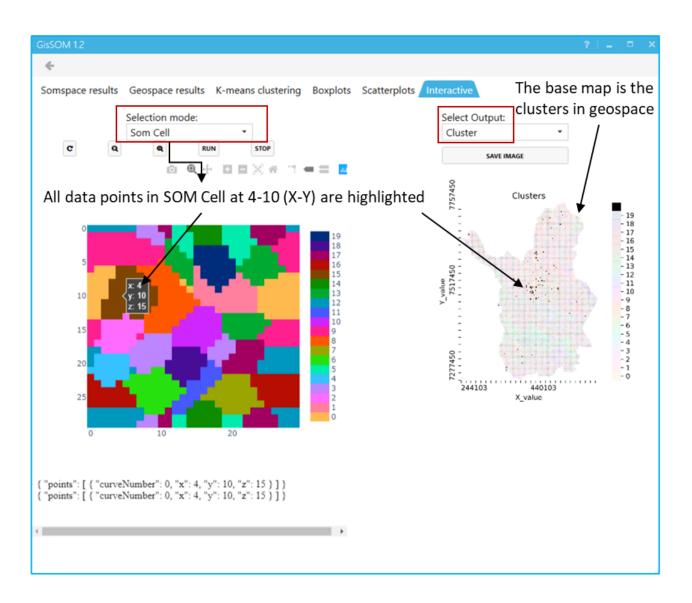


Figure 14. Interactive plot highlighting a single SOM cell

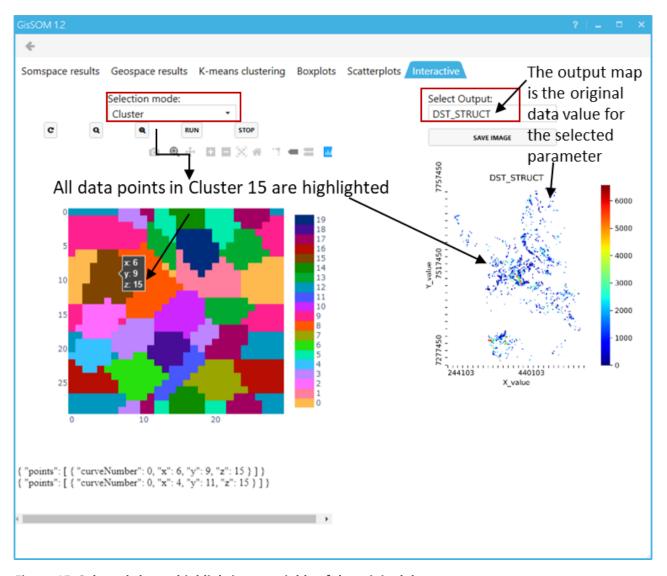


Figure 15. Selected cluster highlighting a variable of the original data

In some cases, the built-in web browser that GisSOM relies on, might not display the interactive plot. In this case you can try to click the "Refresh"-button, or if this doesn't work, you can try stopping the plot ("Stop"-button) and running it again ("Run"-button). After the loading icon for the new plot has completed, the plot may require refreshing to display. If all else fails, you open the plot in a web browser. The interactive plot should work on any up-to-date version of most modern web browsers (Edge, Chrome, Firefox...), and can be opened either by clicking the "Open in web browser"-button in the bottom of the interactive window, or by manually navigating to the web address "http://localhost:8050/" (Error! Reference source not found.). The plot will work the same in both the GisSOM window and the web browser, where clicking on any SOM cell in the interactive plot will highlight the corresponding data points on the main window's interactive geospace plot.

3.5 Visualizing previous results

Results from previous SOM runs can be viewed in GisSOM by selecting the "Old Results" -option form the data selection drop down menu in the data preparation view (Figure 19). Selecting a result folder (a folder prefixed "Out_" in the "GisSOM" main folder) will open the Results-window, showing the selected results. You can use the interactive plot, re-do clustering and save the new clustering scheme in the results folder of the previous SOM run. You can also run the SOM calculation again for the same input data that was used for the previous SOM run. In this case, a new results folder is generated in the "GisSOM" main folder. If the input data for the previous SOM run had been in geoTIF format, saving the geotiff output of the new SOM run requires that the path to the original geoTIF input files has not been changed.

It is recommended not to navigate back to the main "Input data" window unless a new project with new input data needs to be started. The original data of the previous SOM run will not be displayed here, and it cannot be re-preprocessed (Figure 20).

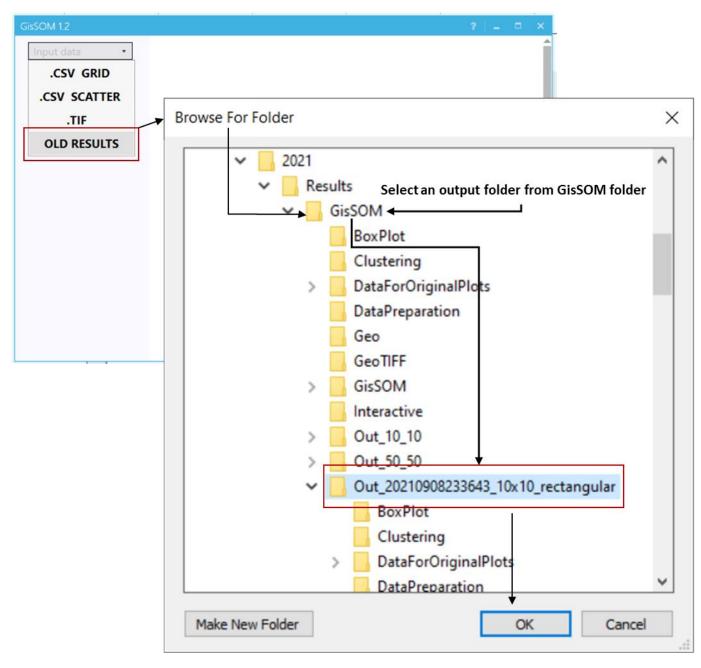


Figure 16. Visualizing old results in GisSOM

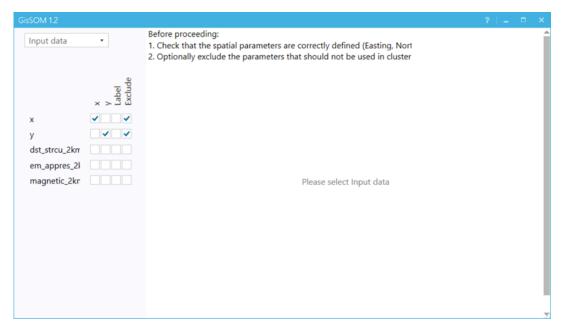


Figure 20. Loading old results in GisSOM – The original data cannot be visualized and re-preprocessed in the main window, when using old results.

4 REFERENCES

Davies, D. L., & Bouldin, D. W. (1979). A cluster separation measure. *IEEE transactions on pattern analysis and machine intelligence*, (2), 224-227.

Deliverable 4.11 Appendix 1: Technical Specification – nextsomcore

Deliverable 4.11 Appendix 2: Technical Specification – GisSOM.

Deliverable 4.12: SOM tool for advangeo® (under preparation, due in M18)

Deliverable 4.13: SOM tool for ArcGIS (under preparation, due in M18)

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