

Instructions for use of the crossvalidation.py script

- 1) Load the file with measuring data into SGeMS twice (Menu - Objects - Load Object): once as data and then under a different name, e.g. "points", as an "interpolation grid". Next, to make things clear, it might be useful to remove properties from the other object (serving as the "interpolation grid") (Menu - Objects - Delete Properties), which will now only contain "empty" locations (Fig. 1).

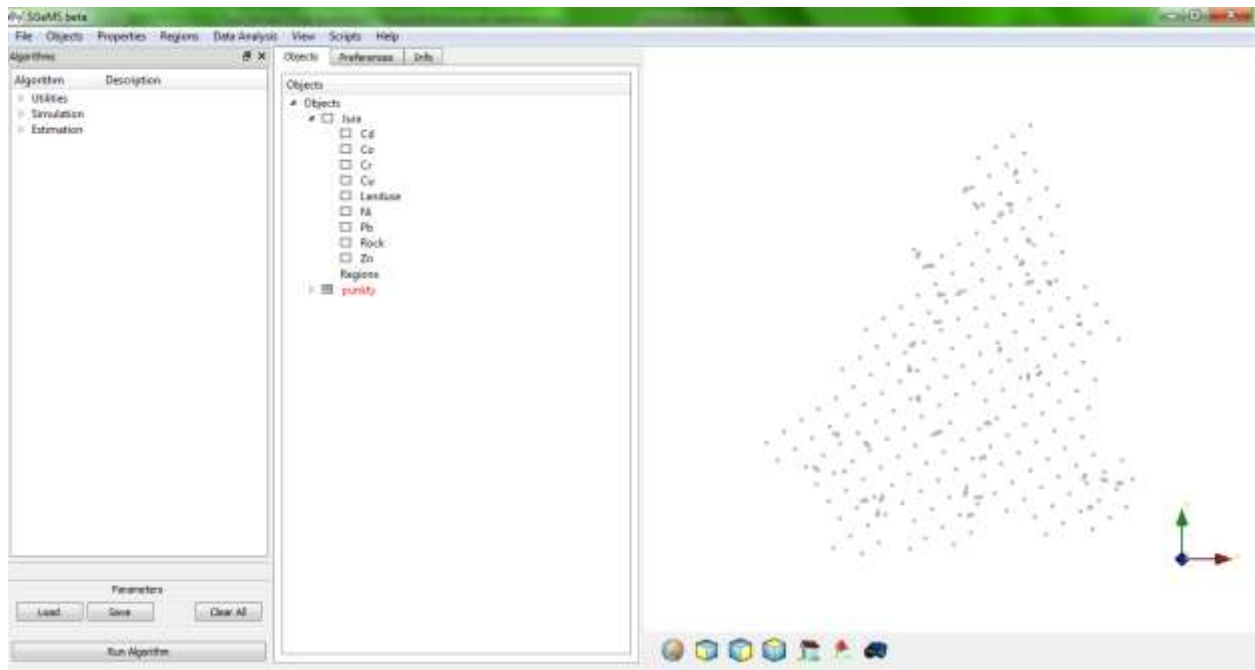


Fig. 1. View of the Objects Panel and "empty" locations ("punkty") - the "interpolation grid"

- 2) Perform kriging on the loaded data using those "empty" locations (Algorithms - Estimation - Kriging) (Fig. 2):
 - in the "General and Data" tab, in the "Kriging grid" section, in the "Grid Name" dialogue box choose the name of the point-set - the "interpolation grid", and in the "New Property Name", enter the name of the new property under which the estimation results are going to be saved;
 - choose the type of kriging: Simple Kriging, Ordinary Kriging, or Kriging with a Trend;
 - in the "Hard Data" section, in the "Object" dialogue box, choose the point-set with measurements in the given locations, and in "Property", the estimated property;
 - provide the remaining parameters in this tab and the "Variogram" tab;
 - press the "Run Algorithm" button.

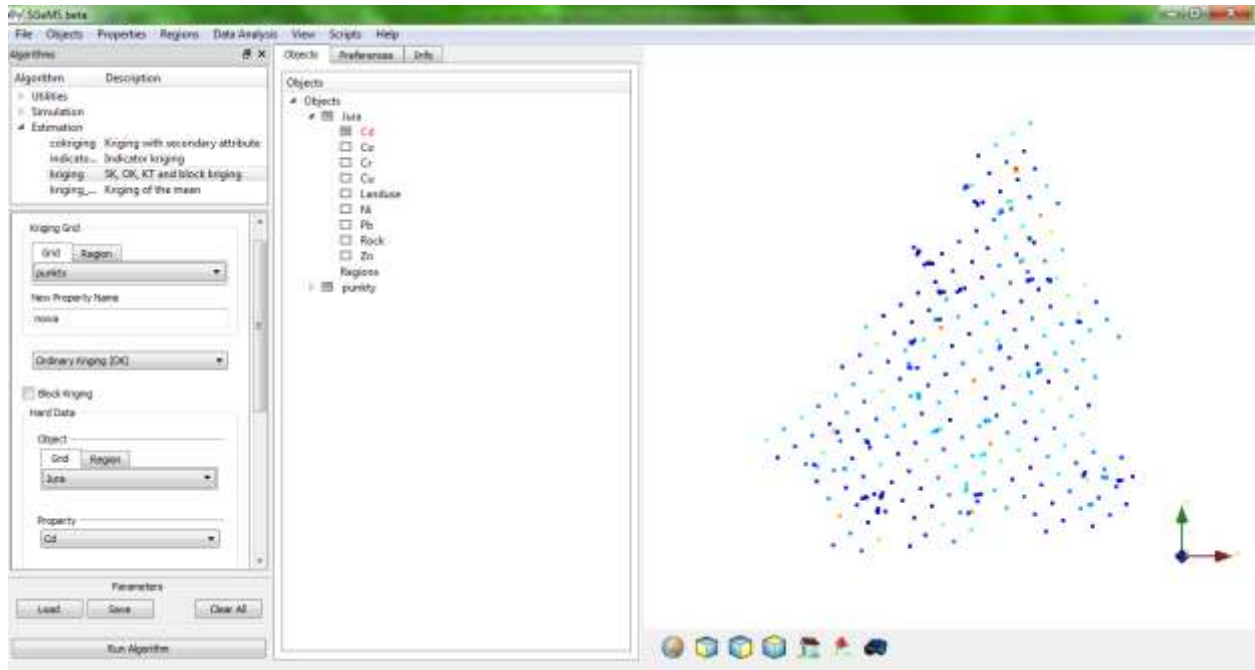


Fig. 2. Supplying the required kriging parameters in SGeMS

- 3) Open the Command panel (Menu - View - Commands Panel) and from the "SGeMS Commands History" window copy the entire last command, starting with "RunGeostatAlgorithm kriging:: ..." to "...</Variogram> </parameters>" (Fig. 3).



Fig. 3. View of the Commands History panel and the copied "RunGeostatAlgorithm" command

- 4) Open the crossvalidation.py script in a code editing program¹ and save it under a new name with the extension .py (the command "Save as...").
- 5) Following the instructions given in the comments, complete the script saved under the new name with names of grids and properties as well as the copied code of the kriging algorithm (Fig. 4):
 - in comments nos. 3, 9, 14, 15, 21, 23, 27, 42, 44, and 45, instead of "object" and "property" enter the exact names given in the "Object" and "Property" dialogue

¹ This can be e.g. the Python script editor in SGeMS (Scripts - Show Script Editor) or any other program, but the author suggests the Notepad++ program.

boxes in the "Hard Data" section during kriging;

- in comments nos. 2, 17, 20, and 24, instead of "grid name" and "new property name" enter the exact names given in the "Grid Name" and "New Property Name" dialogue boxes in the "Kriging Grid" section during kriging;
- to minimise the risk of error when writing the names, you can use the option "Change" to change all the words "object" into the name of the data set, "property" into the name of the estimated property, "grid name" into the name of the point-set, and "new property name" into the name of the new property;
- in comment no. 16, paste the algorithm code; be sure to place the symbols: ') right after the copied algorithm (as in Fig. 4), and not in the next line;
- in comments nos. 37 and 45, in the appropriate places enter the path to the file together with its name and extension (.txt in comment no. 37 and .png in comment no. 45);
- on completion of the entire code, you may want to compare it with the completed script given as an example in Appendix no. 2;
- on completion of editing, save the whole (command Save).

Fig. 4. Editing the crossvalidation.py file saved under a new name

- 6) If this has not been done earlier, open the Python script editor in SGeMS (Scripts - Show Script Editor) and load the script saved under the new name (File - Open). Then activate it by pressing the Run button (Fig. 5a).

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41. importing the necessary modules
import sgems
from math import *

42. deleting the estimation and kriging variance
values calculated by running the kriging
algorithm, which is needed to copy it into the
script - instead of "grid name", the exact name
given in the "Grid Name" dialogue box should be
entered, and instead of "new property name",
the exact name given in the "New Property Name"
dialogue box in the "Kriging Grid" section when
performing kriging, but the "New Property Name"
should be supplemented with _krig_var, e.g. "grid
name", "name krig var"
sgems.execute ('DeleteObjectProperties
punkty:nowa')
sgems.execute ('DeleteObjectProperties
punkty:nowa krig var')

```

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433. displaying the real and estimated values and
errors and other estimation quality statistics
print 'real values:', r_val

print 'estimated values:', new_value

print 'errors:', error
print 'standardised errors:', st_error
print 'mean error (ME):', ME
print 'mean absolute error (MAE):', MAE
print 'mean squared error (MSE):', MSE
print 'root mean squared error (RMSE):', RMSE
print 'mean square standard residual (MSSR):',
MSSR
print 'minimal error:', min_er

```

Script Output Messages

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0.259209767548844, 0.32626887579740604, 0.8283541297705782,
-0.4871188113573745, -0.058852638309720095, 2.974472120305903]

mean error (ME): 0.0033781187097

mean absolute error (MAE): 0.518052082

mean squared error (MSE): 0.534026127919

```

Fig. 5. Script editor in SGEMS: (a) the script; (b) the results of the script execution

7) When the script has finished running, its results: all real and estimated values and estimation quality statistics, will be saved to a file and place indicated by the user (Fig. 6). The results also appear in the "Scripts Output Messages" window of the editor (Fig. 5b). If the script has been filled in erroneously complete, an error message will appear in the window instead. Then go back to point 5 and check if all the names have been entered correctly.



Fig. 6. The file with the results of the script execution

8) In the Objects panel, display an object with data, where four new properties have been added: "estimated values", "errors", "kriging variance", and "standardised errors" (Fig. 7).

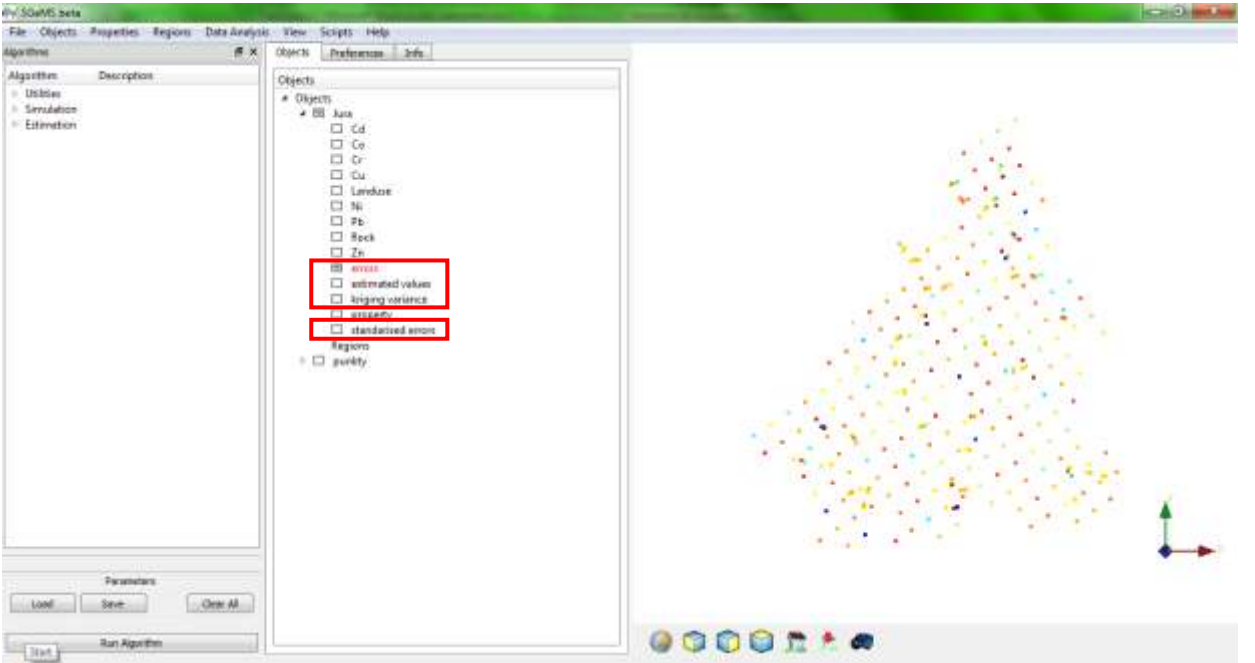


Fig. 7. New properties in an object: error, standardised errors, kriging variance, and estimated values

- 9) Running the script also produces a histogram of standardised errors as well as a scatter diagram of estimated and real values and another one of estimated values and standardised errors (Figs 8-10). Each diagram is saved to a file and place indicated by the user. In addition, the histogram will appear on the screen immediately after the script has finished.

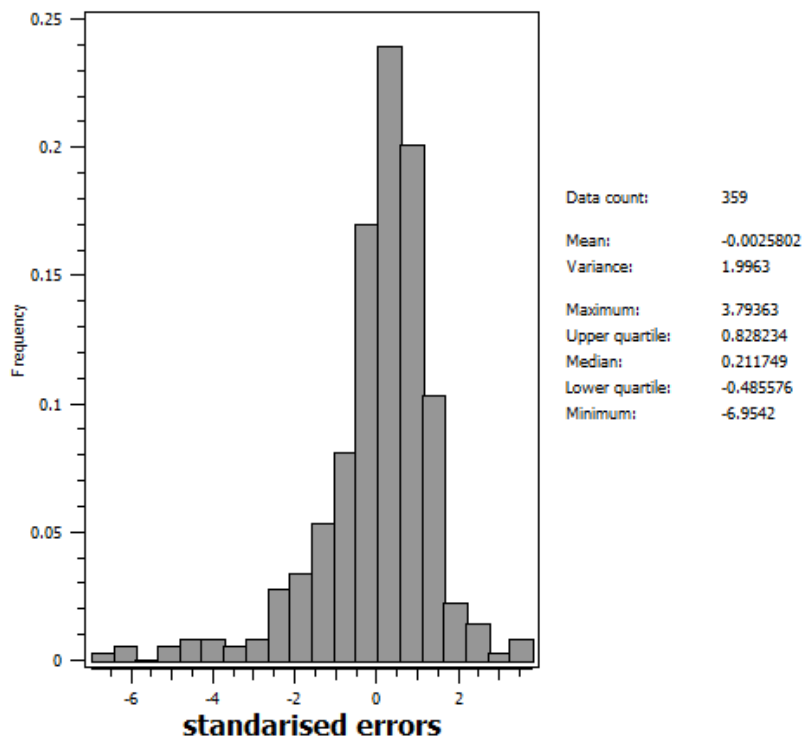


Fig. 8. Histogram of standardised errors

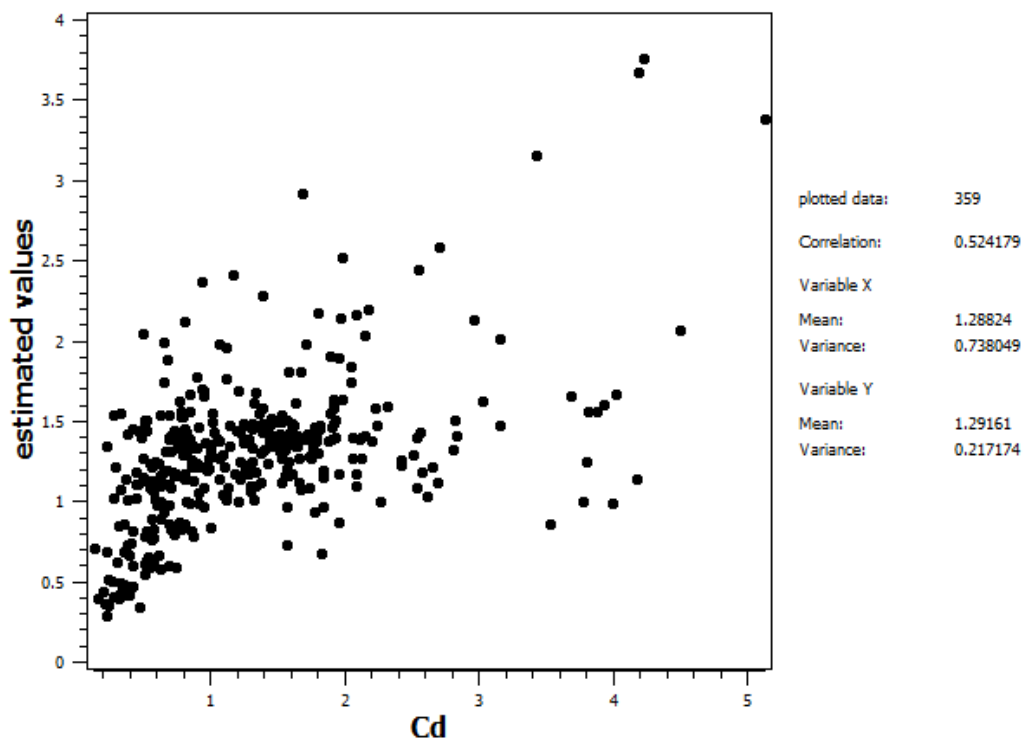


Fig. 9. Scatter diagram of estimated and real values. On the right, the correlation coefficient is given ("correlation")

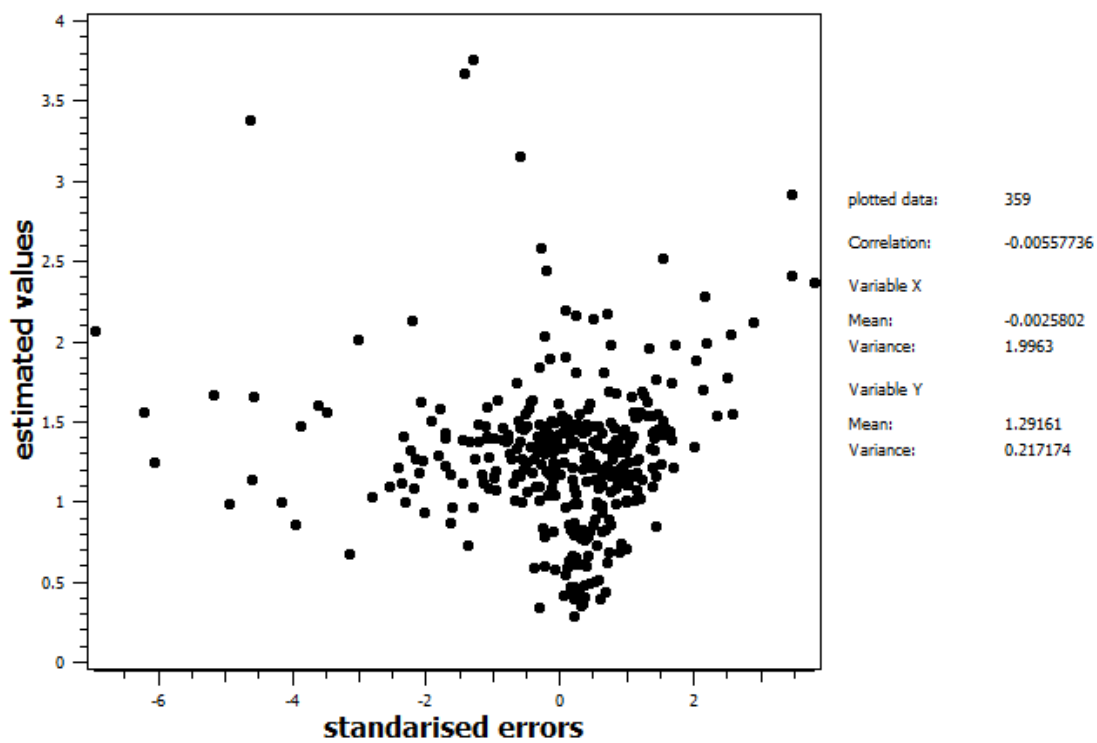


Fig. 10. Scatter diagram of estimated values and standardised errors