ZEISSLER, K.-O., Th. HERTWIG:
Artificial Neural Network instead of Kriging? A Case Study with Soil Contamination of Complex Sources.

Heavy Metal Contamination Maps - The geoscientific task

The soils of the Ore Mountains in Saxony (Germany) have a high concentration of several contaminant elements (As, Pb, Cd, U and others) over large areas. This is caused by geogenic conditions, mining and other industrial activities in the past.
For recultivation and regional planning, soil contamination maps which are indicating the location of these contaminations are needed. Several methodical rules with recommendations for planning of the sampling campaign, analytics and data processing were developed, e.g. in the German States of North Rhine Westphalia and Saxony (/2/, /3/, /4/).
In a first step, the methodical rules where applied to the areas outside the settlements. This was the simple case. In the next step, the modified rules had to be applied to the settlement areas. Due to the complexity of possible sources and small-scale variability of contamination within urban areas, modeling of contamination maps for settlement areas is a sophisticated task. In addition to defining the boundary of the study area, sampling and analytics, both recent and historical land use has to be analyzed. Also, the knowledge about the geological underground is of great importance. The results of several regionalization methods like Voronoi mosaic, IDW, Kriging and others must be combined with the knowledge of the spatial characteristics of the contamination sources. In some cases this is rather difficult, e.g. for linear geological structure sources like veins in combination with Kriging. For such cases a new software was developed: advangeo®. It was applied the first time to prediction tasks of regionalization in the frame of the reserach project "Contamination maps in settlement areas" /1/.

Study area and Sampling

The city of Annaberg-Buchholz was selected as one of two study areas. Silver mining has a history of more than 500 years there. Annaberg has about 22000 inhabitants. After defining the sudy area, it was divided into land use classes captured from aerial images. These data played an important role during modeling of the Pb concentrations. Fig. 1 shows the land use classes and the sampling program. This program consisted of three parts:

- Old samples before 2009 (101)
- New samples in 2010 (32)
- Check samples for proof of the model results (10)

The sample points had to represent the area ratio of the land use classes. Some problems with sample locations occurred within settlements. That's why the "Gardens" are slightly overrepresented.

At each sample point, two samples were taken: upper (0-30 cm) and lower soil sample (30-60cm). The depth values are average values and depend on land use.

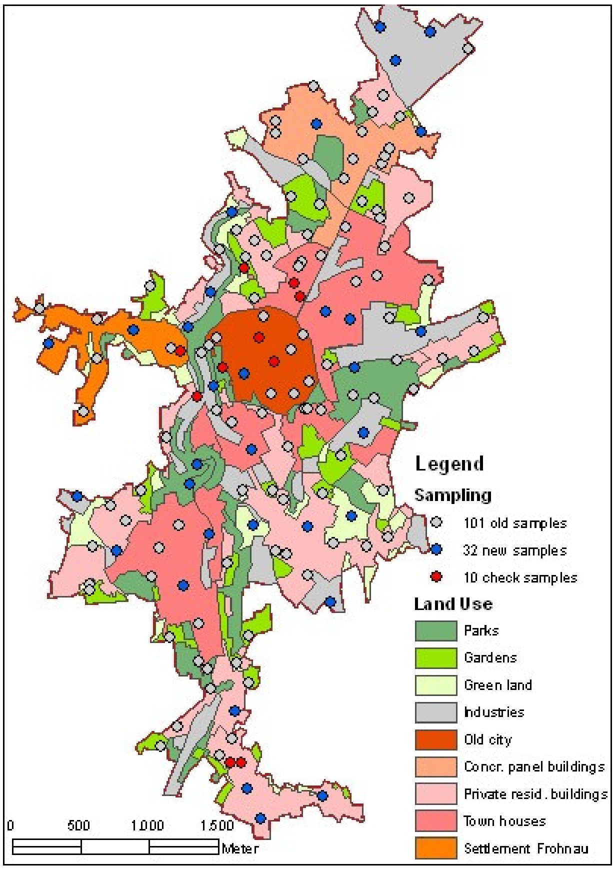

Fig. 1: Study area Annaberg-Buchholz: Land use classes and sampling.

The regionalization was done by using the old and the new sample data. The 10 check samples for proofing the modeling results were defined after modeling .

Several additional pieces of information were available and used during the modeling steps:

- DEM
- Geological map
- Deposit outline
- Vein map

Fig. 2 shows schematically the mineral veins inside the study area.

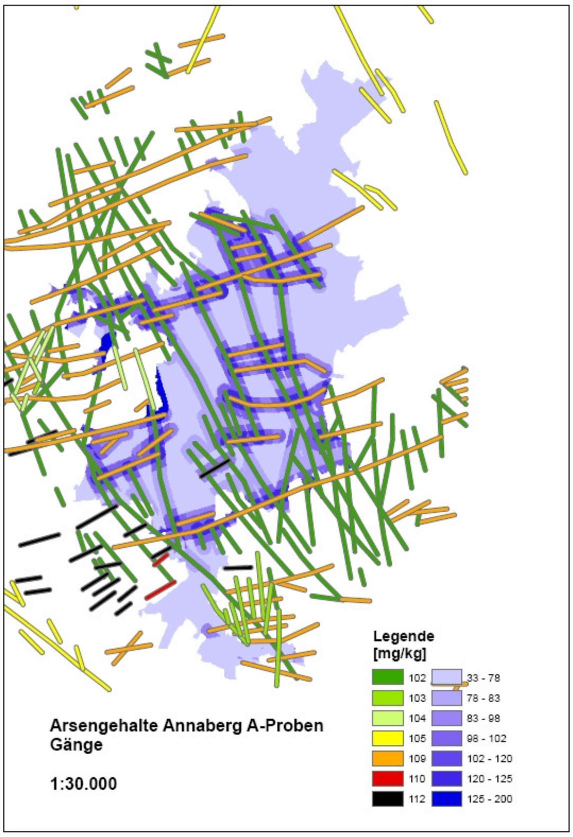

Fig. 2: Mineral veins inside the study area.

Inside the settlement area are some more samples with much more higher concentrations of contaminant elements from former industrial waste territories. These samples are only of local interest. Thus, they were excluded from the data processing.

Regionalization methods and Software

The regionalization methods are based on the functionality of the ArcGIS Extension “Geostatistical Analyst”. The following methods were applied:

- Voronoi Mosaic
- Inverse Distance Weighting (IDW)
- Ordinary Kriging
- Universal Kriging
- Indicator Kriging

The results of the different methods are shown for the example of As in figures 3-6 .

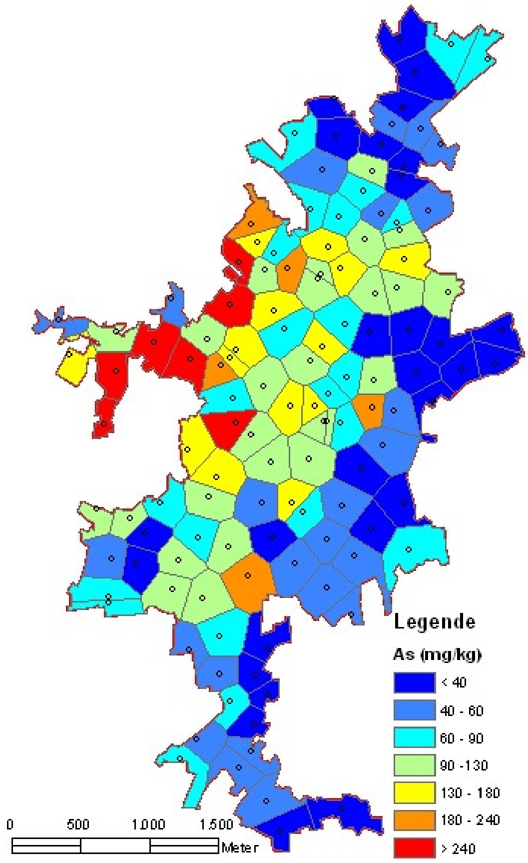

Fig. 3: Regionalization of As values from the upper soil samples by Voronoi mosaic

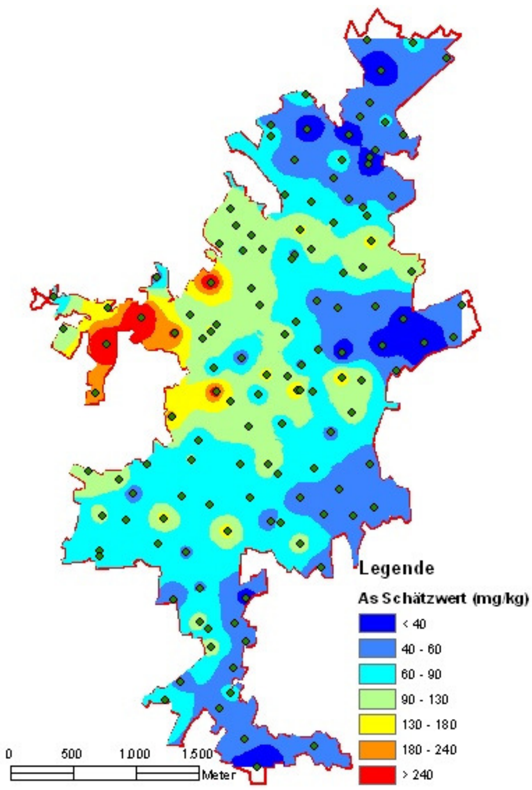

Fig. 4: Regionalization of As values from the upper soil samples by IDW

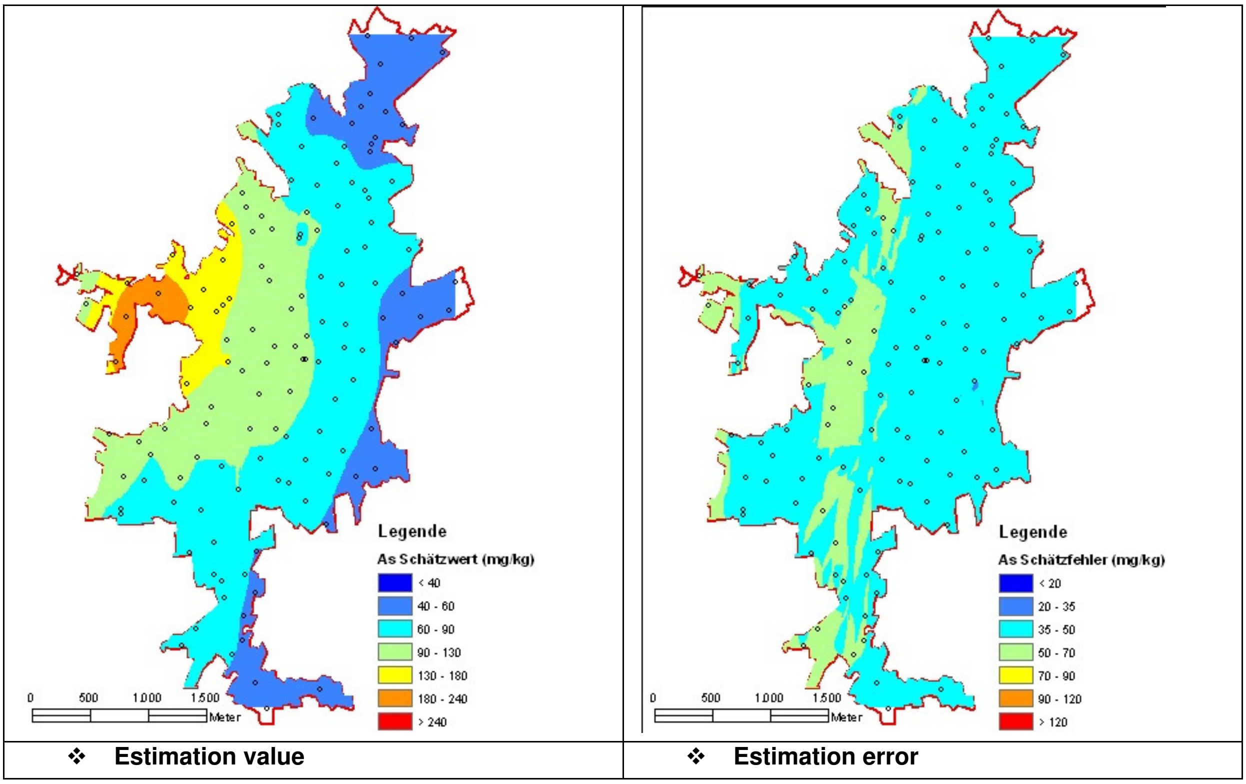

Fig. 5: Regionalization of As values from the upper soil samples by Ordinary Kriging

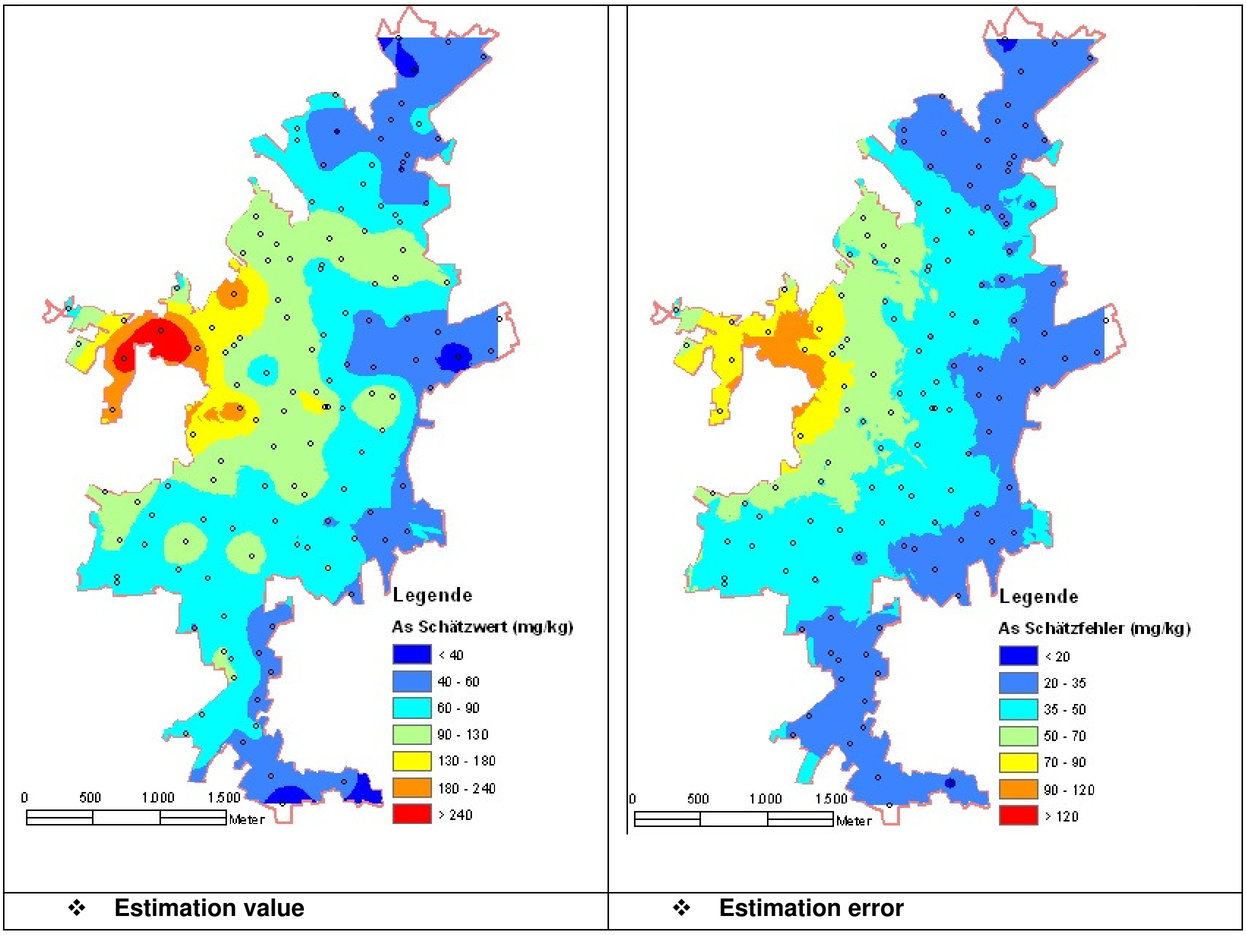

Fig. 6: Regionalization of As values from the upper soil samples by Universal Kriging

Universal Kriging delivered the most suitable regionalization result of the 133 upper soil samples. None of the method gave reasonable results using the mineral vein data (fig. 2).

Artificial neural network and advangeo®

A neuron is an object that receives from different other neurons or from outside signals, transforms them and sends the transformed signal to other neurons or to the outside. Several connected neurons form a neural network. A neural network is structured into layers. A layer consists of neurons with equal functionality. They distinguish between input layer, output layer and hidden layer.

- Input layers receive signals from outside.
- Output layers send signals to the outside.
- Hidden layers receive signals from input layers or from other hidden layers and send transformed signals to other hidden layers or output layers. They have no connection to the real outside world, but they map the real world.

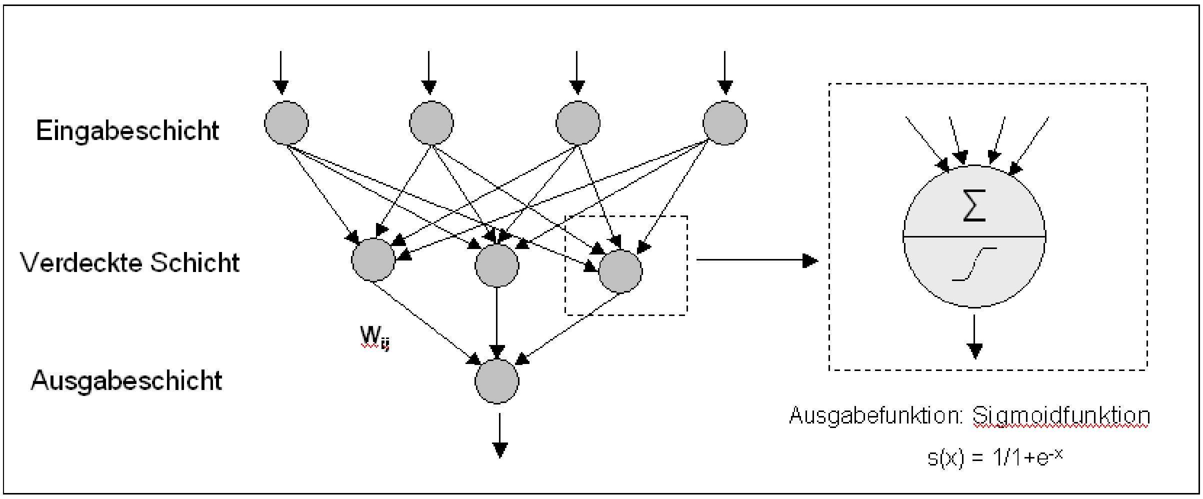

Fig. 7: Neural network with one hidden layer and the transformation function

Each connection between 2 neurons has a weighting factor. The signal of the transmitter will be multiplied by the factor received by the other neuron. All received signals of a neuron will be added. The summarized signal will be sent after transformation by the special transformation function.

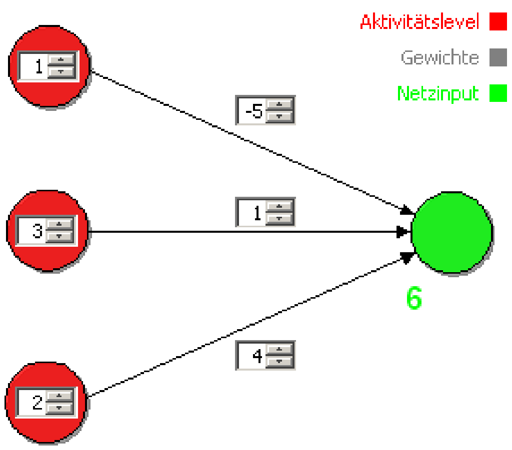

Fig. 8: Example of output signals, weights and input signals
(from ***http://www.neuronalesnetz.de/index.html***)

A complex signal which is coming from outside into a neural network passes through 5 processing steps (in case of an input layer, one hidden layer and an output layer):

- **Transormation of the signal in the neurons of the input layer to an output signal**
- **Weighted sums of the output signals of the input layer become the input signals of the neurons of the hidden layer**
- **Transormation of these signals in the neurons of the hidden layer into the output signals of the hidden layer**
- **Weighted sums of the output signals of the hidden layer become input signals of the neurons of the output layer**
- **Transormation into the output signals of the output layer**

This can be illustrated by two matrix equations and three signal transformations.

- $i_a = t(i_e)$
- $h_e = i_a \bullet W_{IH}$
- $h_a = t(h_e)$
- $o_e = W_{HO} \bullet h_a$
- $o_a = t(o_e)$

where

- i_e, h_e, o_e **– input signals of the neurons of the input, hidden- and output-layers**
- i_a, h_a, o_a **– output signals of the neurons of the input, hidden- and output-layers**
- **t(...) – transformations of the input signals into output signals**
- W_{IH}, W_{HO} **– matrixes of the weights of the connections between the neuron layers**
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An artificial neural network analyses the signals from outside and processes new signals for outside. For this task training data are needed. Training data consist of known input signals (for example land use, geological layers soil layers) and also known output signals (for example element concentrations). This type of training is called supervised training. The task of the training is to define the weights for the connections between the neurons and known output values. The summarized differences between output signals and known output values have to reach a minimum. One of the solution models is called backpropagation. After successful training the system is able to process output values from other known input signals with unknown output values.

This solution process is a multivariate statistical method. The advantages of the artificial neural networks are:

- mapping of complex nonlinear links
- combined input of continuous values and discrete values
- find correlations by training
- to generalize
- noise tolerance

The software advangeo® (/5/) realizes the described model of artificial neural networks. The following input layers were used in the case study:

- DEM
- Land use
- Geological maps
- Soil maps
- buffered mineral veins

advangeo® received for As the following solution (fig. 8).

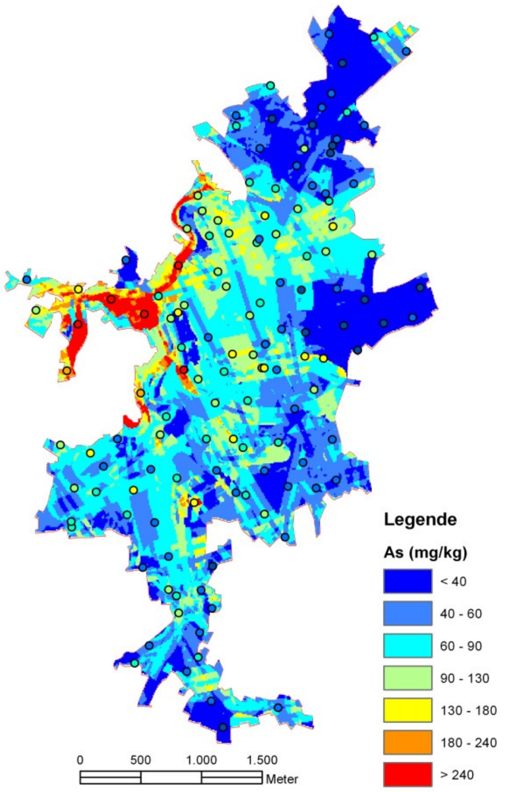


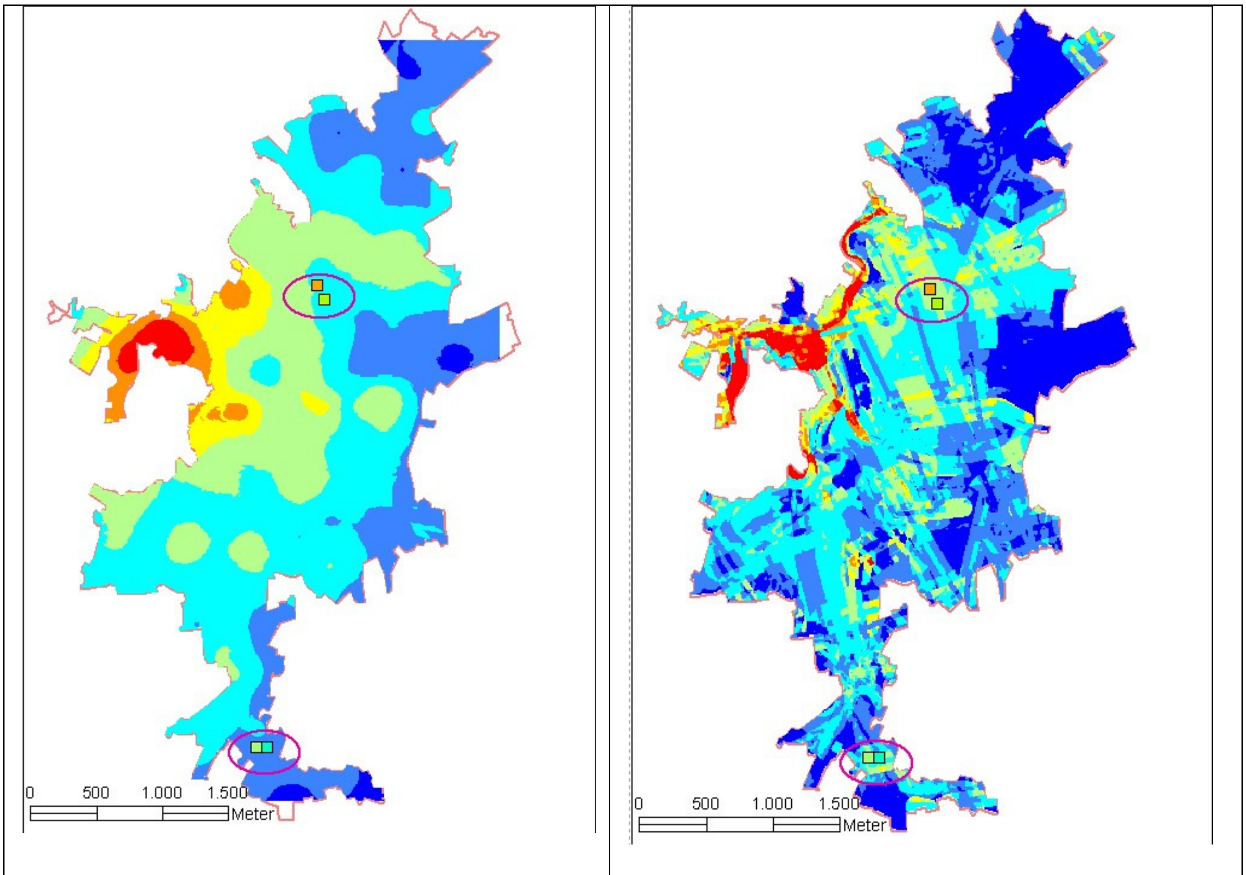
Fig. 8: Regionalization of As values from the upper soil samples by advangeo®

This picture shows the influence of the mineral veins on the results.

Comparison of the results

The comparison was done with the 10 check samples. Four of them at two locations were taken for proofing the As concentrations in the upper soil layer. Fig. 9 shows the real sample concentrations in comparison to the prediction values of Universal Kriging and advangeo®. The prediction of advangeo is closer to the check samples than Universal Kriging because the As concentration at this locations depends on the mineral veins.

A similar result was reached for Cd, but it could not be reached for Pb. The Pb concentration seems to depend on other input values than the ones used in this case study.



❖ **Universal Kriging**	❖ **advangeo®**

Fig. 9: Comparison of the 2 prediction results at two locations with 4 check samples

Literatur

/1/ HERTWIG, Th., ZEISSLER, K.-O.: Schadstoffkarten für Siedlungsbereiche. Landesamt für Umwelt, Landwirtschaft und Geologie, Dresden 2011. 78 S. (in print)

/2/ Leitfaden zur Erstellung digitaler Bodenbelastungskarten – Teil I: Außenbereiche, Landesumweltamt NRW, Essen 2000, 116 S.

/3/ Leitfaden zur Erstellung digitaler Bodenbelastungskarten – Teil II: Siedlungsbereiche, Landesamt für Natur, Umwelt und Verbraucherschutz NRW, Recklinghausen 2007, 107 S.

/4/ Erstellung digitaler Bodenbelastungskarten zur flächenhaften Darstellung und Beurteilung von Schadstoffen in sächsischen Böden – Leitfaden – Stand 05/2007, Materialien zum Bodenschutz, Sächsisches Landesamt für Umwelt und Geologie – 71 S.

/5/ For advangeo® see: http://www.beak.de/advangeo/.