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Remarks to the debate on mapping heavy metals in soil and soil monitoring in the European Union

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Reimann et al. (2017) published a correspondence in which the authors debate the validity of the methodology and results from the LUCAS Topsoil Survey of the European Commission, by commenting our publication on mapping heavy metal content of European soil (Tóth et al., 2016b). In that correspondence a number of issues are raised, including from the views of the authors on the current trends in soil mapping and monitoring to methodological questions on the evaluation of soil survey results.

One of the first critics of Reimann et al. (2017) is that the commented article did not include reference to earlier work of Reimann et al. and to EuroGeoSurvey in general. To miss a reference to a scientist's own publication in a correspondence might be regarded as a taste issue. However, this statement is factually incorrect too. In fact, our paper referred to the related work, including the GEMAS project and cited a number of publications (Demetriades et al., 2010, Lado et al., 2008; Ottesen et al., 2013; Salminen, 2005) of EuroGeoSurvey, which introduced the sampling and the use of collected data of the surveys. Reimann et al. (2017) later in their correspondence finally dubiously recognized the existence of these references - which first they missed to found the attempts to discredit our work. Although later efforts were made to slightly modify the initial sampling by EuroGeoSurvey by the participating institutes, it was not the aim of our article to clarify the situation of changing nomenclature and referencing of these exploratory, low density datasets.

Reimann et al. (2017) tries to give the reader to believe that any round of the FOREGS/GEMAS surveys went beyond low density sampling and that 4000 points on a larger area means higher sampling density than 20,000 points in a smaller area.

Reimann et al. (2017) ambiguously refer to the EC REACH Regulation (EC No 1907/, 2006), as to the protocol to follow at sampling. In fact, there is no prescription for the sampling design nor to sampling density in this regulation.

The correspondence of Reimann et al. (2017) continues the attempt to discredit the findings based on the LUCAS Topsoil Survey by suggesting that only its preferred geological survey have reliable quality control. In reality the survey design and sampling procedure of LUCAS, the laboratory test and interpretation of its results are all subjects of rigorous quality control, which are also supplemented by quality control of obtained data against pedological criteria, which, by the way, was never released for the data of EuroGeoSurvey. In fact, this rigorous quality control procedure of the LUCAS project resulted disregarding of certain samples from the dataset, which did not qualify to any one or more of the assessed criteria, and as a consequence, some spatial hiatus is experienced at the first round of the LUCAS Tospsoil Survey, which was then filled-in at the second sampling campaign. Full documentation of the quality control procedure of the LUCAS topsoil data is available from the references (Carre et al., 2013; Eurostat, 2015; Guicharnaud, 2013; Tóth, 2013) cited in the article. It is worth noting, that a balanced scientific assessment by a commenting article should include reading the literature listed among the references of the commented article.

As soil functions are manifold, soil monitoring can have multiple purposes as well. Reimann et al. (2017) look from a very narrow view, when – in contradiction to other publications from the same authors (e.g. Smith and Reimann, 2008) - suggesting in their current correspondence that detection of hazardous elements with a low density on a continental scale would be an adequate tool to soil resources monitoring. The citation of the REACH regulation as it was the only document which has relevance to soil sampling is also factually incorrect. Although the REACH regulation is an important regulatory document, there are a number of other key EU and international policies, which require soil sampling, for the purpose of carbon sequestration, climate change effects, biodiversity etc. ((EC) No 2152/2003; IPCC - Intergovernmental Panel on Climate Change, 2003, Stolbovoy et al., 2007). A comprehensive soil monitoring system has to serve all these requirements on the possible highest quality.

The ignorance of Reimann et al. (2017) to the multiple objectives of LUCAS becomes evident from the incorrect statement saying "The whole LUCAS project was undertaken in order to detect contamination". Let us call the attention to the facts. First, the LUCAS project is a land use and land cover survey (Eurostat, 2015), which is supplemented by a soil component, which is becoming the soil monitoring in Europe, in association with the land use and land cover monitoring. Second, LUCAS topsoil samples were analyzed for heavy metals only at the second phase of the tests, three years after the measurement of properties of major interest, - such as organic carbon content, or macronutrients - started, on which a series of publications were published, prior to the studies on heavy metals.

Reimann et al. (2017) criticize our statement which specifies the LUCAS Topsoil Survey as "The European Union's first harmonized topsoil sampling", then refer to low density, unharmonized samplings of GEMAS.

Since the independence of soil science from agronomy and geology in the late 19th century, the theory of soil mapping and monitoring went through considerable development and resulted internationally accepted protocols and standards. Such protocols and standards, first of all, cover sampling design. National soil monitoring systems in Europe apply either stratified sampling or sampling based on a regular grid (Jones et al., 2005). Both have their merits, but once the monitoring becomes operational, the basic system of sampling points should be kept. The LUCAS topsoil survey, which becomes an operational soil monitoring in the European Union, having its second sampling campaign in 2015, choose the approach of stratified sampling, based on the grid of the Land Use and Land Cover Survey (LUCAS), which allows

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complex monitoring with land use and land cover patterns. Soil component of the LUCAS applies soil-relevant parameters for the stratification to determine sampling sites. The EuoGeoSurvey on the other hand, is using a non-harmonized approach when collecting samples. Some samples come from regular grid points of national geological surveys, some others from locations identified using different criteria, according to the data provider's traditions, possibilities etc. Therefore, in contrast to the claim of Reimann et al. (2017), the sampling of the EuroGeoSurvey fails the first criteria, namely the harmonized sampling design of a soil survey and/or monitoring protocol. The preconception and scientific quality of the corresponding article is best reflected by its maps on Fig. 1 (Reimann et al., 2017) which, applies the "bigger dot at the sampling point on the map would give an impression of better reliability" approach, which still cannot hide the inconsistency of the sampling design of the GEMAS project.

Nevertheless, even if we would overlook this important criterion, we cannot neglect another one. Density of topsoil sampling of the Geological Surveys is an order of magnitude below the density to qualify for reconnaissance scale, therefore it can be only used for orientation purposes (see Table 1.). Even if digital soil mapping enables to refine the scale of soil maps by using auxiliary information (Boettinger et al., 2010; Dobos et al., 2006; Hartemink et al., 2008; Hengl et al., 2004; Hengl and Husnjak, 2006; Lagacherie et al., 2007; McBratney et al., 2003; Zhang et al., 2016) the sampling density applied by the EuroGeoSurvey is inadequate for even national scale reconnaissance of soil resources, at least with the required reliability for countries having the size of those in the European Union. It is no surprise that country soil maps were not based on this data.

On the other hand, we have to declare that LUCAS data are representative on regional (NUTS 2) to country level for areas below 1000 m elevation across the EU (Carre et al., 2013). This is already detailed enough to detect human-induced changes, which is not possible based on the low density sampling (Smith and Reimann, 2008), done by the EuroGeoSurvey and which is partly financed by Eurometaux, the metal producers' association of Europe.

Reimann et al. (2017) criticized the applicability of spatially exhaustive auxiliary information in digital soil mapping (DSM). Thus, we would like to highlight its advantages. In DSM the role, as well as the application of auxiliary information have been showing an increasing trend since the well-known Jenny's factorial model of soil formation has been formulated by McBratney et al. (2003), which is known as the scorpan model. In DSM the aims of using auxiliary data are twofold (Minasny and McBratney, 2007): (1) to remove the trend to achieve spatial stationarity, and (2) to enhance spatial prediction of soil properties by making use of auxiliary variables as environmental covariates. These environmental covariates are spatially exhaustive information from the area of interest, as well as these covariates are related to the spatial distribution of the soil properties of interest, which make them profitable for DSM. In general, the application of auxiliary information as spatially exhaustive environmental covariates improves spatial predictions, as it was illustrated by numerous papers (e.g. Dobos et al., 2006; Simbahan et al., 2006; Hengl et al., 2007).

Reimann et al. (2017) criticized the applied method. Thus, we would like to highlight several theoretical, as well as practical consideration and consequences of the applied method. We applied regression kriging (RK) in our research (Tóth et al., 2016b), which is a widely and frequently applied geostatistical prediction method in soil, earth and environmental sciences (e.g. Lado et al., 2008; Hengl, 2007; Kempen et al., 2014). The basic assumption of this technique can be originated in Matheron (1969). In case of RK we assume that the adopted random function $Z(\mathbf{u})$ can be decomposed into a residual component $R(u)$ and a trend component $m(\mathbf{u})$:

$$Z(\mathbf{u}) = m(\mathbf{u}) + R(\mathbf{u}) \qquad \text{Eq. 1}$$

where the residual component is modeled as a stationary random function with zero mean and covariance $C_R(\mathbf{h})$. RK combines the regression of the target soil property on spatially exhaustive auxiliary information with kriging of the regression residuals in order to estimate the value of the target soil property at unvisited (unsampled) location $\boldsymbol{u_0}$ (Hengl, 2007):

$$\hat{Z}(\boldsymbol{u_0}) = \mathbf{q}_0^{\mathbf{T}} \times \boldsymbol{\beta} + \boldsymbol{\lambda}_0^{\mathbf{T}} \times (z - \mathbf{q} \times \boldsymbol{\beta}) \qquad \text{Eq. 2}$$

where β is the vector of the regression coefficients, $\mathbf{q}_0$ is the vector of the covariates at the unvisited location $\boldsymbol{u_0}$, $\boldsymbol{\lambda}_0$ is the vector of the kriging weights, z is the vector of the observations and q is the matrix of the covariates at the sampling locations. RK is frequently referred to as the best linear unbiased predictor (BLUP) (e.g. Hengl, 2007) since it minimizes the local error variance; furthermore, the expected value of the difference between the predicted and the true value is zero. As it follows from the RK's equation (Eq. 2.), the "krigged" residuals are the key to represent the so-called "extraordinary effects" of the spatial distribution of the element concentrations, as it was criticized by Reimann et al. (2017). Moreover, RK is an "exact interpolator" therefore it gives back exactly the measured data at the sample sites. That is follows implicitly from its equation (Eq. 2.).

Apparently, the correspondents do not want to deal with the scale issue at all. However, scale and sampling density is the essence of any monitoring, and it has to be designed according to the targeted resolution of the information needed from the monitored environmental compartment. The quoted sampling campaigns from large countries from other parts of the world, like Australia, the USA but also those in China and the GEMAS in European have sampling densities of 1 site/5500 km^2, 1 site/1600 km^2, 1/2000 to 3000 km^2 and 1/2500 to 5000 km^2 respectively (Caritat and Cooper, 2011, Smith et al., 2014., Wang et al., 2015, Salminen, 2005, Reimann et al., 2014). To illustrate how low this density is: the latest studies based on the data of EuroGeoSurvey (Birke et al., 2016) use 148 points for Germany, while in Hungary, the country with one fourth of the territory of Germany operates a state soil monitoring on 1200 sites, but also the LUCAS dataset has >1500 points exclusively for the agricultural area of Germany.

Table 1
Relationships between the goal of the soil survey, sampling density and scale of derived soil maps*
(The table is indicative to soil surveys designed for soil mapping).

Kind of survey or map and level of intensity	Purpose and use of the survey results	Area represented by one sample (km^2)	Indicative scale of published maps
Precision farming (intensive, level1)	Special; executive purpose - within parcel	<0.01	>1:1000
Detailed (field scale, level 2)	Special; executive purpose - for parcel	0.01–0.5	1:1000–1:10.000
Semi-detailed (farm to regional scale, level 3)	General and special; planning purpose	0.5–10	1:10.000–1:100.000
Reconnaissance (regional scale, level 4)	General; planning purpose	10–50	1:100.000–1:250.000
Reconnaissance (regional to national scale, level 5)	General; orientation purpose on national scale	50–200	1:250.000–1:500.000
Exploratory surveys and compilations (national to continental scales, level 5)	General; orientation purpose on continental and global scale	>200	<1:500.000

* Based on the works of: Baranyai et al. (1989), Dent and Young (1981) Legros (1996), Curlik and Surina (1998), Garkusa (1958), Hengl and Husnjak (2006), Rasio and Vianello (1995) Szabolcs (1966) and Western (1978).