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Geostatistical filtering to map a 3D anthropogenic pedo-geochemical background for excavated soil reuse

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Abstract

The safe reuse of excavated soils in urban areas requires the guarantee of geochemical compatibility between this scarce resource and the local pedo-geochemical background. Previous works have shown that the usual statistical tools (high order quantiles, upper whiskers) are not always adequate for separating anomalies from background contents, especially when there are many anomalies.

This paper presents an application of factorial co-kriging (geostatistical filtering) used to separate anomalies from the pedo-geochemical background, according to their different scales of spatial variability. The hypothesis is that the background corresponds to long distance variations, while the anomalies, which can be either positive or negative, represent short distance variations.

The variable of interest is the lead content (Pb) in the subsoils of the “Ile de Nantes” urban area, where some areas were previously dedicated to industrial activities. The data were collected from different surveys, not specifically aimed at determining the pedo-geochemical background, but rather in a context of pollution diagnostics. The lengths of the samples were strongly variable. In a first step, only the samples having approximately the same length were retained for the estimation, which significantly reduced the amount of data. In a second step, the geostatistical estimation was performed using all the data. The resulting maps are significantly more accurate for the total Pb and its background component. The distinction between anomalies and background is discussed based on the calculated maps.

Factorial co-kriging appears to be relevant to map the anthropogenic pedo-geochemical background, using data acquired for other purposes. It allows separating anomalies and background for any parameter presenting significant contrasts.

Keywords: separation, background, anomalies, geostatistics, filtering, geochemical

1 Introduction

Soils are located at the interface between the hydrosphere, the biosphere and the atmosphere, and are thus exposed to influences from various phenomena. Referring to Standard ISO 11074, the term “soils” will be used hereafter as it encompasses both soils and subsoils, including anthropogenic deposits. Soils can be heterogeneous and are known to show even greater heterogeneity in urbanized areas due to important anthropogenic impacts (Cicchella et al., 2008; Le Guern et al., 2016a, 2016b ; Madrid et al., 2006; Pouyat et al., 2007; Rodrigues et al., 2009). Heterogeneity may cause major difficulties when identifying general properties of the environment

47 or building reference databases (Ander, 2013; Demetriades and Birke, 2015). This is why the data
48 acquisition step is typically focused on a specific phenomenon, e.g. the measurement of metal
49 content (Ander, 2013; de Fouquet, 2011; Lark and Scheib, 2013; Saby *et al.*, 2006), the evaluation of
50 carbon stock (Edmondson *et al.*, 2012; Raciti *et al.*, 2012) or the determination of biological
51 indicators (Hartley *et al.*, 2008). Faced with the problem of soil heterogeneity, previous authors; e.g.,
52 Demetriades and Birke (2015) for urban topsoils, have proposed sampling strategies focused on the
53 “most representative sampling sites” for determining threshold values to define the urban pedo-
54 geochemical background. However, anomalies may often still be present in the final data. Such
55 anomalies are related either to the specificities of the particular medium (local contamination,
56 different soil composition or rearrangement) or to analytical errors: therefore they are not
57 representative of the studied environment and phenomena. The presence of anomalies is even more
58 pronounced when using preexisting data, since the sampling strategies were not defined for the
59 specific objective of the study at hand. This is the case for instance in France for redevelopment
60 projects. In France, in the absence of generic soil quality thresholds at a national level, the reuse of
61 excavated soils must refer to local soil background values. However, the geochemical data available
62 to determine this local background mainly come from pollution diagnostic studies.” Therefore such
63 data contain many “outliers” also referred to as “anomalies”. The objective of this paper is to
64 propose a coherent methodology for addressing such anomalies in the context of pedo-geochemical
65 background determination.

66
67 A manual data sorting, performed by an expert with detailed knowledge of the issues and
68 settings, may be efficient although time-consuming and results may vary from one operator to
69 another. Semi-automatic sorting methods are thus preferred in order to separate the background
70 (i.e. the studied feature) from the anomalies. Threshold values used to separate anomalies within a
71 set of representative data are usually calculated using statistical criteria. Such thresholds are often
72 based on higher-order quantiles (Q90 or Q95; Ander, 2013; Cave *et al.*, 2012; McIlwaine *et al.*, 2014;
73 Rothwell and Cooke, 2015) or on the sum of two terms; i.e., a “central” term (mean or median) and a
74 dispersion-dependent term. Common examples are the upper whisker (Jarva *et al.*, 2014; Leys *et al.*,
75 2013; Reimann *et al.*, 2005, 2018; Reimann and de Caritat, 2017; Rothwell and Cooke, 2015;
76 Tarvainen and Jarva, 2011) and the MAD (Median Absolute Deviation) thresholds (Leys, 2013;
77 Reimann *et al.*, 2018). However, “outliers” isolated in this manner only include “extreme” values
78 (which are usually the largest). Among other factors, the results are influenced by the distribution,
79 the sample size, the censoring rate and the actual anomaly rate of the data (Reimann *et al.*, 2005;
80 Rothwell and Cooke, 2015; Sauvaget, 2019; Sauvaget *et al.*, 2020). These statistical criteria may
81 ultimately prove to be inappropriate in determining anomalous data in the case of data collected in a
82 different context with different objectives (Sauvaget *et al.*, 2020).

83
84 The classical framework for estimating statistical thresholds consider data as randomly and
85 independently drawn Butdata can also be interpreted as realizations of a sampling process applied to
86 a regionalized variable displaying some inherent spatial variability. This spatial variability is described
87 and quantified by the variogram, which expresses the relationship (up to the factor 1/2) between the
88 mean quadratic deviation of the data and their spatial distance. This variogram is then used to
89 estimate the variable at unknown locations by co-kriging. Even though geostatistics was initially
90 developed for mining applications (Matheron, 1965), the factorial kriging or co-kriging designed for
91 the search of local anomalies has a wide range of applications in soil sciences (Matheron, 1982;
92 Goovaerts, 1992; Wackernagel and Sanguinetti, 1993 ; Bourennane *et al.*, 2003 ; Rivoirard, 2003;
93 Saby *et al.*, 2009). The approach relies on the different scales of spatial variability present in the data.
94 A variable component associated to each given scale can then be estimated by factorial kriging or co-
95 kriging.

96
97 The pedo-geochemical background (Ademe Agency, 2018; Baize, 2008; Daniau *et al.*, 2009;
98 Reimann *et al.*, 2005) reflects the full set of usual soil contents throughout the study area. It

99 represents either natural phenomena or diffuse contamination and differs from localized
100 contamination or natural anomalies. Given that systematic sampling campaigns for determining
101 pedo-geochemical background values in urban areas are not currently pursued in France, the use of
102 preexisting non-specific data (primarily stemming from pollution diagnostic studies characterizing
103 soils and subsoils) is necessary. This constraint introduces a lack of representativeness in the data,
104 which can be expected to contain a larger proportion of anomalies due to the initial sampling
105 objectives. This introduces additional difficulties for the determination of a local pedo-geochemical
106 background, as it requires a careful separation of anomalies. The development of appropriate
107 methods is therefore needed. In the context of the reuse of excavated (sub)soils in France, an
108 additional difficulty lies in the 3D approach needed to determine the volumetric pedo-geochemical
109 backgrounds that will be used as reference values (Coussy *et al.*, 2020).

110 In this paper, the relevance of factorial co-kriging (geostatistical filtering) for estimating
111 pedo-geochemical background values is examined in the context of local volumetric analysis for
112 guiding the reuse of excavated (sub)soils. The underlying hypothesis is that the “background”
113 corresponds to long-distance variations (i.e. long range), while the “anomalies” correspond to short-
114 distance variations (short range) with respect to the working scale.
115

116 2 Presentation of the site and collected data

117
118 The data were collected within an urban district located in central Nantes (France). This
119 district is composed of former islands on the Loire River, backfilled during the 20th century to form a
120 single island in the middle of the river, measuring 4.9 km long by 1 km large and covering a land area
121 of 337 hectares. District population is approx. 18,000, representing on the order of 6% of total city
122 population. The geological context is mainly composed of a thick layer of anthropogenic deposits,
123 with a thickness varying between 2 and 5 m. These deposits are classified according to the intrinsic
124 contamination potential of the backfill material (Le Guern *et al.*, 2016 a, b): i) man-made grounds
125 with a high intrinsic contamination potential, ii) various man-made grounds with a medium intrinsic
126 contamination potential iii) natural sandy deposits (corresponding to sediments dredged from the
127 Loire River) showing a low intrinsic contamination potential. Below this layer, Loire River alluvia (up
128 to a thickness of 20 m) are lying on micaschists (Le Guern *et al.*, 2016a, 2016b).
129

130 The previous industrial activity on the site is related primarily to the port and shipbuilding
131 yards located in the western part of the island. This activity gradually declined until the closure of the
132 last yards around 1987. It was followed by a district revitalization plan (2000-2030). The volume of
133 excavated soils linked to renovations in the district's southwest sector has been estimated at roughly
134 100,000 tons per year from 2015 to 2025. In order to reuse the excavated soils, the land developers
135 need to refer to the local volumetric pedo-geochemical background, with respect to individual trace
136 element and persistent organic substance contents of the soils and subsoils. In the absence of a
137 information at this scale based on existing national sampling campaigns, the local office of the French
138 Geological Survey (BRGM) used readily available data from existing soil studies (Le Guern *et al.*,
139 2016a, 2016b, 2017a). The data are from 2,570 boreholes and 2,120 samples, mostly in relation with
140 soil contamination diagnostics. The boreholes are georeferenced in a database built using Microsoft
141 Access 2010 which also provides the descriptions of the various layers identified, the top and bottom
142 depths of the collected samples and the analytical sampling results. Figure 1 shows the distribution
143 of these data with an indication of the type of study. The geochemical data come from the pollution
144 diagnostic studies.
145

146 In a first approach, the data processing was simplified by considering a vertical succession of
147 2D-layers, corresponding to various types of anthropogenic deposits and alluvia, with different
148 properties. Most samples refer to one layer, within the first five meters of depth. This depth

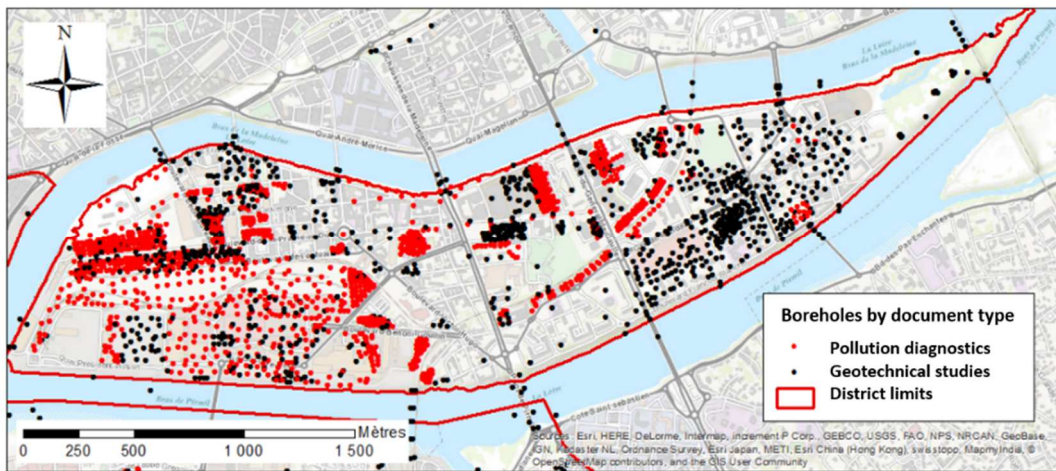
149 corresponds to the maximum depth for future buildings, and therefore of excavation or reuse of soil
 150 materials. The compositions of the samples serve to assign them to the different types of deposits. A
 151 sample crossing several types of materials (at the interface between two layers) is not taken into
 152 account in the analysis since the objective is to define a pedo-geochemical background per individual
 153 layer.

154 We first focus on the natural-like made-grounds composed of sandy Loire River dredged
 155 sediments, which are present within the entire district. 589 samples are associated with this type of
 156 made-ground, among which 581 show copper, lead and zinc contents analysed by ICP-MS following
 157 extraction with *aqua regia*. These three metals are indicative of anthropogenic impacts (Alloway,
 158 1990; Birke and Rauch, 1997, 2000) within this district. Because their contents present a high level of
 159 linear correlation (Table 1), only the results for lead will be presented in this paper.

161 Table 2 gives the statistical summary of the Pb contents. For reference, the statistical
 162 thresholds of the pedo-geochemical background obtained for lead on the processed data (all the 581
 163 samples) are given in Table 3. The MAD is lower than the other statistical thresholds, and just over
 164 the median (10 mg/kg_DM).

165 It is important to note that the length of the samples is highly variable, because they have
 166 been collected by different operators (see §3.2.1). This variation of the “support” has an influence on
 167 metal content variability (variance, variograms) and hence on the statistical and geostatistical
 168 processing. It was therefore necessary to take this data variability into account and a reduced dataset
 169 was considered where all samples have similar length (303 samples). We will refer to the whole
 170 dataset (581 samples) when using the complete dataset where all samples have different lengths.

171
 172



173
 174 Figure 1: Map of the borehole data locations, with an indication of the type of study

175 Table 1: Correlation matrix of the copper, lead and zinc analyses on the hydraulic sandy made-grounds sampled
 176 within the Ile de Nantes district. Results in bold are based on the 581 samples of the whole dataset (whole dataset),
 177 while those in italic are based on the 303 samples with similar sample lengths (reduced dataset).

CORRELATION MATRIX			
	Cu	Pb	Zn
Cu	1	<i>0.85</i>	<i>0.89</i>
Pb	0.86	1	<i>0.84</i>
Zn	0.88	0.83	1

178
 179 Table 2: Statistics of Pb contents on the hydraulic sandy made-grounds within the Ile de Nantes district. Whole

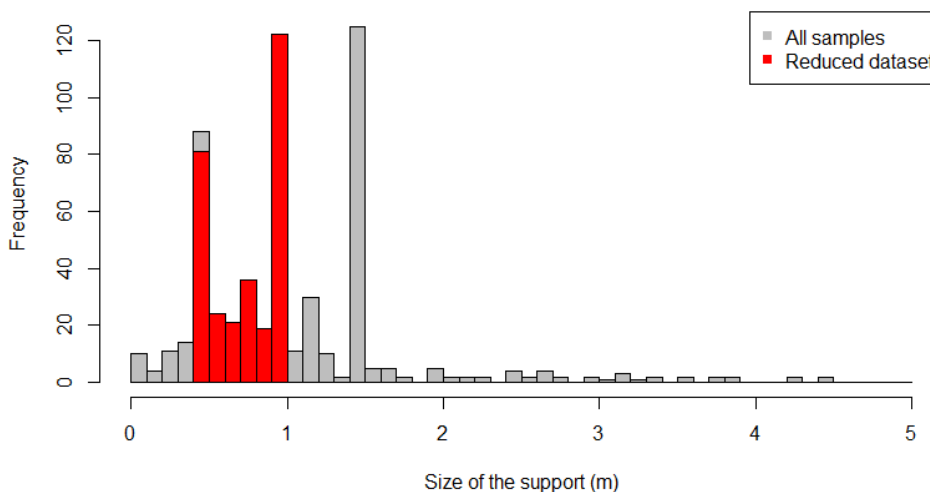
180 dataset (581 data) and reduced dataset (303 data). Units are mg/kg of dry matter.

Pb	Min	Max	Median	Mean	StDev	CV
Whole dataset (581)	3.0	240	10	20.4	27.6	1.35
Reduced dataset (303)	5.6	240	13	27.5	35.0	1.27

181
 182 **Table 3: Pedo-geochemical background threshold values of Pb contents calculated by different statistical methods on**
 183 **the hydraulic sandy made-grounds over the Ile de Nantes district. Units are mg/kg of dry matter.**

Pb	Upper whisker	MAD	Q90	Q95
Whole dataset (581)	28.4	15.4	32.5	40.3
Reduced dataset (303)	57.5	21.9	56.9	92.3

184
 185



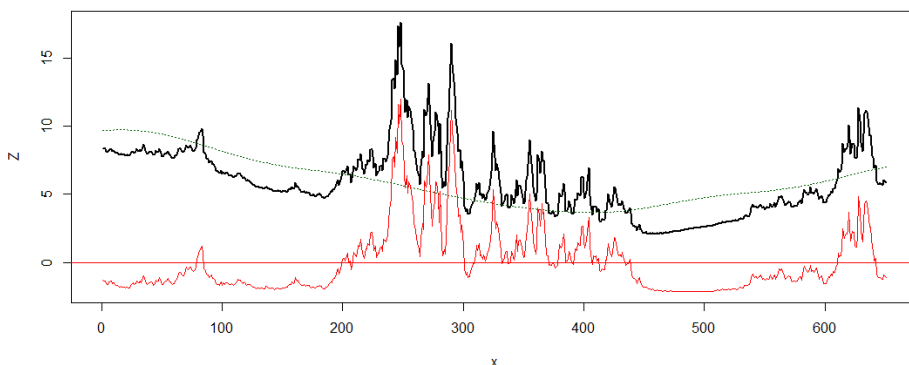
186
 187 **Figure 2: Thickness of the 581 samples (whode dataset). In red, the 303 samples of the reduced dataset.**

188 3 Methodology

189 3.1 Geostatistical filtering by factorial co-kriging

190
 191 The aim of the proposed methodology is to separate the anomalies from the background as
 192 illustrated schematically in Figure 3. Factorial co-kriging provides a geostatistical technique to filter
 193 the anomalies characterized by short-distance variations, from the geochemical background
 194 associated with long-distance variations.

195



196

197 **Figure 3: Decomposition of total content $Z(x)$ (bold black line) as the sum of short-distance $Y^1(x)$ (red thin line) and**
 198 **long-distance $Z^2(x)$ variations (green dots). Long-distance variations are interpreted as the geochemical background.**
 199 **The spatial mean of anomalies equals zero. The distance unit in abscissa is arbitrary.**

200
 201 Factorial co-kriging relies on an interpretation of the variogram model with several structures (in the
 202 monovariate case) and of the linear model of coregionalization (in the multivariate case). The
 203 monovariate case is first discussed, and the multivariate case is presented later. Hereafter, co-kriging
 204 will refer to the usual co-kriging of the total content, and filtering to factorial co-kriging of the long-
 205 range component.

207 3.1.1 Monovariate case

208
 209 The Pb content is modeled as a random function $Z(x)$ which is assumed to be stationary of
 210 order two (for the sake of simplicity): i.e. its expectation (probabilistic mean) m is constant and the
 211 spatial covariance between $Z(x)$ and $Z(x + \vec{h})$ only depends on \vec{h} (simply denoted h in the
 212 following). The variogram $\gamma(h)$ is assumed to be the sum of two structures γ^1 and γ^2 (where 1 and 2
 213 refer to indices in all the subsequent equations):

$$214 \quad (1) \quad \gamma(h) = \gamma^1(h) + \gamma^2(h)$$

215
 216 The random functions $Z(x)$ may be written as the sum of a constant expectation m , and a
 217 linear combination of two spatially uncorrelated components $Y^1(x)$ and $Y^2(x)$ with a zero
 218 expectation (yielding a zero cross variogram):

$$219 \quad (2) \quad Z(x) = Y^1(x) + Y^2(x) + m$$

220
 221 In this decomposition the variogram of Y^1 is γ^1 and that of Y^2 is γ^2 .

222
 223 When the ranges of the two components are significantly different, it is reasonable to
 224 regroup the expectation with the longest-range $Y^2(x)$ component (Rivoirard, 2003):

$$225 \quad (3) \quad Z(x) = Y^1(x) + Z^2(x)$$

226
 227 where $Z^2(x) = Y^2(x) + m$.

228
 229 Each component may be estimated by co-kriging from the Z data (Wackernagel and
 230 Sanguinetti, 1993). In classical terms, the co-kriging matrix involves the variogram γ between Z data,
 231 whereas the right-hand side of the system considers the cross variogram between Z data and the
 232 variable to be estimated, i.e. $\gamma^1(h)$ for the "anomalies" Y^1 and $\gamma^2(h)$ for the "long-range"
 233 component Z^2 associated with the pedo-geochemical background.

234
 235 To estimate the long-range component Z^2 (with the same expectation as Z), the non-bias
 236 condition imposes that the sum of the factorial co-kriging weights equals 1. Conversely, the
 237 expectation of $Y^1(x)$ being zero, then the non-bias condition for estimating anomalies imposes that
 238 the factorial co-kriging weights add up to zero.

239
 240 These results can be generalized to the intrinsic case; for example when the variogram of the
 241 "background" presents a linear structure (i.e. unbounded variogram). In this case, the non-bias
 242 conditions become authorization conditions (Chilès and Delfiner, 1999).

243
 244
 245

246 **3.1.2 Multivariate case**

247

248 The following discussion relies on the properties of the linear model of coregionalization
 249 (Bourennane *et al.*, 2003; Goovaerts, 1992; Rivoirard, 2003; Saby *et al.*, 2009; Wackernagel and
 250 Sanguinetti, 1993). As for the monovariate case, the presentation is made in the case of stationarity
 251 of order two.

252 According to this model, the simple and cross variograms of all variables are linear
 253 combinations of the same basic structures (Chilès and Delfiner, 1999). For the pair of variables
 254 denoted i and j , all simple and cross variograms are written as follows:

255

256 (4)
$$\gamma_{ij}(h) = \sum_k b_{ij}^k \gamma^k(h)$$

257

258 where γ^k stands for the normalized variogram with rank k (sill equal to 1).

259

260 The set of simple and cross-variograms can be written in a synthetic way using a matrix form, i.e.:

261

262 (5)
$$[\gamma_{ij}(h)] = \sum_k [b_{ij}^k] \gamma^k(h)$$

263

264 where the sill matrices $[b_{ij}^k]$ must be symmetrical and of a positive type. Therefore, a structure is
 265 present in a cross-variogram only if it is present in the two related simple variograms. Conversely, a
 266 structure can be present on simple variograms without necessarily appearing in the cross-
 267 variograms.

268

269 In this model, the variables themselves are decomposed into linear combinations of spatial
 270 independent components corresponding to the full range of variability scales:

271

272 (6)
$$Z_i(x) = m_i + \sum_k Y_i^k(x)$$

273

274 where the expectations of the spatial components Y_i^k are null.

275

276 Like in the monovariate case, the "mean" m_i is regrouped with the long-range component of
 277 each variable. Thus we wish to estimate the values linked to the longest-range component(s), in
 278 order to filter out short-range variability.

279

280 **3.1.3 Use of "explanatory" covariates**

281

282 To specify the choice of the component(s) to be assigned to the "background" or to
 283 "anomalies", some attention should be drawn to the correlation matrix deduced from the variance-
 284 covariance matrices that can be calculated either globally or by structure using the relevant formula:

285

286 (7)
$$r_{ij} = \frac{Cov(Z_i, Z_j)}{\sqrt{Var(Z_i)} \sqrt{Var(Z_j)}} \text{ and } r_{ij}^k = \frac{b_{ij}^k}{\sqrt{b_{ii}^k} \sqrt{b_{jj}^k}}$$

287

288 where r_{ij} is the linear correlation coefficient between variables i and j , and r_{ij}^k the regionalized
 289 coefficient associated with component k , with $Cov(Z_i, Z_j)$ representing the covariance between
 290 variables i and j , and $Var(Z_i)$ and $Var(Z_j)$ their respective variances.

291

292 The correlation matrix per spatial structure reflects the various links between variables, with
 293 respect to the spatial variability scale. This result is of special interest herein because it enables

294 drawing the link between the targeted contents and the covariates. This in turn can be used to select
 295 the component(s) retained to estimate the pedo-geochemical background: for example, correlated
 296 components present for different metal associated with the same anthropic contamination (eg. Pb,
 297 Zn, Cu).

298
 299 According to the formula (6), by solely selecting the longest-range component Z_1^2 for the
 300 content Z_1 background estimation, we can express:

$$(8) \quad Z_{1,BG}(x) = Y_1^2(x) + m$$

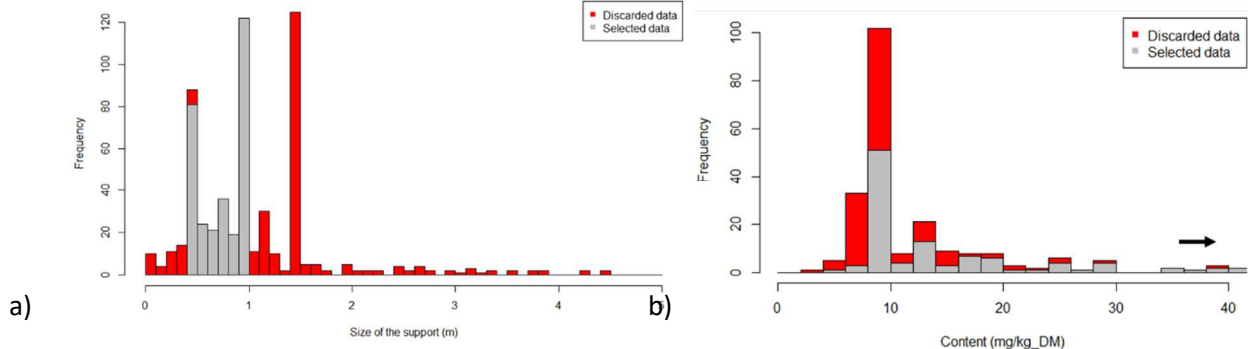
303
 304 This component is estimated by factorial co-kriging based on the Z_1 data (eg. Pb) with one
 305 covariate Z_2 (eg. Cu or Zn) or several covariates $Z_{i>1}$ (eg. Zn and Cu) potentially known more densely
 306 (eg. land use) and whose "long-range" component is adequately correlated with that of the
 307 Z_1 contents.
 308

309 3.2 Taking into account sample lengths

310
 311 As mentioned in section 2, the data used here correspond mainly to pollution diagnostic studies.
 312 They were collected by different operators and were not originally acquired for the determination of
 313 an anthropized pedo-geochemical background. Therefore, the lengths of the samples do not
 314 correspond to the heights of the soil formations. We therefore do not have sufficient information to
 315 use an accumulation model. As a consequence, in order to take into account the variable lengths of
 316 the samples, two approaches are compared. The first one is a selection of the data with a length
 317 close to the mode of the length histogram. The second approach consists in introducing explicitly the
 318 sample support in the co-kriging (and filtering) calculations, using data discretization (Lark & Scheib,
 319 2013; de Fouquet, 2019).
 320

321 3.2.1 Selection of data based on length

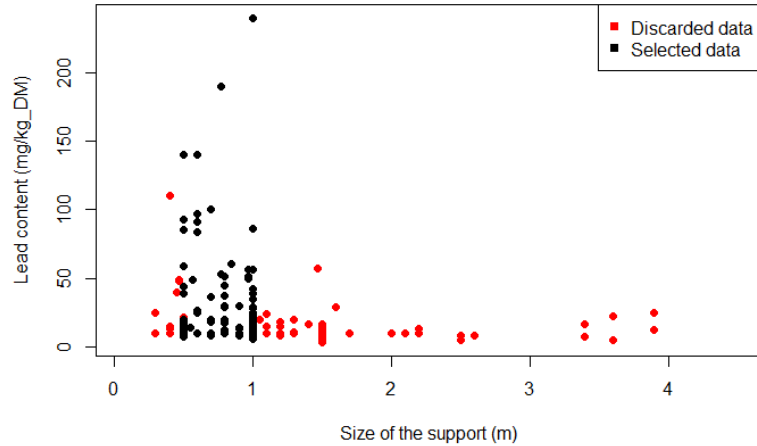
322
 323 In this approach, only the samples with an almost similar length are retained. The sample lengths
 324 of the whole dataset lie between 0.1 and 4.5m with three modes on the histogram: 0.5m, 1m and
 325 1.5m (Figure 4). To keep most of the samples while preserving the spatial distribution of the data and
 326 a relatively constant sample length, we consider samples with support between 0.5m and 1m
 327 inclusive. This selection reduces the number of samples from 581 (whole dataset) to 303 (reduced
 328 dataset). This selection discards a large proportion of low contents and influences the general
 329 statistics of the Pb contents as can be seen in Table 2: the median, the mean and the standard
 330 deviation increase, whereas the coefficient of variation slightly decreases. However, the correlation
 331 coefficients of Pb with Cu or Zn remain similar.



332
 333 **Figure 4: Histogram of sample length (a) and of Pb contents (b) for the complete (581 data) and the reduced (303**
 334 **data in grey) datasets.**

335
336
337
338
339
340
341

The statistical thresholds of the pedo-geochemical background for Pb, calculated on the selected 303 samples, are much higher than for the initial sample set (Table 3), especially for the Upper whisker and the Q95 (57.5 vs 28.4 mg/kg_DM, 92.3 vs 40.3 mg/kg_DM respectively). This shows the important sensitivity of those criteria to the sample population. This variation reflects the fact that discarded data mainly correspond to lower Pb values as shown in Figure 4 and 5.



342
343
344

Figure 5: Scatter plot between sample length and Pb contents for the complete (581 data) and the reduced dataset according to length (303 data in black).

345

3.2.2 Co-kriging with a multi-support dataset

346

347
348 The aim is to enable the use of all 581 samples for the estimation by co-kriging and filtering
349 despite their different support. However, the variographic analysis is performed with data having
350 roughly the same support, i.e., the reduced dataset with sample lengths between 0.50 m and 1 m.
351 For the calculations explained hereafter, this length L is supposed to be equal to 0.75 m. As only one
352 sample per borehole generally belongs to the target layer, only the horizontal sample variogram is
353 calculated, but this sample variogram will be assumed to be isotropic for 3D calculations. To take into
354 account the various sample lengths in the estimation step, the samples are discretized into segments
355 of smaller length d (here $d=0.1$ m). The d support variogram is deduced from the L support model of
356 variogram. The d support variogram is supposed to be horizontally isotropic. The nugget effect is
357 increased by the factor L/d . The vertical ranges are reduced by the distance d ; the horizontal ranges
358 are not modified, as cores are vertical. This modeling approach involves a slight approximation
359 because it does not take perfectly account for the modification of the variogram shape at the origin.

360 The modeled d -support variogram is then used for the estimation. The sample length is taken
361 into account in the matrix and in the right-hand side of the co-kriging system thanks to the length
362 sample discretization into d -length segments.

363

3.3 Variographic analysis of the Île de Nantes data

364

365
366 The simple and cross horizontal variograms for Cu, Pb and Zn, are calculated for the district
367 (15 calculation steps span 90m each, Figure 6). The fitted model comprises a nugget effect and two
368 spherical structures with ranges of 200m and 1000m.

369

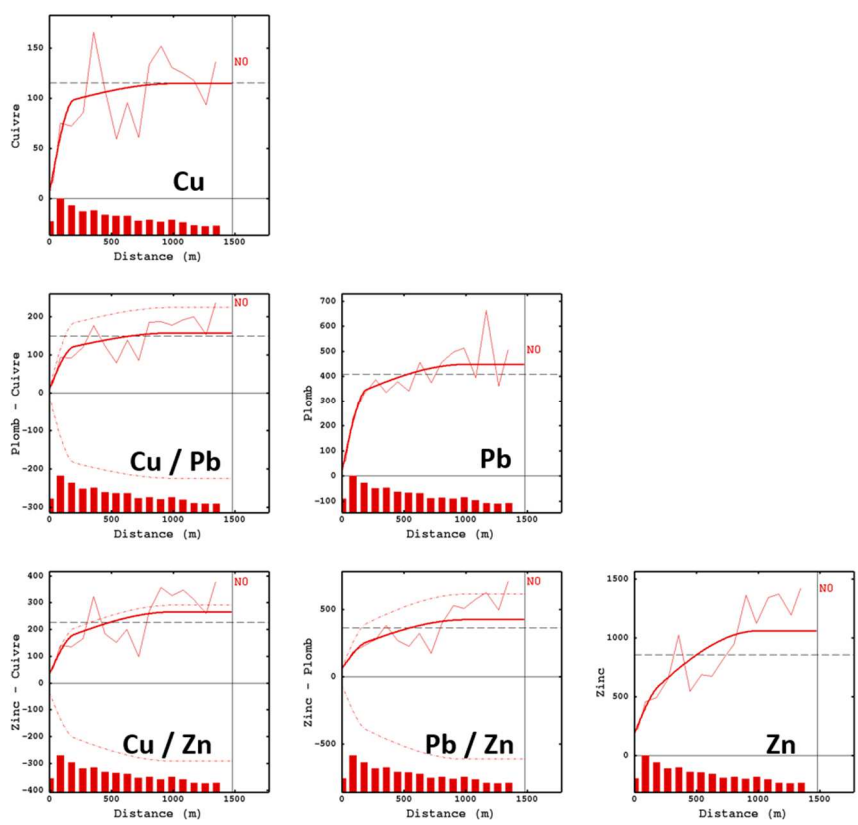
370 To determine long-range structures associated with the “background”, the regionalized
371 correlation coefficients are examined (Table 4). The nugget component presents a strong correlation
372 among the three metals. As stated before, the point-source contaminations are expected to be

373 similar for Cu, Pb and Zn. This nugget component reflects short-distance variations (vs horizontal
 374 distance between samples of about 90m) or other causes of heterogeneity.

375 The intermediate spherical component (200m range) shows correlation coefficients smaller
 376 than those of other components and those of the metals. Then the variations taken into account by
 377 this component differ between the three metals. We have chosen to filter this component out so as
 378 to only retain the highly-correlated variations for the pedo-geochemical background.

379 Lastly, the 1000m range spherical component exhibits a correlation between Cu, Pb and Zn
 380 larger than for the 200m range spherical component. The lower correlation between Pb and Zn, is
 381 mainly explained by the presence of a few samples with large Zn values and lower Pb contents. The
 382 long-range correlation among the three metals remains strong overall (Pb-Cu 0.89, Pb-Zn 0.77, Cu-Zn
 383 0.98), compared to the coefficient correlations between total contents (Pb-Cu 0.85, Pb-Zn 0.89, Cu-
 384 Zn 0.89) (Table 1).

385



386
 387 **Figure 6: Simple and cross sample variograms of the Cu, Pb and Zn contents based on the reduced dataset (303**
 388 **samples). The fitted model is shown as a solid red line. The histogram of the pairs is indicated. The grey dashed horizontal**
 389 **line indicates the variance in simple variograms and the covariance in cross variograms. The maximum correlation**
 390 **envelope (spatial correlation coefficient respectively equal to +1 or -1 for all structures) is indicated with a dashed red**
 391 **line.**

392
 393 **Table 4: Regionalized correlation coefficients of Cu, Pb and Zn from the linear coregionalization model based on the**
 394 **reduced data set (303 samples)**

	NUGGET EFFECT			SPHERICAL: 200M			SPHERICAL: 1000M				
	Cu	Pb	Zn	Cu	Pb	Zn	Cu	Pb	Zn		
Cu	1.00			Cu	1.00		Cu	1.00			
Pb	1.00	1.00		Pb	0.61	1.00	Pb	0.89	1.00		
Zn	1.00	1.00	1.00	Zn	0.83	0.51	1.00	Zn	0.98	0.77	1.00

395 **3.4 Tools and estimation domain**

396 All calculations were carried out using the Isatis© geostatistical software and RGeostats. To
 397 perform the estimation, a modified version of the RGeostats co-kriging function was developed by
 398 MINES Paris Tech.

399 The estimations are performed at block support, on a grid covering the whole study area. The
 400 grid mesh is 10m by 10m by 0.75m. The estimations carried out with the reduced dataset (303 data,
 401 length between 0.5 to 1m) rely on a 2D approach: all the sample centers are assigned to the same
 402 horizontal depth at the center of the unique vertical mesh. The estimations carried out with the
 403 whole dataset (581 data) are based on a 3D approach, considering the exact vertical locations of the
 404 (discretized) samples.

405 **4 Results and discussion**

406 Table 5 presents the statistics of the block estimations of the total Pb and of the long-range
 407 components, for the whole and reduced datasets. It will help to discuss the estimation of the total Pb
 408 contents (co-kriging) and the Pb "background" component (filtering), based on the multivariate
 409 approach (using contents of Pb, Cu and Zn). The negative values are related to the negative weights
 410 of the kriging system. Post-processing would be necessary for these values. As this point is not
 411 specific to the methods of estimation used, it will not be discussed here. A possible correction would
 412 be to substitute these values by 0 or the limit of quantification (LQ) of the estimated parameter.

413
 414 **Tableau 5 : Statistics of Pb total content (co-kriging) and long-range components (filtering) according to dataset**

	Estimated total content		Estimated long range component	
	<i>whole dataset</i>	<i>reduced dataset</i>	<i>whole dataset</i>	<i>reduced dataset</i>
Min	10.66	-5.26	-5.61	7.18
Max	124.84	173.02	58.27	70.03
Median	12.34	18.62	5.56	7.89
Mean	11.93	18.39	4.91	7.18
Standard deviation	12.33	17.37	6.58	5.25

415

416 **4.1 Comparison of Pb background with total content estimations based on the**
 417 **reduced dataset**

418

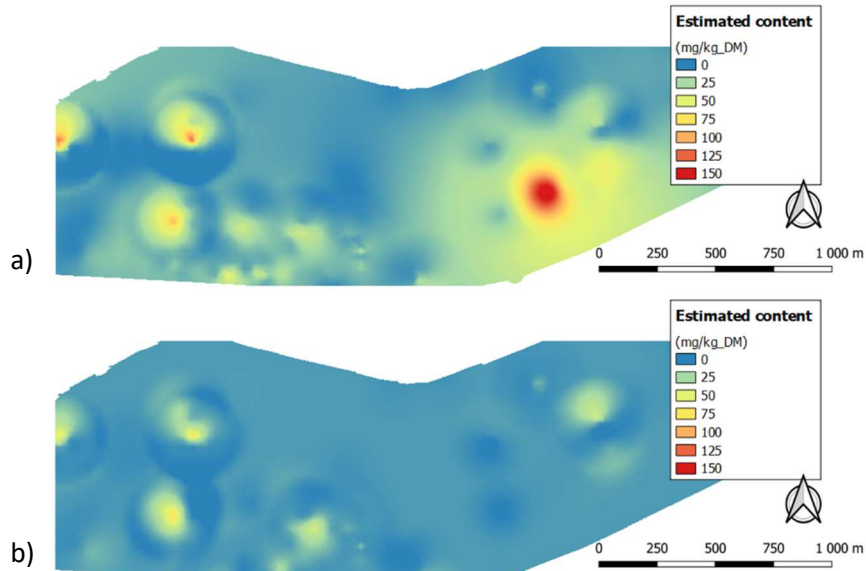
419 The maps of total Pb contents estimated by co-kriging and of the estimated Pb background
 420 values estimated by filtering using the reduced dataset (303 data), are presented in Figure 7. The
 421 estimated Pb contents (Figure 7) show highly contrasted areas (red and light blue spots). These spots
 422 indicate point-source contamination within the zone, as well as sites with abnormally low Pb
 423 contents compared to global statistics over the whole district. This is consistent with the extensive
 424 industrial past within the district's western sector and the presence of gasoline stations in the
 425 central-eastern part, as described in Le Guern *et al.* (2016a, 2017b). These spots with high or low
 426 contents are much smoother in the background estimation, which exhibits more homogeneity. The
 427 most homogeneous zones correspond to historical housings or former meadows now transformed
 428 into housings.

429

430 The higher-content areas seen in the estimated background in the western portion of the
 431 district can be explained by the presence of an industrial zone that has caused Pb contamination (Le

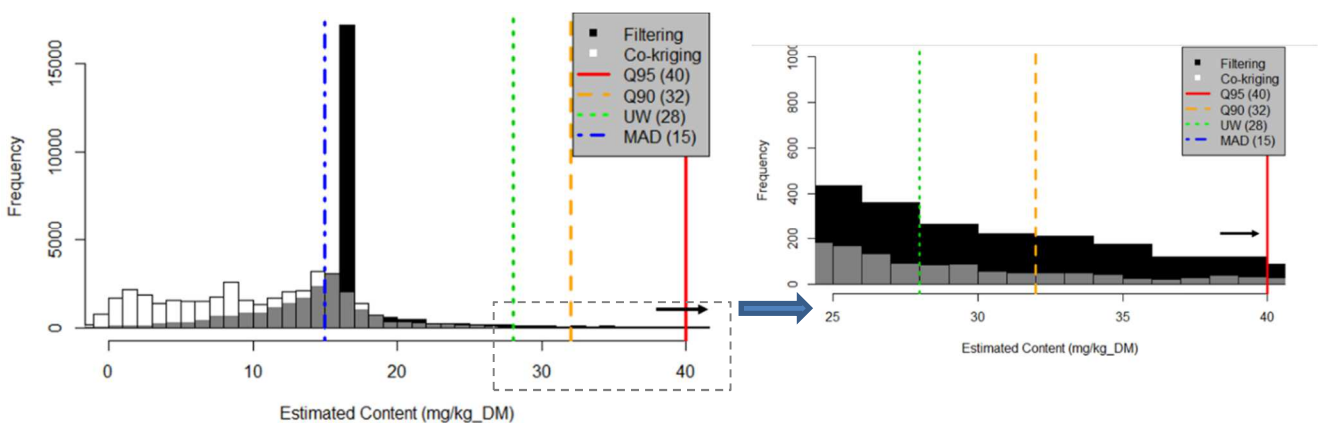
432 Guern *et al.*, (2016a, 2017b). This contamination, which affects a broad zone, is interpreted as diffuse
 433 contamination at the scale of the district.
 434

435 The background estimation is less dispersed than the total Pb estimation (Figure 8). More
 436 specifically, since the estimated pedo-geochemical background only includes long range variations,
 437 the local contrasts are reduced out. The maximum estimated total content level is greater than that
 438 of the estimated background, which is consistent with the filtering of positive anthropic anomalies.
 439



440
 441 **Figure 7: Block estimation of Pb contents by co-kriging (a) and pedo-geochemical background by filtering (b) based**
 442 **on the reduced dataset (303 data).**

443
 444 In Figure 8, the reported standard statistical thresholds (Q90, Q95, upper whisker and MAD
 445 threshold) are those calculated based on the whole dataset (581 data) in order to facilitate the
 446 further comparison with Figure 10 (cf. section 4.3). The MAD threshold (15 mg/kg_DM) is slightly
 447 lower than the mode of the background estimation (15 mg/kg_DM), whereas the upper whisker and
 448 the 90th quantile correspond to the high background estimated values. The 95th quantile is slightly
 449 lower than the maximum of the estimated long-range component.
 450



451
 452 **Figure 8: Histograms of estimated total Pb contents (grey and white) and estimated background (grey and black)**
 453 **based on the reduced dataset (303 data). The black arrow indicates graphic truncation (largest content around 140 is not**
 454 **shown). Standard statistical thresholds values calculated on the whole dataset (581 data) are reported. MAD: median**
 455 **absolute deviation, UW: upper whisker, Q90: 90th percentile, Q95: 95th percentile. Units are mg/kg_DM.**

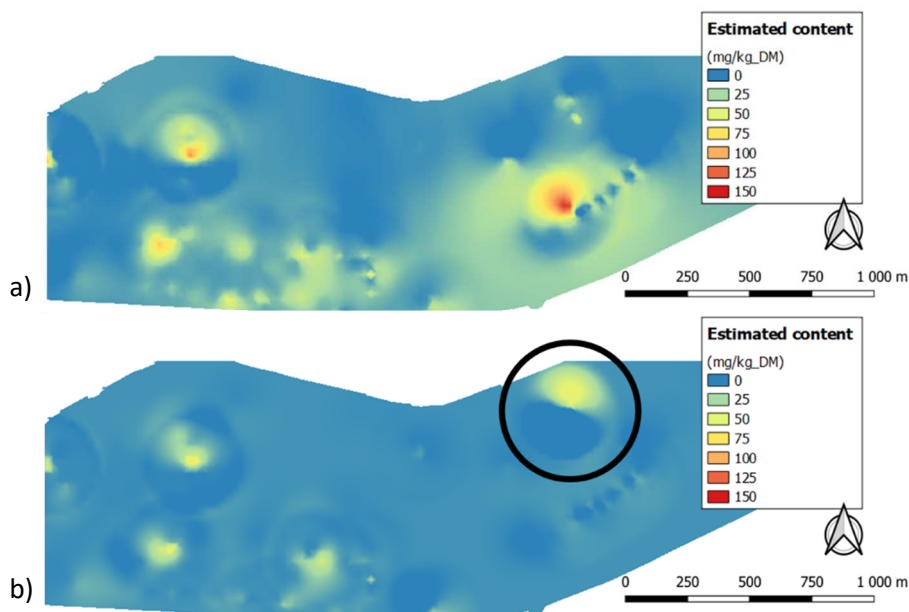
456

457 **4.2 Comparison of Pb background with total contents estimations based on the**
458 **whole dataset**

459
460 The maps of the total Pb contents and of the Pb background estimated using the whole dataset
461 (581 data) are presented in Figure 9. As in the case of the reduced dataset (Figure 7), the map of
462 estimated total Pb contents shows highly contrasted values (red and light blue spots). Local
463 contaminations are indicated by orange and red spots. Again the estimated background is more
464 homogeneous than the estimated total contents.

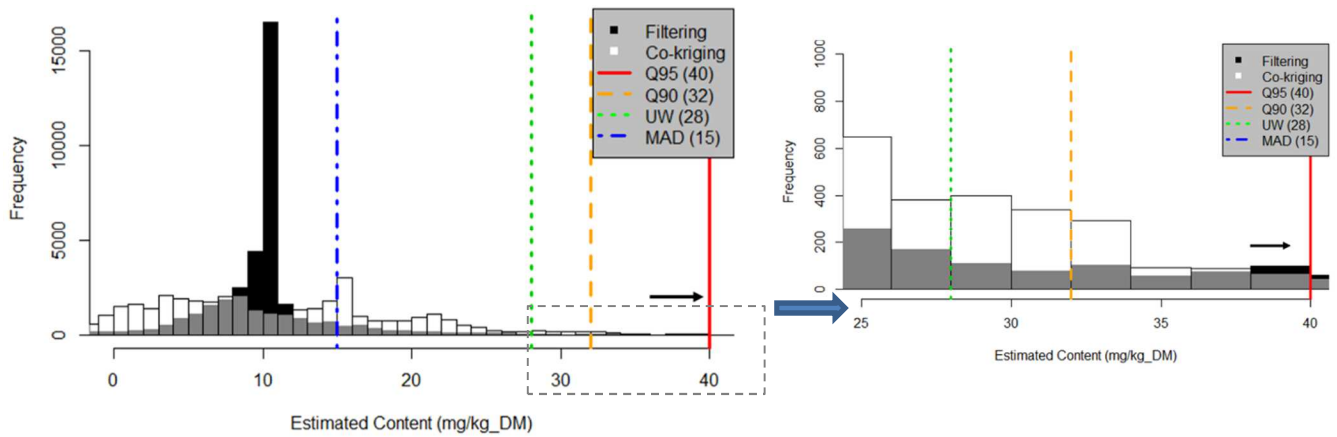
465
466 However, some “polarized” background estimations (rapid changes from low to high values)
467 appear in the area marked with the black circle in Figure 9. This is explained by the presence of a
468 sample with large Pb content close to one with a lower content. This was not apparent when the
469 reduced dataset was used because the sample with the largest value was discarded.

470
471 The histogram (Figure 10) confirms the lower dispersion of the estimated background compared
472 to the estimated total contents. The total estimated contents show secondary modes around 15 and
473 22 mg/kg_DM. The mode of the estimated background values lies around 11 mg/kg_DM. The MAD
474 threshold (15 mg/kg_DM) is higher than the main mode of the background component, and lower
475 than the secondary modes of the estimated total Pb. The upper whisker and the 90th percentile are
476 higher than the estimated background and the secondary modes of the estimated total Pb.



477
478 **Figure 9: Estimated total Pb contents (a) and background (b) based on the whole dataset (581 data). The black circle**
479 **shows the local highly “polarized” estimations explained by the presence of a sample with high Pb contents (discarded in**
480 **the reduced dataset).**

481

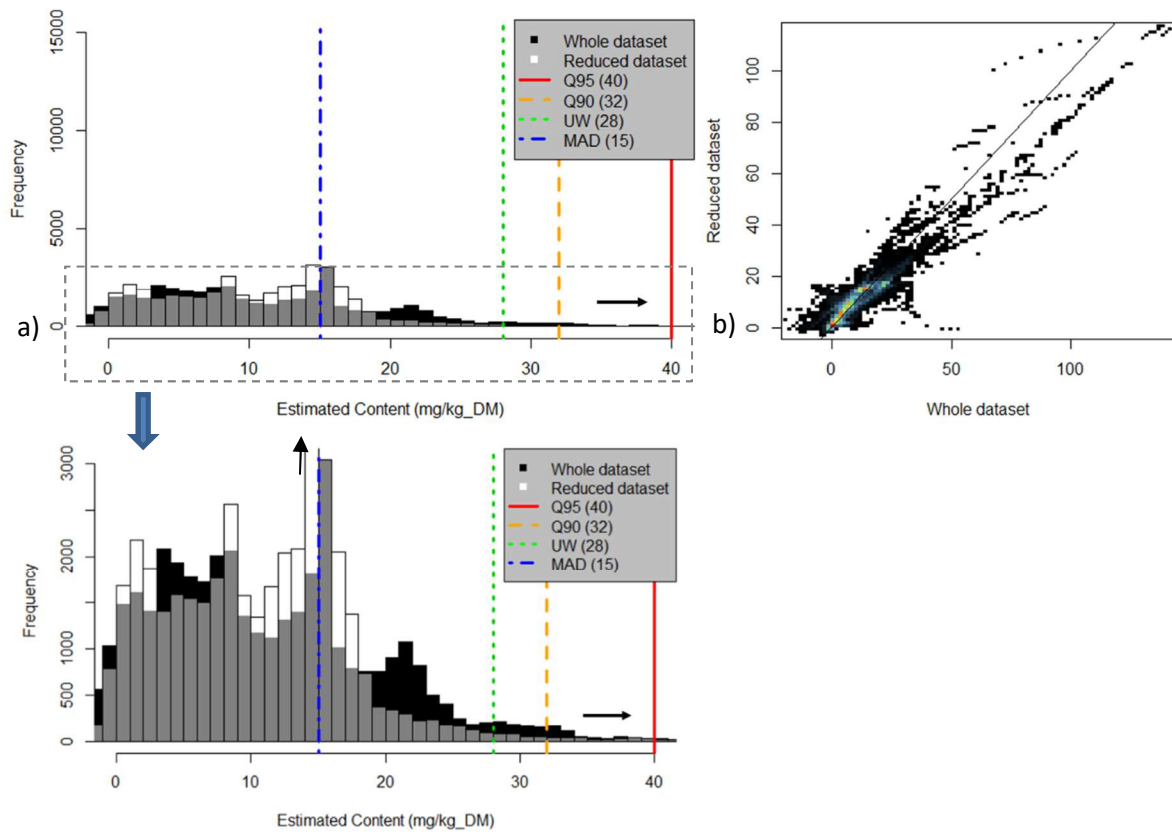


482
 483 **Figure 10: Histograms of estimated total Pb (grey and white) and background (grey and black) based on the multi-**
 484 **support dataset (581 data). The black arrow indicates graphic truncation (i.e. higher content not shown). Standard**
 485 **statistical thresholds values calculated on the whole dataset (581 data) are reported. MAD: median absolute deviation,**
 486 **UW: upper whisker, Q90: 90th percentile, Q95: 95th percentile. Units are mg/kg_DM.**

487 **4.3 Influence of the whole versus reduced datasets**

488
 489 Keeping only the data corresponding to similar sample lengths (reduced dataset) discards a
 490 significant portion of the data, which implies a significant loss of information (from 581 to 303 data).
 491 While the co-kriging maps based on the whole dataset (Figure 9) are relatively similar to those
 492 obtained with the reduced dataset (Figure 7), local differences appear nevertheless between the
 493 estimations, particularly at locations of point-source contamination. The histograms and correlation
 494 diagrams (Figure 11) confirm these differences. The histogram of the total Pb content estimations
 495 calculated with the whole dataset shows a higher proportion of extreme values, whereas the
 496 proportion of medium values is larger with the reduced dataset.

497 These differences can be explained by two phenomena. The first one is the influence of the
 498 discarded data in the reduced dataset. The second phenomenon is the influence of the vertical
 499 discretization of the sample support. When considering the whole dataset, each sample has its
 500 vertical variable extension and its gravity center is set at its “exact” vertical location (3D approach). In
 501 the 2D approach on the other hand, all samples are considered with the same lengths and at a
 502 common depth. The 3D approach distributes the data more faithfully along the vertical axis.
 503

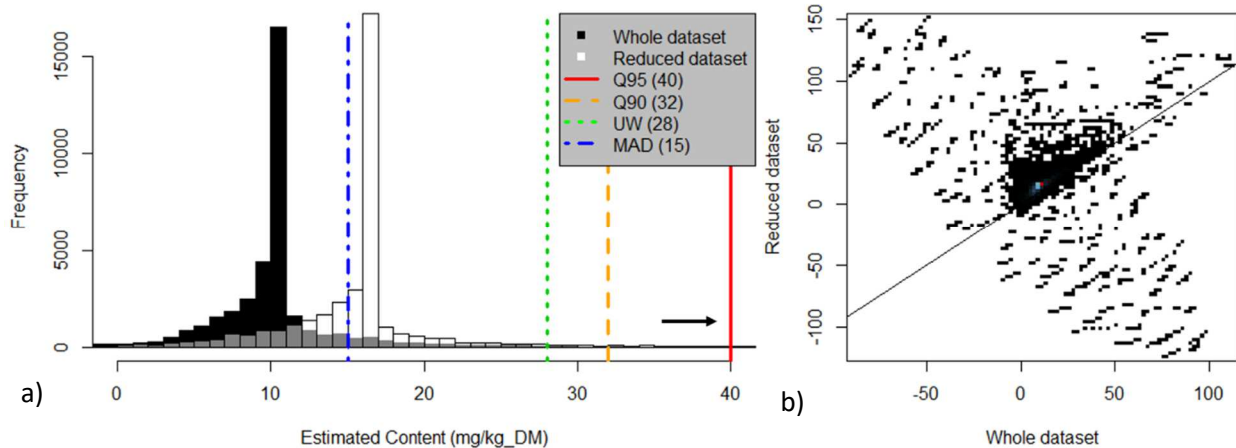


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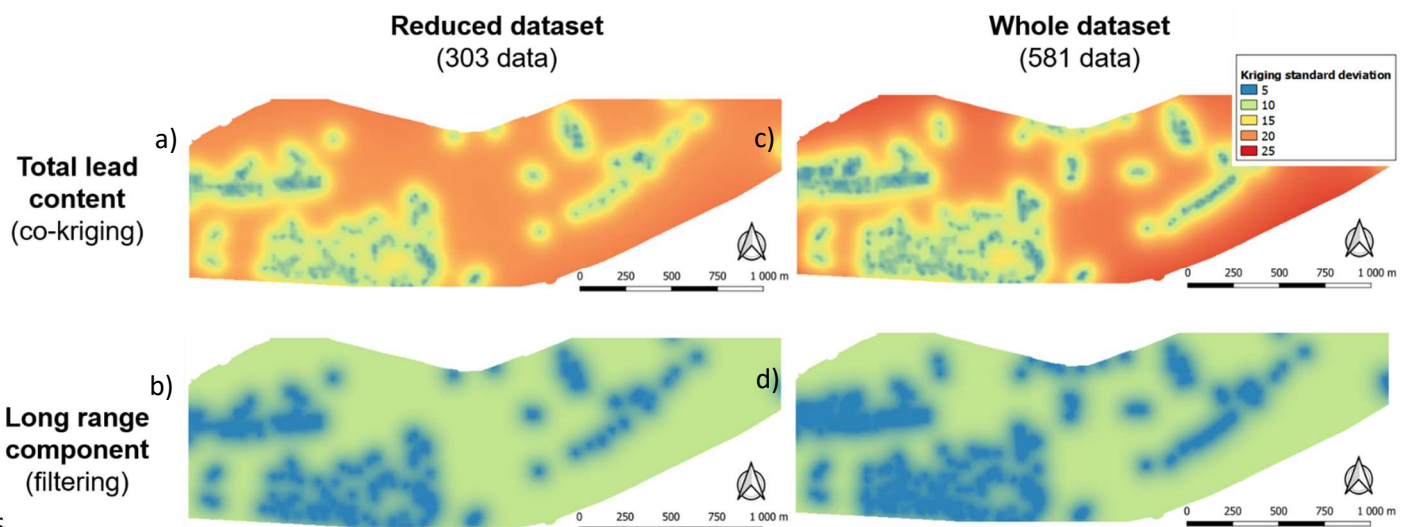
Figure 11: a) Histogram of the total Pb contents estimations with the reduced dataset (white and grey) and the whole dataset (black and grey). Bottom figure is a zoom. The black arrows indicate that higher values are not shown. Standard statistical thresholds values calculated with the whole dataset (581 data) are reported. UW: upper whisker, Q90: 90th percentile, Q95: 95th percentile. Units are mg/kg_DM. b) Correlation diagram between estimations obtained with whole dataset (abscissa) and reduced dataset (ordinate).

511 The differences are more significant on the background estimations (Figure 12). Some large
512 background estimations generated using the reduced dataset become low (and even negative) when
513 estimated from the whole dataset (Figure 11). As mentioned previously, the additional samples of
514 the whole dataset led to local strongly “polarized” estimations with high and low values (black circle
515 on Figure 9). On the correlation cloud (Figure 12b), the high estimates with the whole dataset are
516 thus associated to low estimates with the reduced dataset, which generates a local negative
517 correlation. In addition, the histogram (Figure 12a) clearly reflects the influence of discarding the low
518 values in the reduced dataset (Figure 4). Indeed, the mode is clearly lower for the whole dataset
519 (581 data), than for the reduced one (303 data). This is consistent with the observations from the
520 general statistics in Table 2. It emphasizes the influence of the data pre-processing (selection and
521 discretization).



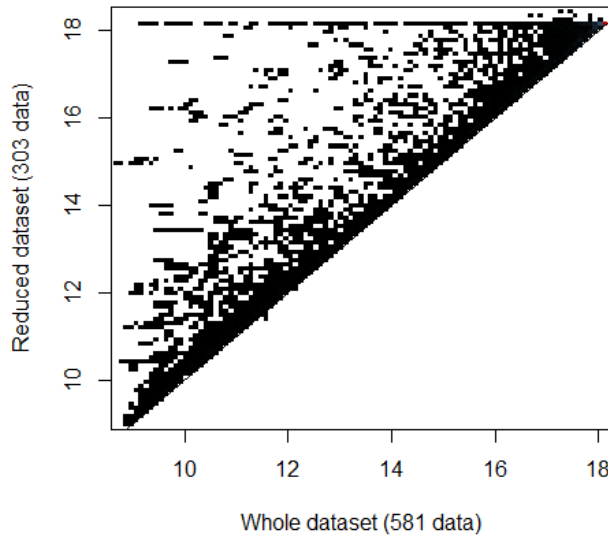
522
 523
 524 **Figure 12: a) Histogram of the Pb background estimated by filtering based on the reduced dataset (white and grey) or**
 525 **on the whole dataset (black and grey). The black arrow indicates data truncation (i.e. highest values not shown).**
 526 **Standard statistical thresholds values calculated on the whole dataset (581 data) are reported on the histogram. UW:**
 527 **upper whisker, Q90: 90th percentile, Q95: 95th percentile. Units are mg/kg_DM. b) Scatter diagram between the**
 528 **estimation with the whole dataset in abscissa and the reduced dataset in ordinate.**

529
 530 Finally, the standard deviations of estimation error maps (Figure 13) are different for both
 531 estimations (co-kriging vs. filtering) and depend on the dataset used. The blue spots (low standard
 532 deviation) are more frequent in the background map based on the whole data set than in the case of
 533 the reduced dataset. Figure 14 clearly shows that adding data decreases the standard deviation of
 534 the estimation errors. The opposite effect may sometimes occur, due to the consideration of the
 535 exact sample location in 3D.



536
 537 **Figure 13: Standard deviation of the estimation error maps for Pb total contents by co-kriging (a & c) and background**
 538 **by filtering (b & d) based on the reduced dataset (a & b) and on the whole dataset (c & d).**

539



540 **Figure 14: Correlation diagram of standard deviation of the background estimation according to the dataset (reduced**
 541 **dataset versus whole dataset).**
 542

543

544 **4.4 Discussion**

545

546 Since the data originate from pollution diagnostic studies, the whole dataset introduces
 547 biases related to the specific initial objectives of the data. This approach does not fulfill the
 548 recommendations issued by the group of geochemical experts (Demetriades and Birke, 2015) who
 549 advise a systematic strategy for mapping the urban pedo-geochemical (URGE) background. Another
 550 difference is due to the investigation depth. The sampling used to determine the pedo-geochemical
 551 background (whether urban or not) typically focuses on topsoils (Albanese, 2007; Demetriades and
 552 Birke, 2015; Karim *et al.*, 2015; Lark and Scheib, 2013; Reimann and al., 2012; Saby *et al.*, 2006). But,
 553 given the reuse guidelines for excavated soils (Coussy *et al.*, 2020), the subsoil must be taken into
 554 account and therefore, all available subsoil samples have been used with depths up to 5m. Then
 555 Geostatistical filtering appears as a relevant solution when the sole use of samples dedicated to the
 556 determination of the pedo-geochemical background is not possible.

557

558 Based on the variability scale, the filtered anomalies present not only high values
 559 (contamination) but also low values (areas with abnormally low metal contents), as opposed to
 560 statistical thresholds, which are only intended to highlight the highest "outliers". Therefore, in the
 561 presence of estimated negative anomalies, the background estimation produces values locally
 562 greater than those of the total content estimation. This may correspond to deposits of materials with
 563 lower contents than those of the surrounding materials in place.

564

565 It should also be noted that the estimated contents are influenced by data means, which
 566 themselves reflect the influence of large values. This effect could lead to a bias in the estimations
 567 (total and background contents) especially when the data come from surveys aimed at polluted site
 568 characterization. In such cases, the sampling may be biased, with a lack of low contents.

569

570 Moreover, the variable sample length may cause practical problems since the content variability
 571 depends on the support. Selecting samples with similar support facilitates the variogram modeling if
 572 the data are numerous enough, but should be avoided for the estimation, because it reduces the
 573 number of data. There is no theoretical difficulty to introduce the support explicitly in the co-kriging
 574 or filtering equations, which allows the utilization of all available data. This represents a significant
 575 gain in precision, and the estimations become more faithful to reality.

575

576 Also, taking into account the vertical extension and location of the samples is a more accurate
577 reflection of the data. This leads to a reduction of the estimation error's standard deviation , in
578 particular for the background component (Figure 14). However, taking into account the support
579 implies working on variographic models (adaptation of the range and the nugget effect) and requires
580 conceptual choices (size of the reference support, size of the discretization step) based on
581 geostatistical expertise. In addition, the integration of new data can have consequences on the
582 estimations; either globally (lower estimated values of the background component, Figure 12) or
583 more locally (zone of contrasted estimates, Figure 9). The integrated data require an in-depth study
584 to validate their use. In all cases, a preliminary exploratory data study constitutes a key
585 methodological step.

586
587 The choice was made herein to assume that anomalies could be either positive or negative,
588 which is relevant in a context of excavated soil reuse: the total content may be lower than the local
589 background value. This model is therefore different from a description of the contents as the sum of
590 positive quantities. It corresponds to a background content to which the natural or anthropic
591 "anomalies" are rather superimposed. This latter description makes it necessary to add information,
592 such as the absence or presence of local anomalies, or the local ratio between the mean of each
593 spatial component (background and anomalies).

594 **5 Conclusions**

595
596 It is possible to separate out background from "anomalies" based on the estimation of the long-
597 range component by filtering, relying on an interpretation of the linear model of coregionalization.
598 For this, the use of correlated covariates makes the estimation more representative of the long-
599 distance variations of the variable of interest. This methodology may be applied at various scales, but
600 this has an influence on the type of anomalies being filtered. A phenomenon seen as an anomaly at a
601 large scale might be considered as the background at a smaller scale.

602
603 Geostatistical filtering can also be applied to the data themselves, in order to detect high or low
604 "outliers". Nevertheless, geostatistical estimations require a large amount of data, which is generally
605 incompatible with the sampling budgets dedicated to the estimation of pedo-geochemical
606 backgrounds in urban areas. To remedy this problem of data paucity, the use of pre-existing data is
607 required, even though it may have been collected with different objectives than that of defining a
608 pedo-geochemical background. Different sampling protocols rely on different supports and therefore
609 influence the variability, complicating the variographic study. Taking into account the size of the
610 support in the estimation represents a viable alternative in order to avoid a loss of information such
611 as is the case if only considering data with similar support.

612 Several parameters, such as the spatial distribution of the samples or inter-variable correlations,
613 must be taken into account and need a preliminary exploratory data analysis. These parameters help
614 building the variogram model and identifying the additional data ultimately needed.

615
616 In conclusion, filtering is a common practice in fields requiring a separation between point and
617 diffuse phenomena. It appears especially useful for creating reference values or studying the general
618 properties of soils and subsoils, assuming that the linear model of coregionalization is relevant. It
619 provides the opportunity to mine existing data, collected in different contexts, thus reducing the
620 burden associated with additional sampling campaigns and associated costs.

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629

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