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Anticipating geochemical compatibility to reuse excavated soils at urban scale: Are usual statistical tools effective?

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ABSTRACT

Reusing low to moderately excavated soils within land redevelopment projects necessitates among others to verify the geochemical compatibility of these soils with the receiving site. Optimizing excavated soil reuse at redevelopment project or urban scale is compelled by comparing their concentrations with threshold values based on quarter or urban geochemical background. Because urban soil geochemistry varies both at horizontal and vertical scale, background might vary spatially. It is thus necessary to consider also the vertical dimension of the geochemical background. However, available in depth data on urban soils consist mainly in pollution diagnoses. The representability of these data is then called into question, along with the method employed to determine geochemical background.

To answer this question, we compare herein three standard statistical computation algorithms and examine their sensitivity to various parameters: probability distribution, number of data, proportion of values below the limit of quantification, and sampling schema heterogeneity. After performing a set of theoretical computations, simulations are run and application tests are conducted on actual datasets.

Results reveal a variability in the calculated thresholds depending not only on the applied statistical methods used, but also on the distribution law, number of samples and sampling heterogeneity. It appears to be impossible therefore to apply these statistical methods on datasets that are not dedicated to the geochemical background without conducting a preliminary data study, ultimately followed by a data sort. It is in fact necessary to verify dataset consistency with the notion of an anthropogenic geochemical background. In addition, according to the objectives associated to the valorisation of excavated soils (economic benefit of excavated soils and/or environmental/health protection being prioritized), the thresholds (based on background) targeted may be more or less conservative by virtue of adapting both the computational method and algorithm used.

1. Introduction

Given the socioeconomic changes and demographic pressures, many countries are reorganizing their urban zones. In order to limit encroachment on farmland and natural habitat, cities are densifying and transforming their former urban fabric (Kasanko et al., 2005; Inostroza et al., 2013). This urban renewal effort generates significant volumes of excavated soils (Cadiere and Masselot, 2011; Magnusson et al., 2015). The reuse of low to moderately contaminated soils constitutes a major economic and ecological challenge (Blanc et al., 2012; Chittoori et al., 2012; Le Guern et al., 2016; Kenley et al., 2011; Magnusson et al., 2015). This is the case for the low and moderately contaminated soils present in many places in the city. Diffuse contamination of soils occurs indeed on the whole city, due to the impacts of the various anthropic activities (industrial, domestic, agricultural, traffic, material or waste deposits) (Le Guern, 2017). Point-source contamination are frequent also e.g. in derelict industrial land (Lark and Scheib, 2013; Limasset et al., 2018; Manta et al., 2002; Sun et al., 2010).

Reusing low to moderately contaminated excavated soils within land redevelopment projects necessitates among others to verify their geochemical compatibility with the receiving site. Actually, we notice two main approaches in Europe to allow or even enhance the reuse of

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such excavated soils. In the first one, the adequacy of the geotechnical properties of the soils to be reused with the needs of the receiving site is first studied (eg. in Sweden). Once this criteria is fulfilled, the geochemical compatibility with the receiving site is verified. In the second approach the geochemical compatibility between the excavated soils and the receiving site is first verified (eg. in France). Once the geochemical criteria is fulfilled, as well as potential environmental and sanitary impacts (at least in France), then the geotechnical compatibility is verified. In France, the aim of the geochemical verification is to avoid degrading soil quality of the receiving site (Blanc et al., 2012; Coussy et al., 2017*)*.

Anticipating the reuse of low to moderately contaminated excavated soils at redevelopment project or urban scale is an opportunity to optimize their reuse. This is possible by fixing threshold values based on quarter or urban geochemical background. Because a) urban soil geochemistry varies horizontally and vertically due to urban soils heterogeneity and b) excavation and reuse of soils occurs in 3D, it is thus necessary to consider also the vertical dimension of the geochemical background.

There have been however until recently nore dedicated in depth geochemical sampling protocol neither campaigns, especially in France. It is necessary thus to use available data. Most of them are acquired for other purposes, mainly within the frame of pollution diagnoses.

From the standpoint of reusing excavated soil within an urban setting, the urban soil layer is considered to extend several meters deep and is likely to generate excavated soils during land development projects. This layer incorporates the anthropogenic deposits that are widely encountered in urbanized areas (Le Guern et al., 2016). The urban geochemical background is defined for purposes herein as all soil contents related to either natural or anthropogenic phenomena spread throughout the target zone. It thus encompasses typical contents (i.e. diffuse natural content and anthropogenic pollution) yet excludes the geochemical anomalies it is supposed to separate (Guillén et al., 2011; Matschullat et al., 2000; Reimann et al., 2005; Salminen and Gregorauskien, 2000). For the sake of convenience, this value range is typically represented by its upper bound, or threshold limit, whose determination in an urban setting is complicated by the extreme soil heterogeneity and high level of spatial geochemical variability (Guillén et al., 2011; Jarva et al., 2014; Karim et al., 2015). Moreover, the anomaly herein, and hence the computed threshold limit, depend of the area of the investigated territory. Defining this anomaly will depend on the scale chosen to proceed with the background determination, e.g. urban district, metropolitan area. This scale must in particular be large enough to have real local significance yet still enable generating a sufficient number of data points to yield a robust statistical computation.

The literature presents several computational methods for deriving the upper bound of the geochemical background, which will be referred to below as “threshold”. The graphical methods (Matschullat et al., 2000) rely on identifying inflection points in the cumulative frequency curves. Overly sensitive to operator interpretation, these methods will not be addressed herein. Among the statistical computational methods focused on the threshold value, the three most common algorithms are: 1) a high-order percentile, in practice 95% or 90% (Ander et al., 2013; Cave et al., 2012; McIlwaine et al., 2014; Rothwell and Cooke, 2015; ISO Standard 19258, 2005), 2) the whisker obtained with the Tukey percentile (Jarva et al., 2014; Reimann et al., 2005; Reimann and de Caritat, 2017; Rothwell and Cooke, 2015; Tarvainen and Jarva, 2011), and 3) the median absolute deviation or MAD (Reimann et al., 2005; Reimann and de Caritat, 2017; Rothwell and Cooke, 2015). In light of the differences among these three algorithms, their applicability to non-dedicated datasets in determining the geochemical background becomes a cause for concern. We check therefore the possibilities of use in this context of unspecified data, with unknown rates, likely to be high anomalies.

This paper examine the properties and sensitivity of these three statistical thresholds and evaluate their consistency with respect to the urban geochemical background. The influence of data probability distribution is first assessed by means of theoretical computation for well-known distributions. The sensitivity of thresholds to the number of samples and the limit of quantification is then studied by simulation. Next, an application to a real-world case reusing data not specifically dedicated to the geochemical background will serve to evaluate the influence of the directed sampling, its heterogeneity as well as the importance of taking descriptive data into account. Based on these results, we discuss the notion of anomaly and the pertinence of computing a threshold from data that have not been acquired for this specific purpose.

2. Equipment and methodology

The three criteria most frequently found in the literature are recalled first, followed by a presentation of the study approach. In relying on the literature and various regulations proposing two thresholds associated with percentiles, computations are performed using percentiles at 90% and 95%. It is important to notice that these calculation do not take into account the localization (geographic coordinates) of the samples.

2.1. Definition of the three statistical thresholds

Let Z be the studied variable (representing a chemical substance concentration in the soils and subsoils). Let's denote Q_{50} as its median ($P(X < Q_{50}) = 1/2$) (with P: Probability), and respectively Q_{25} and Q_{75} as the other two quartiles ($P(X < Q_{25}) = 1/4$ and $P(X < Q_{75}) = 3/4$). The three criteria most widely used in order to establish geochemical background thresholds are as follows:

– threshold associated with a high-order percentile (90% or 95%) (Ander et al., 2013; Cave et al., 2012; McIlwaine et al., 2014; Rothwell and Cooke, 2015; ISO Standard 19258, 2005):

$$S_{95} = Q_{95} \textit{ and } S_{90} = Q_{90} \tag{1}$$

– threshold associated with the whisker, by means of Tukey's centile (Jarva et al., 2014; Reimann et al., 2005; Reimann and de Caritat, 2017; Rothwell and Cooke, 2015; Tarvainen and Jarva, 2011) defined as:

$$S_{whisker} = Q_{75} + a\,(Q_{75} - Q_{25}) \textit{ with } a = 3/2 \tag{2}$$

– threshold associated with the MAD, median absolute value of the deviations from the median, by means of the median method (Reimann and de Caritat, 2017):

$$S_{MAD} = Q_{50} + (b\ MAD) \textit{ with } MAD = median\,(|\,Z - Q_{50}\,|) \textit{ and } \mathrm{b} = 2 \tag{3}$$

2.2. Test cases

The empirical distributions of geochemical data for a given site, metropolitan area or region do not systematically follow the same statistical distribution (Karim et al., 2015; Reimann et al., 2005).

In order to study the influence of data distribution on the computed geochemical background threshold, three basic probability distributions are examined herein: uniform, normal, and log-normal distributions. This investigation will determine if a systematic orderly relationship exists between the thresholds values obtained should the study population conform to any of these distributions. Emphasis is placed on identifying whether one of the three thresholds is more conservative (i.e. systematically yields the minimum value) regardless of the associated distribution.

The subsequent step will focus on the case of a mixing of distributions. We verify whether the thresholds can differentiate the two modes of a statistically heterogeneous population.

The influence of the number of samples collected is scrutinized next. It is a well-known fact that some statistics, like low- or high-order percentiles, are extremely sensitive to this number (see, for example, Bernard-Michel and de Fouquet, 2005; Bernard-Michel, 2006, regarding an environmental context). The question is also raised over the influence of the limit of quantification (LQ) actually present in the "background" geochemical data. Several publications have underscored this influence (Reimann et al., 2005; Rothwell and Cooke, 2015; Sancho, 2016), yet without accurately quantifying it. Simulations will be run to analyze the effect of the proportion of data below the limit of quantification as well as that of the substitution value for such data.

The influence of spatial heterogeneity within the samples is then examined on actual BRGM databank entries. The considered site is a district in the French city of Nantes spanning approximatively 340 ha with a land use historically dominated by industrial activity. The subsoil is characterized by a deep alluvial layer covered by various types of fill material with a thickness of two to four meters. The volume of soil to be excavated for the district restoration project was evaluated at approximatively 100,000 tons/year during the renovation works initiated in 2015 and scheduled to last through 2025. The data stem from pollution assessments and include samples of variable lengths extracted from cored boreholes. The sampling is thus oriented in a particular direction and intended to demarcate the polluted zones, with only few reference samples typically located in a zone assumed not to be impacted. Nearly 2500 boreholes containing 4400 samples between zero and five meters deep were uploaded to the databank. This type of data, which was not originally intended to compute a geochemical background, ultimately serves as the primary source of geochemical data available in France for urban soils.

The computations are initially conducted on samples without taking location into account. They are then replicated, this time in weighting the data to correct for the influence of spatial irregularity in the sampling. As a last step, the typology of fill materials is also incorporated (Le Guern et al., 2016) in order to distinguish the effect of anthropogenic soils on the geochemical background thresholds.

The data of the real site are spatially correlated, whereas the drawings are independent for the theoretical calculations.

Most computations were performed with the software "*Free R*". The Access 2016 and Excel 2016 applications within the Microsoft Office suite plus ArcGis 10.2.2 were used for the computational and mapping steps.

3. Results and discussion

3.1. Influence of the probability distribution

In this part, calculations are made for independent runnings of a random variable.

3.1.1. Homogeneous case

The theoretical computation serves to specify the properties of the three threshold values for a number of typical probability distributions. Three distributions are examined herein: uniform, normal, and log-normal distribution (Fig. 1).

Let's note that for all these distributions (theoretical or empirical), $S_{90} \leq S_{95}$.

3.1.1.1. Symmetrical distribution. Let's denote Q_{50} as the median of the Z distribution. Since the distribution is assumed to be symmetrical about its median, Q_{75}-Q_{50} = Q_{50}-Q_{25}. Consequently,

$$\begin{aligned} \mathrm{MAD} &= \mathrm{median}(|\,Z - Q_{50}\,|) \\ &= Q_{75} - Q_{50}. \end{aligned}$$

$$s_{\mathrm{MAD}} = Q_{50} + 2\mathrm{MAD}$$

which yields:
$$\begin{aligned} &= Q_{50} + Q_{75} - Q_{25} \\ &= Q_{75} + (Q_{50} - Q_{25}) \end{aligned}$$

Since $S_{Whisker} = Q_{75} + a\,(Q_{75}\text{-}\ Q_{25})$, and excluding the case where $Q_{75} = Q_{50}$, it thus follows that:

$$\forall\ a \geq 1,\ s_{MAD} < s_{\mathrm{Whisker}}$$

3.1.1.2. Uniform distribution. Let's now consider the uniform distribution over the interval [0, Z_{max}] (the general case, [Z_{min}, Z_{max}], is presented in Appendix A); while highly unlikely for geochemistry data, this case still provides a basis for analysis. Hence, $Q_{50} = 1/2$ Z max and $Q_{25} = \frac{1}{4}Z_{max}$, $Q_{75} = \frac{3}{4}Z_{\max}$, resulting in (detailed computations are shown in Appendix A):

- $S_{90} = 0.90\ Z_{max}$ and $S_{95} = 0.95\ Z_{max}$
- $S_{Whisker} = 3/4\ Z_{max} + 1.5\ (3/4\ Z_{max} - 1/4\ Z_{max}) = 3/2\ Z_{max}$
- $S_{MAD} = 1/2\ Z_{max} + 2\ (1/2\ Z_{max} - 1/4\ Z_{max}) = Z_{max}$

which yields the following inequalities among the thresholds:

$\mathbf{S_{90} < S_{95} < S_{MAD} < S_{Whisker}}$

The thresholds associated with the percentiles indicate that the upper 10% or 5% of the dataset are not included in the geochemical background. Yet nothing herein actually justifies this differentiation. In contrast, the upper whisker would allow integrating data above Z_{max}: an additional data point higher than Z_{max} would not necessarily be considered therefore as an anomaly.

3.1.1.3. Normal distribution. Let's recall that for a reduced Gaussian distribution, $Q_{75} = 0.6745$, $Q_{90} = 1.282$ and $Q_{95} = 1.645$.

The thresholds associated with the normal variable, $Z = \mu + \sigma Y$ where Y is a reduced Gaussian, μ the mean and σ the standard deviation of Z, are:

- $S_{90} = \mu + \sigma Q_{90}$, hence $S_{90} = \mu + 1.282\sigma$;
  $S_{95} = \mu + \sigma Q_{95}$, hence $S_{95} = \mu + 1.645\sigma$
- $$\begin{aligned} S_{\mathrm{Whisker}} &= \mu + \sigma[Q_{75} + 1.5(Q_{75} - Q_{25})] \\ &= \mu + (1 + 2 * 1.5)\sigma Q_{75} \\ &= \mu + 2.698\sigma \end{aligned}$$
- $$\begin{aligned} S_{\mathrm{MAD}} &= \mu + 2 * \mathrm{median}_i(|Z_i - \mu|) \\ &= \mu + 2\sigma * \mathrm{median}_i(|Y_i|) \\ &= \mu + 2\sigma Q_{75} \\ &= \mu + 1.349\sigma \end{aligned}$$

The order of these thresholds is as follows:

$\mathbf{S_{90} < S_{MAD} < S_{95} < S_{Whisker}}$

It thus differs from that of the uniform case; more specifically, the order of thresholds for the 95th centile and MAD method are reversed.

3.1.1.4. Log-normal distribution. In the case of a log-normal distribution, $Z = e^{\mu+\sigma Y}$ where Y is a reduced Gaussian. Two computation modes are possible: the thresholds calculated for the normal distribution can be exponentiated, leading to:

- $S_{90} = e^{\mu+1.282\sigma}$ and $S_{95} = e^{\mu+1.645\sigma}$
- $S_{Whisker} = e^{\mu+2.698\sigma}$
- $S_{MAD} = e^{\mu+1.349\sigma}$

The order remains identical to the previous case since the exponential function is increasing:

$\mathbf{S_{90} < S_{MAD} < S_{95} < S_{Whisker}}$

The computation can also be performed directly on the log-normal distribution, with the following formulae:

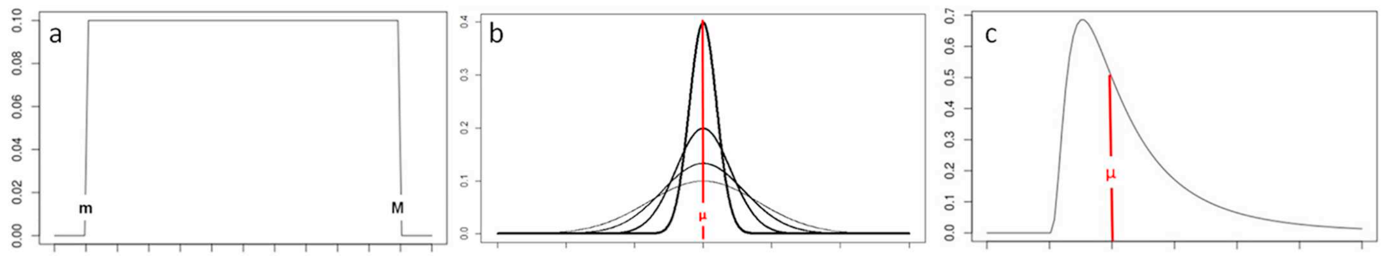


Fig. 1. Distributions: uniform (a), normal (b), and log-normal (c). **m** and **M** denote the minimum and maximum values, and **μ** the average. The normal distribution is illustrated using 4 different standard deviations.

- $S_{90} = e^{\mu+1.282\sigma}$ and $S_{95} = e^{\mu+1.645\sigma}$, i.e. identical results to those of the previous computation.
- $S_{Whisker} = e^{\mu+\sigma Q75} + 1.5\, e^{\mu}\, (e^{\sigma Q75} - e^{-\sigma Q75})$

which yields:

$S_{Whisker} = e^{\mu+\sigma\ Q75}\ (5/2 - e^{-2\sigma Q75})$

- $S_{MAD} = e^{\mu} + 2\, e^{\mu}$ median (I $e^{\sigma Y}$-1 I)

In order to compare results, these thresholds are expressed as a function of σ in the form of a threshold/e^{μ} ratio (Table 1):

These results differ from those of the first computation. The order of thresholds varies now as a function of σ as follows, with S_{MAD} being underlined for easier comparison:

- when **σ** ≤ 0.01, $\mathbf{S_{90}} < \underline{\mathbf{S_{MAD}}} < \mathbf{S_{95}} < \underline{\mathbf{S_{Whisker}}}$
- when **σ** ϵ]0.01; 0.75], $\underline{\mathbf{S_{MAD}}} < \mathbf{S_{90}} < \mathbf{S_{95}} < \underline{\mathbf{S_{Whisker}}}$
- when **σ** ϵ]0.75; 1], $\underline{\mathbf{S_{MAD}}} < \mathbf{S_{90}} < \underline{\mathbf{S_{Whisker}}} < \mathbf{S_{95}}$
- when **σ** > 1, $\underline{\mathbf{S_{MAD}}} < \underline{\mathbf{S_{Whisker}}} < \mathbf{S_{90}} < \mathbf{S_{95}}$

For highly dispersed distributions (**σ** = 5), the percentiles Q_{90} and Q_{95} are far apart; on the other hand, when distributions are very tightly centered around the median (**σ** = 0.01), the median-quartile deviation is reduced. Consequently, for highly dispersed distributions (**σ** = 5), $S_{Whisker} < S_{90}$, and vice versa for distributions with limited dispersion.

As such, not only the probability distribution but also, in the log-normal case, the computational method influences the thresholds obtained. The ranks of the 95th and 90th percentile thresholds vary with respect to the whisker and MAD thresholds; they depend on the data distribution (i.e. level of value clustering). Yet the observation can be drawn that the MAD threshold always lies below the whisker threshold, regardless of σ value. Indeed, whether applied to values above or below the median, the absolute value$|X-Q_{50}|$acts indiscriminately; typically however, since lower values are less widely dispersed than higher values, this deviation is smaller than the Q_{75}-Q_{25} interquartile deviation.

3.1.2. Heterogeneous case

Let's now consider mixing two distributions of the same type with different parameters. The first mode is assumed to correspond to the background while the second to the anomalies.

3.1.2.1. Combination of two uniform distributions. As shown in Fig. 2:

- m_1 and m_2: the minimum values of the first and second mode, respectively;
- M_1 and M_2: the maximum values of the first and second mode, respectively;
- α: proportion of the first mode in the combination.

The two modes are assumed to be disjointed, with $m_1 < M_1 < m_2 < M_2$

The percentiles Qx are expressed as follows:

if $x < \alpha$: $Qx = m_1 + x\,[(M_1 - m_1)/\alpha]$

if $x > \alpha$: $Qx = m_2 + (x - \alpha)[(M_2 - m_2)/(1 - \alpha)]$

We are seeking herein at which conditions a threshold "S" separates the two modes, i.e. M1 < S < m2.

Since the formulae for the three thresholds feature a percentile as their first or only term (i.e. 95th for $\mathbf{S_{95}}$, 90th for $\mathbf{S_{90}}$, 75th for $\mathbf{S_{Whisker}}$, and 50th for $\mathbf{S_{MAD}}$), these percentiles actually constitute the initial inequality constraint. As such, the 90th centile can only be positioned between M1 and m2 if α equals 0.9, or 0.95 for the 95th centile. This condition is rarely verified in a real-world case when using undedicated datasets.

In the case of the upper whisker, a positive term is added to the 3rd quartile; to ensure that the threshold satisfies the target conditions, this quartile must belong to the first mode; hence α must exceed 0.75. This hypothesis remains plausible since it implies that the anomalies account for < 25% of all data. A second mode proportion above 0.25 may in fact undermine its property of being an anomaly. The second condition imposes that the threshold lies below the second mode.

Given that:

$$(Q_{75} - Q_{25}) = m_1 + 0.75\,[(M_1 - m_1)/\alpha] - m_1 + 0.25\,[(M_1 - m_1)/\alpha]$$
$$= 0.5\,[(M_1 - m_1)/\alpha]$$

it can be deduced that:

$$S_{Whisker} = m_1 + 0.75\,[(M_1 - m_1)/\alpha] + 1.5\,(0.5\,[(M_1 - m_1)/\alpha])$$

The condition can thus be written as follows:

$$S_{Whisker} = m_1 + 1.5\,((M_1 - m_1)/\alpha) \quad (4)$$

The final condition for ensuring that $S_{Whisker}$ effectively separates the two modes, in the case where anomalies account for < 25% of the data, is therefore that Expression (4) lie below m2 (i.e. minimum of the second mode).

Moreover, in the case of MAD, the initial constraint pertains to placing the median, imposing an initial condition of α being > 0.5. This requirement means that the background dataset must necessarily be larger than the anomalous dataset. The two cases of α ≥ 0.75 and 0.5 ≤ α ≤ 0.75 will be studied in the following discussion.

- If α is greater than or equal to 0.75, then the threshold is expressed as follows:

Since the uniform distribution is symmetrical, if *α ≥ 0.75:*

$$MAD = Q_{75} - Q_{50}$$
$$= m1 + 0.5[(M_1 - m_1)/\alpha] - m_1 + 0.25[(M_1 - m_1)/\alpha]$$

then:

$$= 0.25[(M_1 - m1)/\alpha]$$
$$S_{MAD} = m1 + 0.5[(M_1 - m_1)/\alpha] + 2(0.25\,[(M_1 - m_1)/\alpha])$$

Hence:

$$S_{MAD} = m_1 + ((M_1 - m_1)/\alpha) \quad (5)$$

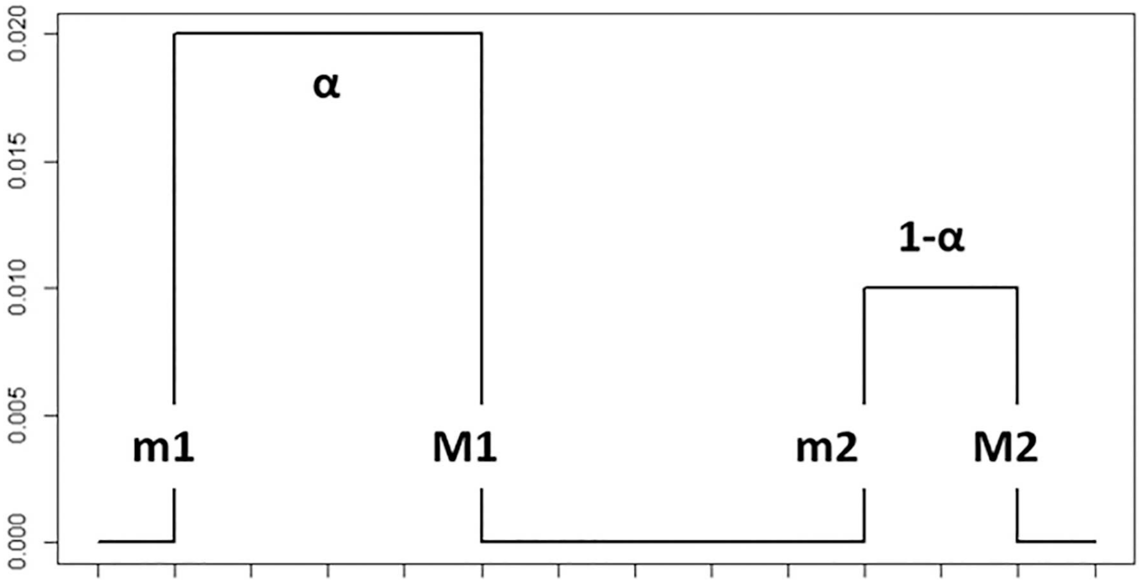


Fig. 2. Combination of two uniform laws, with two disjointed modes featuring minima $\mathbf{m_1}$ and $\mathbf{m_2}$ and maxima $\mathbf{M_1}$ and $\mathbf{M_2}$, and with a proportion of the first mode $\boldsymbol{\alpha}$ used in the mixing.

Since $\alpha < 1$, then $((M_1 - m_1)/\alpha) > (M_1 - m_1)$ and $S_{MAD} > M_1$.
If $S_{MAD} < m_2$, in the case where $\alpha > 0.75$, the threshold may separate the two modes.

- Moreover, if α lies between 0.5 and 0.75, then the threshold may be expressed as follows:

Under the additional condition $(Q_{50} - m_1) < (m_2 - Q_{50})$, i.e. $2Q_{50} < m_2 - m_1$

It can be written:

$$\begin{aligned} MAD &= Q_{50} - Q_{(\alpha-0.5)} \\ &= (1-\alpha)[(M_1 - m_1)/\alpha] \end{aligned}$$

$$S_{MAD} = m_1 + 0.5[(M_1 - m_1)/\alpha] + 2[(1-\alpha)[(M_1 - m_1)/\alpha]]$$

Put otherwise:

$$S_{MAD} = m_1 + 2.5((M_1 - m_1)/\alpha) + 2\alpha((M_1 - m_1)/\alpha) \tag{6}$$

Since $\alpha < 0.75$, then $2.5 - 2\alpha > 1$ and $S_{MAD} > M_1$

When the MAD threshold separates the two modes, α thus lies between 0.5 and 0.75.

Should the result of Eq. (6) be less than m2: this condition assumes however that anomalies account for over 25% of the population, which is only really consistent if the anomalies are being oversampled relative to the background.

Combining two uniform distributions reveals the constraints necessary for the threshold to be consistent with the presumed limit of the geochemical background. It is obvious that these restrictive conditions could in practice go unverified (in assuming that the data correspond to a mixing of uniform distribution).

The outcome of an algorithm does not necessarily correspond to the concept being targeted.

3.1.2.2. Combination of two log-normal distributions. Let's examine the combination of two log-normal distributions with respective means of 1 and 10 and standard deviations of 1 and 1.5. Simulations are used to verify if the thresholds can separate the two modes, testing the α proportions of background data in the combination (95%, 80%, 70% and 50%).

A random sample of 3000 data points is then generated using this combination, with the thresholds being calculated and depicted graphically (Fig. 3).

These results are similar to those obtained for the combination of uniform distributions. The background data proportion α serves as the main parameter defining the consistency of the threshold result with respect to the definition of the pedo-geochemical background.

3.1.3. Discussion

First, the data distribution does influence the order of the thresholds calculated with the three tested statistical algorithms, as the lowest and highest values of the three thresholds depends of the distribution. Second, the results show that the algorithms cannot always separate background and anomalies (cf. definition of the geochemical background). This finding demonstrates that a single statistical criterion, independent of the context, has little chance of yielding the expected result (separating the anomalies from the pedo-geochemical background). On any given polluted site, the "background" dataset may be much smaller than that of the "anomalies"; the same can occur even with surveys using a regular mesh. This outcome may also hold for a district with an extensive industrial past, where the various manufacturing sites containing polluted soils would actually cover a majority of the territory. The notion of background thus clearly depends on the working scale. The study zone must be large enough for the "anomalies" to remain more confined than what is considered as the local "background". In some cases nevertheless, e.g. smelter with impact on a large area, the anomalies at a given scale become a background at a smaller scale. It is preferable therefore to infuse knowledge (notably a historical record) of the medium to understand the variations or even to delimit the study zone. In the case of data derived from an irregular pattern or a preferential sampling protocol, it also becomes necessary to account for sampling irregularities. However this is not always sufficient, especially when the preferential survey fails to adequately sample the low-value mode. These results show the absolute necessity of first exploring the data, verifying their "representativeness" and accuracy for a geochemical background calculation. To achieve this, at least data distribution must be checked and interpreted.

3.2. Influence of the number of samples and limit of quantification

Let's now examine the sensitivity of these three thresholds to the dataset size and the limit of quantification. This study is performed by simulation of a lognormal distribution with mean 1 and standard deviation 2.5 (through an empirical computation on the drawings).

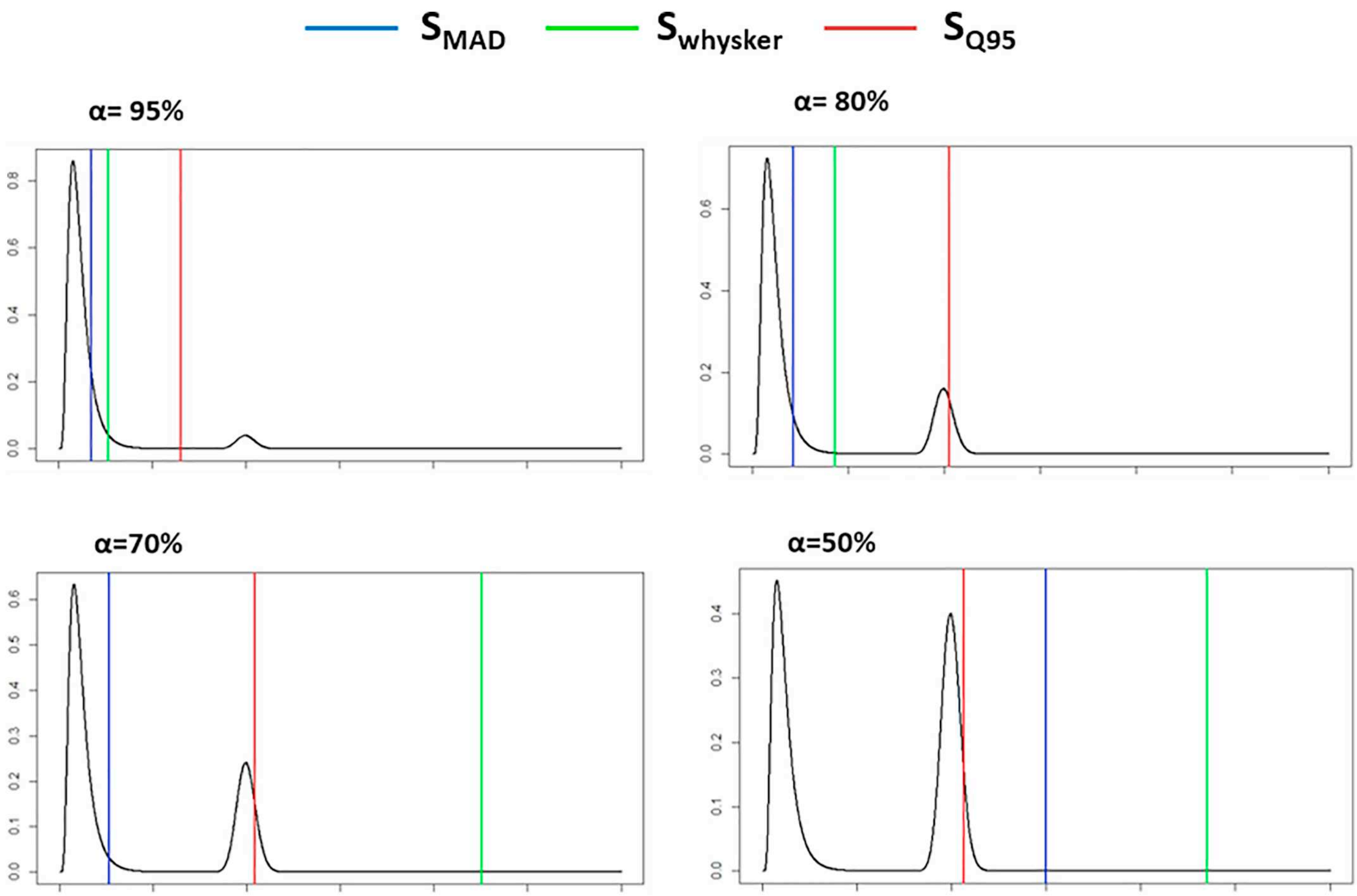


Fig. 3. Calculated thresholds for the three algorithms (MAD, Whisker, Percentile 95) with different proportions "α" of background data (Sauvaget, 2019).

3.2.1. Influence of the dataset size

To assess the influence of the number of data, the thresholds are computed over increasing datasets, with 20, 30, 50, 100, 200, 300, 500, 750, and 1000 data points. The computations are then repeated 1000 times, and the minimum and maximum results for each sample subgroup are depicted graphically in order to show the fluctuation amplitude.

Uncertainty is quantified by the deviation between the calculated maximum and minimum for each of the three algorithms, on all 1000 simulation iterations. Uncertainty thus represents the fluctuation amplitude for the computed threshold values. The results of this step (see Fig. 4) obviously demonstrate a reduction in fluctuations as the number of data points increases.

For each of the three thresholds, uncertainty quickly drops until reaching 100 samples; it then continues to decline more gradually, in stabilizing beyond 200 samples for the MAD threshold and 500 for the other two. As noted above, the MAD threshold appears to be the most conservative.

Computing thresholds on the basis of an overly small dataset size (i.e. fewer than 30 data points) must clearly be avoided. The excessively unstable result would vary with the introduction of additional data. Nonetheless, this scenario remains quite common in environmental studies, which are hard-pressed to produce such a volume of data. The MAD threshold however appears to display the smallest fluctuation amplitude and would thus be the best option under the hypothesis of a computation using a small-sized dataset. The value output must only be considered as a conventional criterium and used for purely informational purposes given the high level of associated uncertainty.

3.2.2. Influence of the limit of quantification (LQ)

The influence of the limit of quantification is assessed using the same set of simulations, but this time by varying the LQ. The data lying below this limit are assumed to be non-quantifiable by means of analytical techniques. The proportion of data less than the limit of quantification is obtained by setting the limit of quantification as the increasing percentiles of the empirical distribution, the values being set to either the LQ or 0.

Fig. 5 shows the simulation results obtained by increasing the limit of quantification, and thus the number of data lying below this limit.

As long as the limit of quantification remains below the Q95 percentile, the S_{95} threshold remains independent of the replacement value: 0, LQ/2 or LQ. This same relationship holds for Q90 and the S_{90} threshold, with a proportion below 90%.

The MAD and upper whisker thresholds are, for one thing, insensitive to LQ at percentages respectively < 20% and 25% of data lying below the LQ. At higher percentages, these thresholds drop. The MAD threshold decreases all the way to 50% while the upper whisker reaches 75%. These declines result from the distance term in the two threshold expressions, which fall all the way to zero for the aforementioned percentages (Fig. 6). Once these percentage levels have been exceeded, the thresholds are reassigned to the LQ value and thus not depicted in Fig. 5.

In the case of replacing data lying below the LQ by 0, it can once again be observed that the 95th centile is not being affected as long as the proportion of values lying below the LQ remains < 95%. Afterwards, it falls to 0. In the same way, the S90 threshold, will fall to 0 once 90% of values are positioned below the LQ. The behavior of the MAD and upper whisker thresholds is less homogeneous than before; the thresholds are notably no longer affected until 20% of data drop

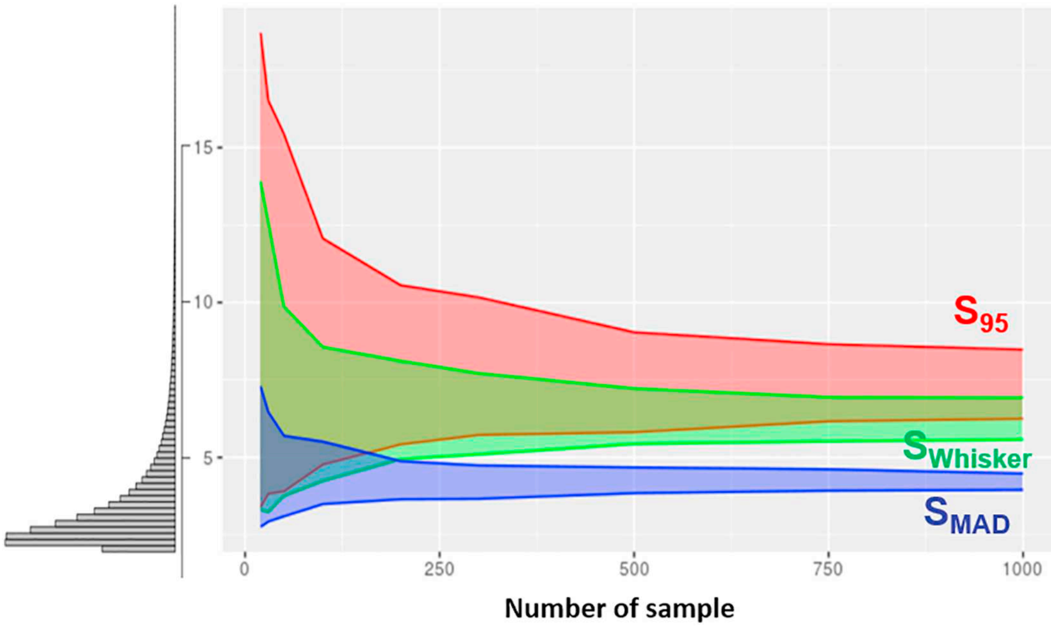


Fig. 4. Influence of the number of data points on the computed threshold. Minimum and maximum results of threshold computations for 1000 iterations on an increasing dataset. Red: Q95, Green: Upper whisker, Blue: MAD threshold. The simulated data histogram has been indicated on the y-axis. Log-normal case (average = 1, standard deviation = 2.5) (Sauvaget, 2019). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

under the LQ. Next, observed thresholds are rising, more quickly for the upper whisker and more slowly for the MAD. This increase can be explained by the distance term of these thresholds, which takes into account the deviation between the replacement value (0 in this case) and the LQ value, hence expanding the distance between LQ and replacement value. Subsequently, the upper whisker displays stability between 30% and 70%, as explained by the fact that both the 1st quartile (0) and 3rd quartile values do not vary. A lowering of the thresholds can then be observed, rather quickly for the whisker and more slowly for MAD, with both reaching 0, at 75% for the whisker and 50% for MAD, respectively. These results remain valid to all cases of substitution by a value less than LQ, e.g. LQ/2, as it is frequently encountered in geochemistry.

The proportion of data lying below the limit of quantification and the substitution value therefore influence the computed thresholds. Even though the choice of substitution by 0 does seem to be more conservative (by virtue of lowering the values), the influence of distances (MAD and interquartile distance) in the MAD and upper whisker thresholds must also be taken into account.

Moreover, in the case most of the data are lower than LQ, all three thresholds correspond to the substitution value. These percentages equal respectively: 50% for the MAD method, 75% for the upper whisker, 90% for the 90th centile, and 95% for the 95th percentile. In case of a majority of data lower than LQ, it is only possible to mention the background threshold is lower than LQ, indicating though the value of LQ.

3.2.3. *Discussion*

These results reveal the importance of taking into account the number of data and the limits of quantification when establishing geochemical background values. The dataset size is a highly restrictive parameter since a small number of samples induces great uncertainty on the computed thresholds (high fluctuation amplitude). The majority of urban studies are confronted with difficult and costly sampling procedures and, quite often, cannot guarantee a sufficient number of data (> 30). It is therefore advised to accompany the computed thresholds with the actual dataset size so that the relevance of these thresholds can be evaluated by the reader. However in the cases of

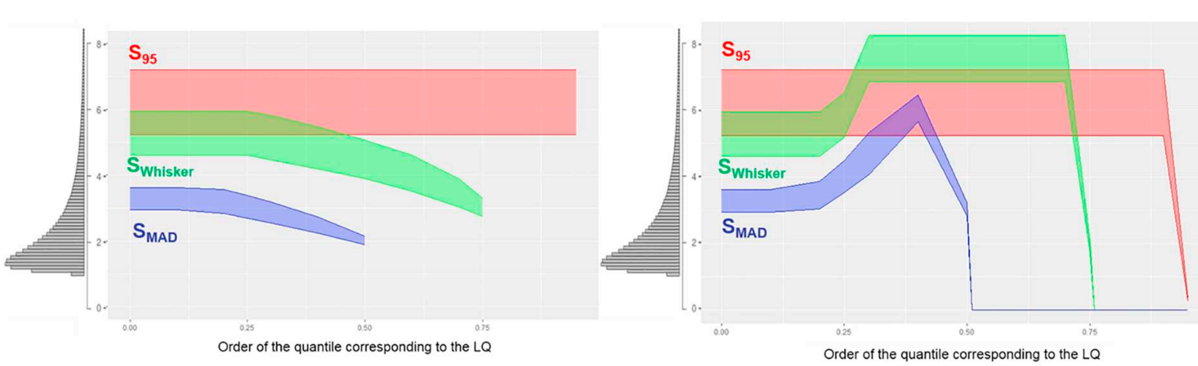


Fig. 5. Influence of the limit of quantification. Minimum and maximum values of the threshold computations on 1000 iterations, in increasing the limit of quantification (LQ) and thus the proportion of samples lying below the LQ Replacement of the values lower than LQ by LQ (left) and by 0 (right). Red: Q95, Green: Upper whisker, Blue: MAD threshold MAD. The simulated data histogram has been provided on the y-axis. Log-normal case (mean = 1, standard deviation = 2.5). On the left, result equals to the LQ are not represented (Sauvaget, 2019). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

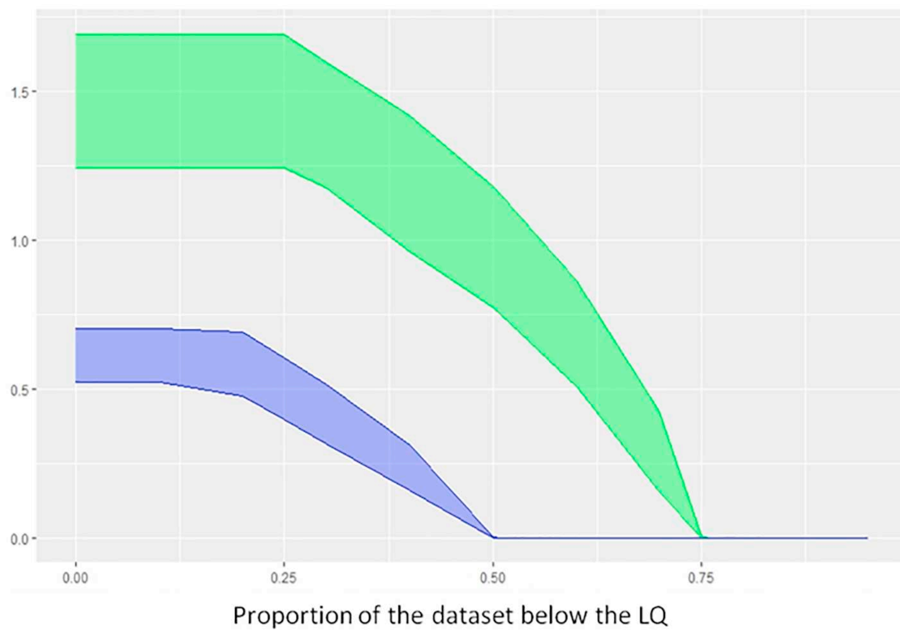


Fig. 6. Influence of the percentage of values lying below the LQ. Empirical minimum and maximum computed thresholds for the interquartile distance (green) and MAD term (blue) on 1000 iterations, in considering a portion of samples lying below the rising limit of quantification and a replacement of values rejected by the LQ (Sauvaget, 2019). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

strongly homogeneous soils, and if this can be proved, less data could be used (e.g. 20).

Many geochemical parameters are subject to censoring from a statistical standpoint (i.e. data lying below the limit of quantification), as it was demonstrated above that such data heavily influence the computed thresholds. It then becomes important to take into account the percentage of censored values in order to make the threshold computation criterion relevant. Lastly, the substitution value of disqualified data must be examined; with the aim of avoiding an overestimation of the thresholds computed when using the MAD or upper whisker methods, it is highly advised to select the LQ value as the substitution value. Furthermore, analytical techniques with low quantification limits are needed.

3.3. Influence of the spatial heterogeneity of sampling

Application to a practical case will expose the influence of a preferential, hence heterogeneous, sampling schema. The case study used herein is the Nantes district described in Part 2.

The three algorithms are first be applied without taking into account data location (Fig. 7) on the whole dataset. The MAD threshold yields the most conservative results. Results from all three algorithms are consistent with this urban environment through pronounced enrichment regarding arsenic, copper, lead or zinc, as influenced by anthropogenic activity. The lower natural geochemical background thresholds of the zone apply to barium, chromium or nickel (of geogenic origin here).

For a second calculation, the data are weighted in order to correct the irregular sampling density, which in this case has been designed to study anomalies and thus tends to oversample the zone of potential anomalies. The sampling is not only irregular, but also preferential. The data are weighted by the inverse of the number of samples present in a square mesh 25 m or 100 m to a side. This weighting reduces the influence of tightly bound samples. According to the initial result (Fig. 8), regardless of sample weighting, the threshold order remains unchanged, the MAD threshold being the most conservative. Next to be noticed is an increase in computed thresholds the bigger the mesh used for weighting. From the histograms presented in Fig. 9, this relationship is explained by a greater proportion of higher values after weighting. This rise is due to the large number of low values in the dataset lying within geographic proximity, a condition that lessens their influence on the weighting. The greater proportion of high values in the weighted data exerts an influence on the percentiles, which in turn raise the computed threshold values. Moreover, the MAD threshold, which is reliant on the median and nearby values, would appear to be relatively insensitive to the weighting.

In this case therefore, sample weighting depending on geographic proximity, increases the computed thresholds, with the effect of limiting the influence of data located nearby and better incorporating the zone's actual geochemistry. Moreover, threshold underestimation in the non-weighting case in actuality reduces the possibilities for reusing excavated soils.

3.4. Taking into account the determinants of urban geochemistry

Urban geochemistry is the result of various determinants (Le Guern, 2017) acting at different levels and scales. Such determinants may pertain to soil and subsoil type (geological data, 583 pedological data) or depend on current or past land use. To better understand urban geochemistry and hence the urban geochemical background, it may prove worthwhile to take these determinants into account as co-variables. For this purpose, a typology of anthropogenic deposits was developed by Le Guern et al., 2016) according to their geochemical specificities. Samples were thus classified according to the following typology of materials composing the soils and adjacent subsoils: natural like anthropogenic deposits (sandy) with a low intrinsic potential of contamination, various or miscellaneous anthropogenic deposits (including demolition waste) with a medium intrinsic potential of contamination, questionable anthropogenic deposits (including e.g. slags or bottom ash) with a high intrinsic potential of contamination, and alluvial deposits. Results are shown in Fig. 10.

Higher thresholds are found in barium, chromium and nickel in the alluvia than in the made-grounds, indicating these elements' geogenic origin. It is the contrary for the thresholds calculated for lead, copper and zinc revealing an anthropogenic origin. Lower thresholds are however detected in the natural type made-grounds than in the alluvia, as explained by the specific type of this fill, composed of Loire sand graded when laid and exhibiting fewer fine particles than alluvia. Including descriptive data then makes it possible to dissociate typologies of soils featuring distinct geochemical properties, hence displaying different geochemical backgrounds.

In contrast, incorporating such descriptive data would herein

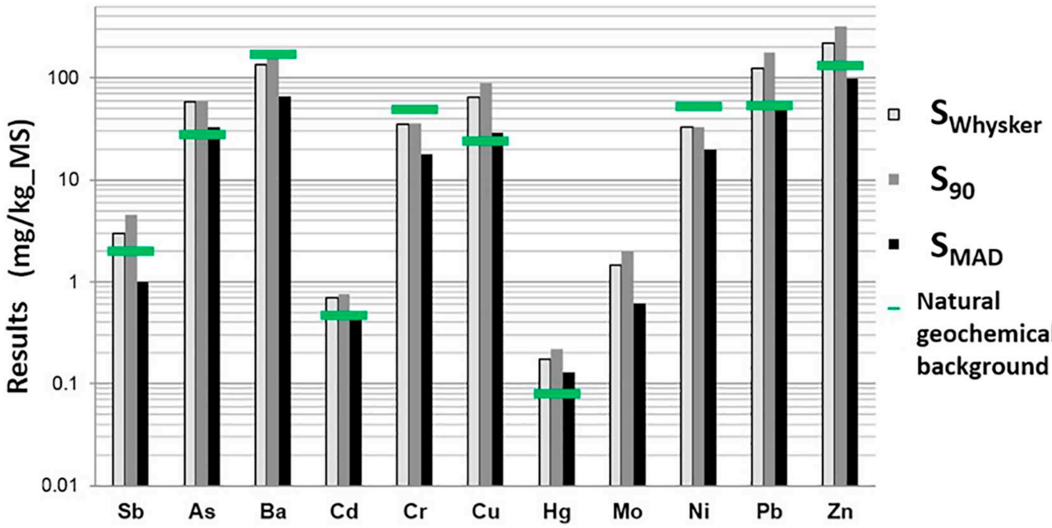


Fig. 7. Results of threshold computations on case study samples for the three methods on whole dataset- Green: Natural geochemical background values (calculated on deep alluvial deposits on the same district) (Sauvaget, 2019). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

segment the data into subgroups. This division thus decreases the number of samples per group that are used to compute the thresholds, with the consequences noted above. There is a need to find a balance when introducing descriptive data so as to build coherent geochemical areas of sufficient size, which is a not so easy due to urban soil heterogeneity. In addition, the descriptive data is likely to provide geochemically homogeneous areas thus allowing the use of statistical thresholds with fewer samples, as seen in the previous discussion (3.2.3).

3.5. Discussion: contributions and limitations of the typical statistical computation methods

The use of statistical thresholds to determine the geochemical background requires taking into account the various parameters capable of influencing the result. A preliminary study of the data, notably sample locations, number, share of non-quantified data along with the covariables describing the medium, is thus necessary. The choice of threshold computation algorithm must be adapted to meet the objective of determining the geochemical background, as well as to the sampling protocol employed (both strategy and mode) and to the data collected.

By definition, the 95th centile considers that the background represents 95% of the data, which corresponds in fact to assigning a margin of error for a sampling protocol dedicated to determining the geochemical background. For example, this step relies on the type of sampling introduced by BGS to produce the G-Base (https://www.bgs.ac.uk/gbase/home.html). Moreover, its insensitivity to values lying below the limit of quantification can yield an initial approach in the specific case of considerable data disqualification (i.e. lying below the LQ). Similarly, the 90th percentile remains a special milestone, regardless of the data distribution. While the margin of error may be greater (10% for Q90 compared to 5% for Q95), it nonetheless remains purely arbitrary and potentially insufficient in the case of data acquired for purposes other than determining the geochemical background, wherein the proportion of anomalies may actually exceed these percentages. Such a case thus overestimates the geochemical background.

The upper whisker highlights the anomaly rate of up to 25% of the dataset. This percentage corresponds more to a non-dedicated sampling protocol in zones only lightly (in retaining a sizable margin of error). This method therefore is quite consistent with the samplings conducted within the scope of the Soil Quality Measurement Network (RMQS) or the Finnish geochemical background program (Jarva et al., 2010). Its use in urban studies that reuse unacquired data available for this purpose is not recommended, despite their utility for an initial preview, over raw data. In contrast, it may prove to be a relevant method for use on sorted data (elimination of obvious anomalies) (Le Guern et al., 2016). Moreover, the limit of quantification is to be assessed by virtue of the threshold sensitivity as of 25% of data lying below the LQ. Replacing data by a value less than the limit of quantification is to be avoided due to the influence exerted on the interquartile distance. Such a replacement would lead in some cases to a background overestimation.

The MAD threshold can differentiate background from anomaly, up to under certain conditions 50% anomalies. This capability integrates

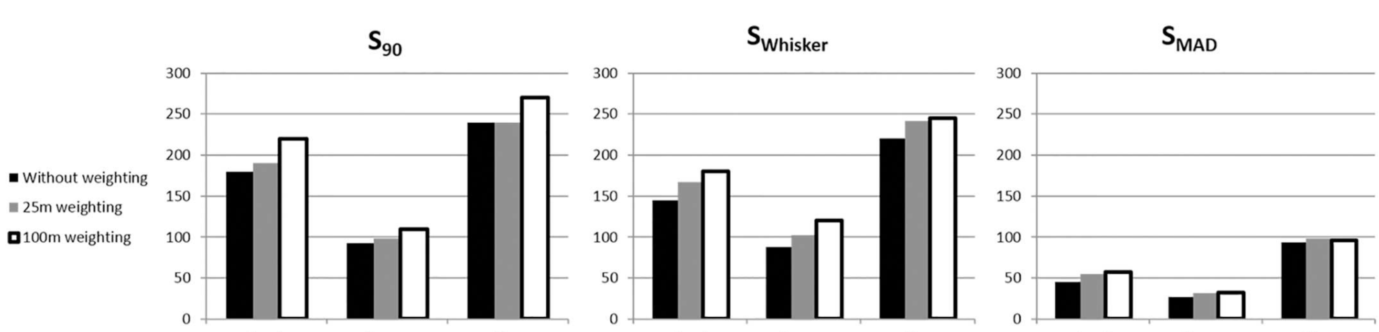
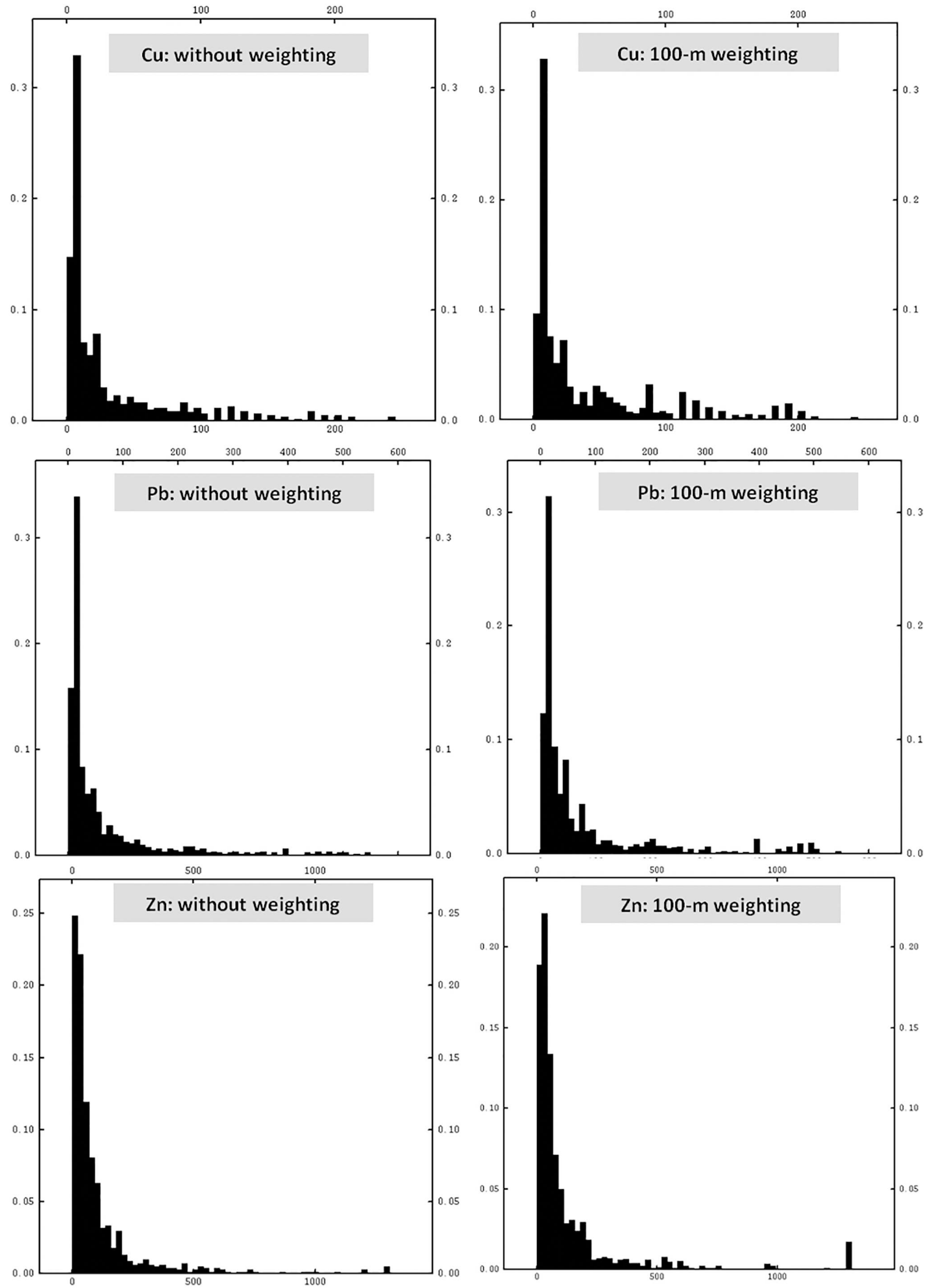


Fig. 8. Thresholds calculated on the case study samples for the three methods: without weighting (black), weighting using the inverse of the number of samples in the meshes either 25 m (grey) or 100 m (white) to a side. Contents of lead, copper and zinc, expressed in mg/kg of DM.



(caption on next page)

Fig. 9. Histograms of the concentrations in copper, lead and zinc, expressed in mg/kg of DM, with or without weighting by the inverse of the number of samples in a mesh measuring 100 m to a side.

data stemming from sampling campaigns dedicated to contaminated sites, including pollution diagnoses. It thus provides an attractive solution for optimizing the use of these data. Since the computed thresholds are relatively low (compared to the other thresholds), it tends to suit a conservative approach to the detriment of reusing excavated earth. Just like the upper whisker, it is somewhat sensitive to the data lying below the limit of quantification (beyond 20% disqualified data), and the replacement value must not lie below this limit to ensure the background has not been overestimated.

The choice among these statistical methods thus relies in part on a dual evaluation of the proportion of anomalies and of the background, which in turn depends on the properties of soils being studied and type of sampling protocol implemented. In this sense, our conclusions are similar to those of Reimann et al. (2005). It demonstrates that for a small proportion of anomalies, the upper whisker can provide adequate threshold values. On the other hand, just as we have also presented, a relatively large proportion of anomalies can only be separated by the MAD threshold.

In the case study cited herein, the vast majority of our data stems from samplings dedicated to the potentially polluted zones, which offers the advantage of better localizing and identifying the anomalies. This being the main divergence from the previous work on the subject (Birke and Rauch, 1997; Cave et al., 2012; Jarva et al., 2010; Reimann et al., 2005; Reimann and de Caritat, 2017) with taking into account the depth and the made-grounds. However, the fact that data are less representative of the geochemical background for the entire study zone must also be taken into account. While a complete and specific sampling, either random or systematic, dedicated to the geochemical background is not currently feasible in France at the moment, it may be carried out for a handful of samples as a data collection complement (e.g. a random, geographically-stratified sampling). This effort would serve to guarantee an enhanced representativeness of the sectors sampled less (yet excluding zones with a strong anomaly potential, like derelict industrial land).

Moreover, the notion of anomaly varies depending on the working scale. As such, an industrial zone may appear to be an anomaly at the scale of a city while included in the background at the scale of a district. Similarly, a former heavily industrialized region constitutes an anomaly at the scale of a country yet part of the background at the metropolitan scale. Such a dichotomy entails a spatial aspect to the anomaly, whereby the anomaly is correlated with the scope of the study zone. Only those phenomena covering a limited surface area (i.e. < 25% of the zone) may be considered as anomalies. The sampling protocol may influence (through over- or underrepresentation) this relationship in the final data.

4. Conclusion

The use of typical statistical methods (MAD, higher percentile Q90 or Q95, upper whisker) for determining a geochemical background threshold value apply the hypothesis that processed data correspond in the vast majority of instances to the geochemical background and only for a small proportion to anomalies. As for datasets non-dedicated to the background, this hypothesis has still yet to be verified, depending on the working scale and type of sampling employed. In this context, the first step to computing a value for an anthropogenic geochemical background consists therefore of verifying both the spatial representativeness and distribution of this dataset. In cases where the data

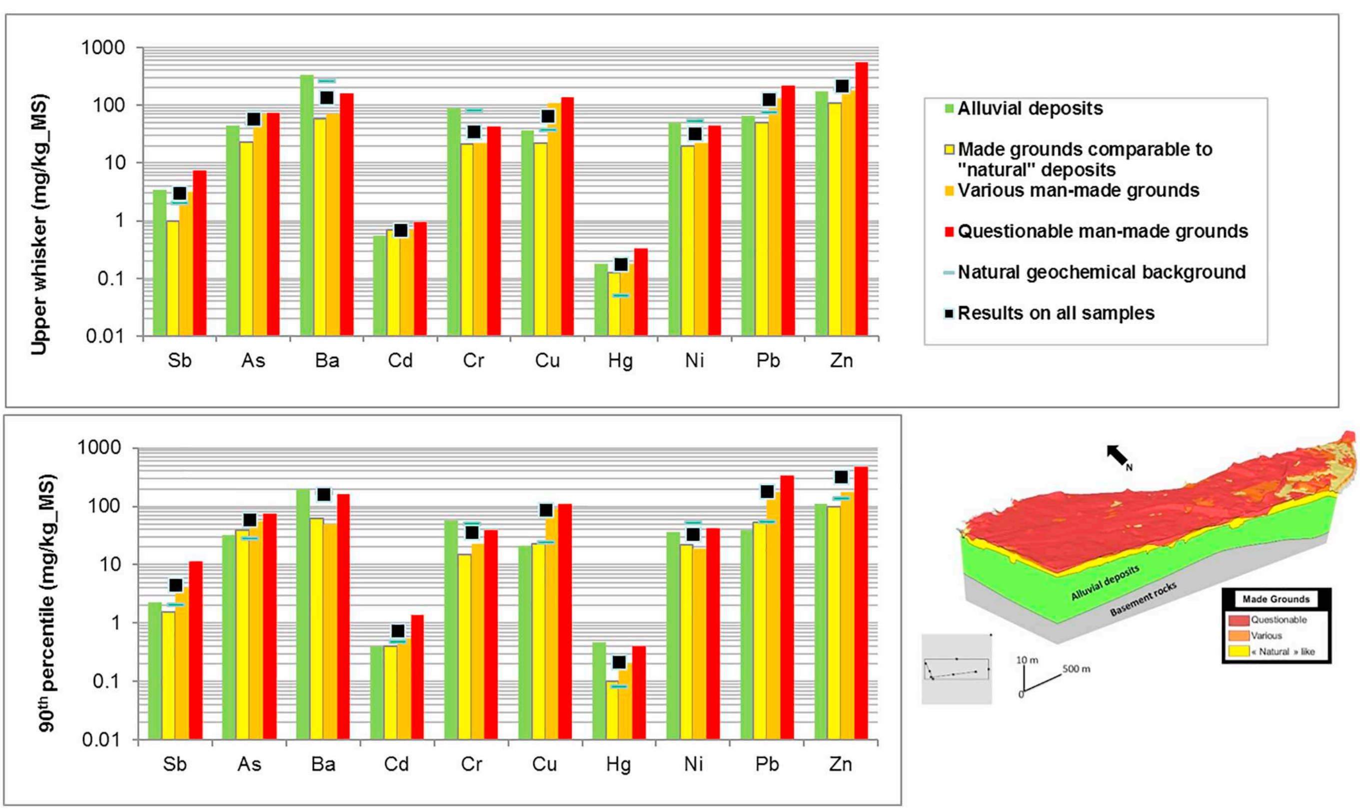


Fig. 10. Thresholds calculated on the case study samples for both the upper whisker and 90th centile methods, relative to the made-ground typology defined in Le Guern et al. (2016). Green marking: Natural geochemical background values (calculated on alluvial samples from a natural zone upstream), black squares: thresholds calculated on all samples, 3D view of the geological model of the district, including the typology employed (modified from Le Guern et al., 2016).

representativeness cannot be guaranteed (e.g. < 15 non-anomalous data points, overly reduced sampling zone), it would be impossible to compute the threshold values.

The mapping of geochemically homogeneous or consistent zones may help evaluate the representativeness of non-dedicated data (e.g. background sampling, overestimation of anomalies) and select, if need be, data that are representative of the geochemical background. For data representative of the zone, the computed threshold values must be accompanied by the dataset size and coverage of the particular zone. In the case of limited data (< 30 samples), it is advised to emphasize the non-binding nature of these threshold values and their inherent uncertainty and to testify the homogeneity of the soils.

The choice of computational method also depends on the objectives associated with the threshold determination. In the case of urban soil data that may have relatively many anomalous values, the MAD threshold will be preferred for reasons of environmental protection since it yields lower thresholds than the other algorithms. On the other hand, the upper whisker provides higher thresholds, which are more oriented toward economic goals by generating reuse opportunities from a greater volume of excavated soil.

Lastly, purely statistical criteria fail to account for the data location, which appears to be essential for the determination of the geochemical background that may vary spatially due to various determinants of urban soils geochemistry. A spatial approach, along with geostatistics, should facilitate the detection of anomalous data and allow mapping the geochemical background. Indeed, the background component can be better isolated from the “anomalies” when considering the scale of the spatial variability of the concentrations.

CRediT authorship contribution statement

Baptiste Sauvaget: Conceptualization, Methodology, Software, Writing - review & editing. **Chantal de Fouquet:** Conceptualization, Methodology, Validation. **Cécile Le Guern:** Conceptualization, Validation. **Jean-François Brunet:** Validation. **Stéphane Belbeze:** Validation. **Hélène Roussel:** Validation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. General case of the uniform distribution

In the case of a uniform distribution on [Zmin, Zmax], the expression of a percentile is:

$$Q_z = (z - Zmin)/(Zmax - Zmin)$$

This expression then yields the following expression of $\mathbf{S_{95}}$:

$$S_{95} = Q_{95} = Zmin + 0.95\,[Zmax - Zmin]$$

In the case of the upper whisker:

- $\mathbf{S_{Whisker}} = Q_{75} + 1.5\,(Q_{75}\text{-}Q_{25})$

with:

$$(Q_{75} - Q_{25}) = Zmin + 0.75\,[Zmax - Zmin] - Zmin + 0.25\,[Zmax - Zmin] = 0.5\,[Zmax - Zmin]$$

$$S_{Whisker} = Zmin + 1.5\,[Zmax - Zmin]$$

For $\mathbf{S_{MAD}}$, since the uniform distribution is symmetrical:

$$\mathbf{MAD} = \text{median}(|X - Q_{50}|) = Q_{75} - Q_{50} = Q_{50} - Q_{25}$$

Leading to:

$$\mathbf{S_{MAD}} = Q_{50} + 2MAD = Q_{50} + Q_{75} - Q_{25}$$

$$\mathbf{S_{MAD}} = Zmin + 0.5\,[Zmax - Zmin] + Zmin + 0.75\,[Zmax - Zmin] - Zmin - 0.25\,[Zmax - Zmin]$$

$$\mathbf{S_{MAD} = Zmin + [Zmax - Zmin]}$$

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