

Analysing the impact of soil spatial sampling on the performances of Digital Soil Mapping models and their evaluation: A numerical experiment on Quantile Random Forest using clay contents obtained from Vis-NIR-SWIR hyperspectral imagery

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| 1 | Analysing the impact of soil spatial sampling on the performances of Digital Soil Mapping |
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| 4 | |
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| 12 | |
| 13 | |
| 14 | Abstract |
| 15 | It has long been acknowledged that the soil spatial samplings used as inputs to DSM models |
| 16 | are strong drivers – and often limiting factors – of the performances of such models. |
| 17 | However, few studies have focused on evaluating this impact and identifying the related |
| 18 | spatial sampling characteristics. In this study, a numerical experiment was conducted on this |
| 19 | topic using the pseudo values of topsoil clay content obtained from an airborne Visible Near |
| 20 | InfraRed-Short Wave InfraRed (Vis-NIR-SWIR) hyperspectral image in the Cap Bon region |
| 21 | (Tunisia) as the source of the spatial sampling. |
| 22 | Twelve thousand DSM models were built by running a Random Forest algorithm from soil |

23 spatial sampling of different sizes and average spacings (from 200 m to 2000 m) and

24 different spatial distributions (from clustered to regularly distributed), aiming to mimic the

various situations encountered when handling legacy data. These DSM models were evaluated with regard to both their prediction performances and their ability to estimate their overall and local uncertainties. Three evaluation methods were applied: a model-based one, a classical model-free one using 25% of the sites removed from the initial soil data, and a reference one using a set of 100,000 independent sites selected by stratified random sampling over the entire region.

31 The results showed that: 1) While, as expected, the performances of the DSM models 32 increased when the spacing of the sample increased, this increase was diminished for the 33 smallest spacing as soon as 50% of the spatially structured variance was captured by the 34 sampling, 2) Sampling that provided complete and even distributions in the geographical 35 space and had as great spread of the target soil property as possible increased the DSM 36 performances, while complete and even sampling distributions in the covariate space had 37 less impacts, 3) Systematic underestimations of the overall uncertainty of DSM models were 38 observed, that were all the more important that the sparse samplings poorly covered the 39 real distribution of the target soil property and that the dense sampling were unevenly 40 distributed in the geographical space, 4) The local uncertainties were underestimated for 41 sparse sampling and over-estimated for dense sampling while being sensitive to the same 42 sampling characteristics as overall uncertainty.

Such finding have practical outcomes on sampling strategies and DSM model evaluation that
are discussed.

45 Keywords

46 Uncertainty, sampling methods, spatial distribution indicators, Quantile Random Forest

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49 **1.** Introduction

50 Digital Soil Mapping has now emerged as a credible solution for providing soil data to 51 decision-makers acting at global or local scales. Following the GlobalSoilMap specifications 52 (Arrouays et al., 2014), a significant number of countries across the world are now covered 53 by a high-resolution (90-m) grid documented with estimates of soil properties and their 54 associated prediction uncertainties. To obtain this spatial soil information, Digital Soil 55 Mapping models relating the targeted soil properties with exhaustively available covariates 56 were built by running learning algorithms onto spatial sampling of available legacy soil 57 profiles with measured soil properties. Numerous different algorithms have been proposed, 58 mainly depending on the availability and type of soil data (e.g. point data (profiles, 59 augerings), soil maps with various scales and detailed legends) and on the availability of 60 covariates (Minasny and McBratney, 2010).

61 It has been largely acknowledged that the main limitation of such digital models is the 62 spatial sampling of the legacy measured soil profiles. The average spacing of such soil spatial 63 sampling used in most operational DSM applications have been very large, e.g. 28 km (Hengl 64 et al., 2017) and 5.5 km (Mulder et al., 2016). Furthermore, these soils' spatial samplings 65 have been constituted by the soil profiles of the different existing soil surveys within the 66 mapped area, which means that their locations were not specifically selected for a DSM 67 application and are often clustered at a few sub-areas of the study region, with large sub-68 areas without any soil information. Consequently, the performances of soil predictions are 69 often severely limited, especially for soil properties whose pattern of variation is largely 70 below the soil profiles' spacing (Vaysse and Lagacherie, 2016; Gomez and Coulouma, 2018). 71 One way to increase DSM performance is therefore to increase the average densities and 72 improve the spatial distribution of the measured soil profiles (Voltz et al., submitted).

Because of their high cost of acquisition, such new locations should be selected with care. For that, the prerequisites are: i) to accurately evaluate the uncertainty of the current soil property maps made from the unevenly distributed legacy measured soil profiles, ii) to determine the expected gain of an increase in the average spatial sampling densities and iii) to identify the spatial sampling characteristics that should be considered in the sampling strategies. These three prerequisites will be examined in this paper and are successively evoked in the following.

80 The uncertainty evaluation of the soil property maps is an intrinsic part of a DSM application. 81 This was theorized very early (McBratney et al., 2003) and translated into specifications in 82 the GlobalSoilMap project (Arrouays et al., 2014). Although there exist guidelines for the 83 assessment of uncertainty of Digital Soil Maps (Heuvelink, 2014), their practical application is 84 not straightforward, which makes the uncertainty evaluation itself uncertain. The spatial 85 sampling from which uncertainty is evaluated is a crucial point: the probability sampling that 86 is advocated to obtain an unbiased estimate of uncertainty (Brus et al., 2011) cannot be 87 obtained with the already fixed legacy soil data locations. Furthermore, uncertain 88 estimations of the uncertainty of soil maps can be non-negligible even when using 89 independent probability sampling (Kempen et al., 2011, Lagacherie et al., 2019). Lastly, it is 90 uncertain that the set of locations used as evaluation data well describes the real pattern of 91 the soil cover that is to be mapped, especially the short-range variations. For all of these 92 reasons, determining the uncertainty of a DSM map is still an open question.

Although there has been a large consensus in the DSM community that the density of soil
data is a clear limiting factor for DSM (Lagacherie, 2008), few experiments showing their
impacts on DSM mapping performances exist in the literature. Somarathna et al. (2017) and
Wadoux et al. (2019) both observed an increase in the performances of Soil Carbon Mapping

97 as the amount of input data increased, regardless the algorithms used to build the DSM 98 models. However, Somarathna et al. (2017) observed that this increase in performances was 99 lower for the highest sampling densities, which may suggest that, beyond a given threshold 100 of density, it would not be worthwhile to add further new locations. Such a threshold was 101 not observed by Wadoux et al. (2019), which means that it should be highly case-dependent. 102 More case studies should therefore be studied to gain expertise regarding fixing this 103 threshold.

104 Apart from their average densities, the soil spatial samplings may vary with regard to their 105 spatial distribution across the study areas, which may also strongly affect the prediction 106 performances of the DSM models that use such data as input. This was acknowledged early 107 on (Brus and de Gruijter, 1993), and sampling algorithms for optimizing the completeness 108 and evenness of the input soil locations within the geographical space (Brus et al., 2007) or 109 soil covariate space (Minasny and McBratney, 2006) have been proposed. Similarly, Zhang 110 and Zhu (2019) observed a slight increase in DSM performances when the spatial sampling 111 was optimized with regard to its representativeness of the distribution of the soil covariates. 112 Lark and Marchant (2018) showed that geostatistical predictions can be improved by adding 113 10% of the closely spaced locations to regular sampling to better represent the short-range 114 spatial structures. Finally, Adamchuk et al. (2011) improved the soil property predictions 115 from soil sensors by developing a sampling strategy that considered the spread among 116 sensor output, the local homogeneity and the physical coverage across an entire field as 117 target spatial sampling properties. All of these works converge towards the idea that 118 sampling strategies can be leveraged to increase DSM performances. However, a recent 119 experiment (Wadoux et al., 2019) showed that this increase could not be obtained by some

sampling strategies, which means that the benefit of sampling strategies could be highlycase-dependent.

122 This paper presents a numerical experiment that relates the characteristics of legacy spatial 123 samplings used as input soil data (spatial density and spatial distribution characteristics) with 124 the DSM performance and the accuracy of their ex-ante evaluation. The study used the 125 pattern of the topsoil pseudo clay content derived from airborne Visible Near InfraRed-Short 126 Wave InfraRed (Vis-NIR-SWIR) hyperspectral data acquired over the Cap Bon region (300 127 km², Tunisia) at five-metre resolution (Gomez et al., 2012). This pattern is composed of well-128 predicted clay values ($R^2 = 0.75$) that are free of visible artefacts and pedologically plausible, 129 which allows it to be considered as a fair representation of the variations of a real soil 130 property across the landscape (Lagacherie et al., 2019). Such a soil dataset provided a quasi-131 unlimited number of pseudo-measured sites, which enabled the testing of a large number 132 (12,000) of spatial samplings. These spatial samplings were used as input data for a Quantile 133 Random Forest algorithm that produced DSM models whose performances in predicting clay 134 values and the associated accuracy were analysed with regard to the sampling 135 characteristics.

136

137

Insert figure 1 here

138 **2.** Case study

139

140 This case study has already been described in a previous paper (Lagacherie et al., 2019).

141 Large excerpts of this paper are used in the following.

142 2.1. The study area

143 The study area is in the Cap Bon region in northern Tunisia (36°24'N to 36°53'N; 10°20'E to 144 10°58'E), which is 60 km east of Tunis (Figure 1a). This 300-km² area includes the Lebna 145 catchment, which is mainly rural (>90%). The Lebna catchment is devoted to the cultivation 146 of cereals in addition to legumes, olive trees, vineyards and natural vegetation for animals. 147 The region is characterized by its rolling hills and elevations between 0 and 226 m. The 148 climate varies from humid to semi-arid, with an inter-annual precipitation of 600 mm and an 149 inter-annual potential evapotranspiration of 1500 mm. The soil pattern of the Lebna 150 catchment is mainly the result of variations in lithology. The variations in the bedrock 151 between Miocene sandstone and Marl cause large variations in the physical and chemical 152 soil properties (Zante et al., 2005). Furthermore, the distance between successive sandstone 153 outcrops decreases significantly as the terrain changes from the ocean to the mountains, 154 which also causes variations in the soil property patterns (Gomez et al., 2012). The soil 155 materials were redistributed laterally along the slopes during the Holocene, which adds to 156 the complexity of the soil pattern. The main soil types are Regosols (IUSS working group 157 WRB, 2006), which are preferentially associated with sandstone outcrops, and Calcic 158 Cambisols and Vertisols, which preferentially formed on marl outcrops and lowlands. The 159 south-eastern region of the study area has a flatter landscape with sandy Pliocene deposits 160 in which Calcosols and Rendzinas prevail.

161

162 2.2. Data

163

164 2.2.1. Hyperspectral image and derived topsoil clay content predictions

The numerical experiment uses an image of topsoil clay content as input. The topsoil clay contents were derived from a Vis-NIR-SWIR hyperspectral image (Gomez et al., 2012). The approach used to produce the data is summarized below. More details regarding the preand post-processing of the hyperspectral image can be found in Gomez et al. (2012).

170 On November 2, 2010, AISA-Dual airborne-based hyperspectral data were acquired over the 171 study area with a spatial resolution of 5 m. The area of the image is approximately 12 km x 172 24 km. The AISA-Dual spectrometer measured the reflected radiance via 359 non-contiguous 173 bands covering the 400- to 2450-nm spectral range, with 4.6-nm bandwidths between 400 174 and 970 nm and 6.5-nm bandwidths between 970 and 2450 nm. The radiance units were 175 converted to reflectance units using ASD spectrometer measurements of uniform surfaces (parking lots, asphalt, concrete) that were collected at the same time during the over flight. 176 177 Topographical corrections were performed using a digital elevation model built from ASTER 178 data and ground control points.

To isolate the bare soil areas, the study masked pixels with normalized difference vegetation index (NDVI) values greater than an expert-calibrated threshold (0.20). Water and Urban areas were also removed. Finally, the bare soil represented 46.3% of our study area, that is, 5,889,847 measured AISA-Dual 5-m x 5-m pixels.

A Partial Least Square Regression (PLSR) technique (e.g. Tenenhaus, 1998) was then applied to estimate the topsoil clay contents from AISA-DUAL reflectance at each location. The PLSR was calibrated from 129 couples of AISA-DUAL Vis-NIR-SWIR reflectance spectra on bare soil surfaces associated with the topsoil clay content measured on a laboratory soil sample collected from the same bare soil surfaces. Before the PLSR model was built, the reflectance was converted into "absorbance" (log [1/reflectance]). In addition, a Savitzky–Golay filter with second-order polynomial smoothing and window widths of 30 nm (Savitzky and Golay,

190 1964) and a mean centring and variance scaling was applied to the spectra to reduce noise. 191 The calibrated PLSR model was then validated using a leave-one-out cross-validation that 192 showed successful predictions (R² = 0.75, Gomez et al., 2012, figure 3). The PLSR model was 193 then applied to all bare soil pixels to estimate the topsoil clay content, thus providing the 194 final predicted topsoil clay properties map (Figure 1b). These treatments were implemented 195 in R (Version 1.17) using the signal and pls packages (Mevik and Wehrens, 2007).

196

197 2.2.2. Digital Elevation Model and derivatives

198

A 30-m ASTER digital elevation model (DEM) with specific ortho-rectification and mosaicking was produced for this area. The classical geomorphometric indicators found in the DSM literature were calculated. These include Elevation, Slope, Aspect, plan Curvature, Profile Curvature, Multi-Resolution Valley Bottom Flatness (MRVBF) and four variables describing the aspect: northness, easterness, northwesterness, and northeasterness. All of these indicators served as covariate candidates for representing the relationships between clay content and the relief.

206

207 2.2.3. Tunisian agriculture map

A set of layers of the Tunisian agriculture map (STUDI-SCOT-SODETEG, 2001) at 1:20,000 scale was considered as covariates. This includes two soil properties, soil colour classes and textural classes, which were mapped by considering existing detailed soil maps completed by manual interpretation of remote sensing images. The other covariates extracted from the Tunisian agriculture map were the parent material (14 classes) and the land use (7 classes).

213

214 2.2.4. Indices from Sentinel-2 images

216 Three spectral indices were used in this work, based on a Sentinel-2 image acquired on the 2nd of November 2016 over the study area. The acquisition date of Sentinel-2 data was 217 218 chosen to fit in the period of more extensive bare soils. Sentinel-2 data are composed by 219 multispectral data in 13 bands covering the Visible, Near InfraRed and Short Wave InfraRed 220 spectral domain with spatial resolutions ranging from 10 to 60 m. The Sentinel-2 data 221 acquired on the 2nd of November 2016 was downloaded from the Muscate platform of the 222 French land data centre, called Theia (https://www.theia-land.fr/) in Level 2A, i.e., corrected 223 from atmospheric effects, thanks to the three bands acquired at 60-m spatial resolution 224 (coastal at 443 nm, water vapour at 1375-nm atmospheric correction, coastal at 443 nm, and 225 cirrus at 1376 nm). The three spectral indices used in this work were the normalized 226 difference vegetation index (NDVI), Redness index (RI) and Colour index (CI), calculated 227 following Pouget et al. (1990) and Ghodalizeh et al. (2016):

228
$$NDVI = \frac{(B8-B4)}{(B8+B4)}$$
 [1]

229
$$CI = \frac{B4^2}{B3^3}$$
 [2]

230
$$RI = \frac{(B4-B3)}{(B4+B3)}$$
 [3]

where B8, B4 and B3 are the spectral bands centred at 842 nm, 665 nm, and 490 nm,respectively.

NDVI was selected as a proxy of the vegetation health and biomass that could be in relation
with topsoil clay contents through the water and nutriment retention properties. CI and RI
were selected as proxies of topsoil colour that could be related to clay content through
different parent materials.

237 3. **Methods**

215

238 3.1. DSM modelling

Three criteria were considered to select the learning algorithm used to produce the DSM models: i) the algorithm should be one of the most used and the most efficient among the recent DSM applications, ii) the algorithm had to provide local uncertainty predictions to be able to test its ability to predict the associated uncertainty, and iii) the algorithm should be run without manual intervention and repeated a great number of times in the numerical experiment. Combining these three criteria resulted in selecting the Quantile Regression Forest as the learning algorithm used in this study.

246 Recent performance testing has found that the Random Forest, from which the Quantile 247 Regression Forest is derived, was among the best algorithm for obtaining predictions of soil 248 properties (Nussbaum et al., 2017), which confirmed a test performed on a wider range of 249 machine learning applications (Caruana et al., 2006). The Quantile Regression Forest has also 250 been demonstrated as efficient for predicting the uncertainty associated with soil property 251 predictions (Vaysse and Lagacherie, 2017). Finally, many authors have adopted this machine 252 learning algorithm for recent large-scale DSM applications (Hengl et al., 2017; Roman 253 Dobarco et al., 2019).

254

255

3.1.1. Random Forests and Quantile Regression Forests

This section summarizes the main characteristics of Random Forests and Quantile Regression Forests, using excerpts of Meinshausen (2006). It was already presented in Lagacherie et al. (2019). More details on these two machine learning algorithms are given in the seminal papers by Breiman et al. (2001) and Meinshausen (2006), respectively.

Let Y be a real-valued response variable and X be a covariate or predictor variable that is likely high-dimensional. A standard goal of statistical analysis is to infer the relationship between Y and X. Random Forests grow a large (>500) ensemble of trees using n

263 independent observations (Y_i , X_i), i = 1, ..., n. Each tree grows via a recursive partitioning of 264 the source set using one predictor variable *X*. At each step, the source set is split into two 265 subsets following a test on the value of *X*. When *Y* is a quantitative variable, the selected test 266 is the one that minimizes the within-subset variance of *Y* (Breiman et al., 1984). The 267 recursive partitioning is limited by a stopping rule, and the subsets are produced by the last 268 split being the leaves of the tree. The ensemble of trees is produced by using a random 269 sample of the training data and a random subset of the predictor variables for each tree.

For the regression, the prediction $\hat{Y}_{\theta}(x)$ of a single tree ?? of a Random Forest for a new data point x can be represented as the weighted average of the original observations Y_{i} , i = 1, \dots , n:

273

274
$$\hat{Y}_{\theta}(x) = \sum_{i=1}^{n} w_{\theta i}(x, \theta) Y_{i}$$
[4]

275

where $w_{\theta i}(x, \theta)$ is the weight vector given by a positive constant that is 1 if the observation Y_i is part of the same leaf and 0 otherwise.

278 By using Random Forests, the prediction is the average prediction of *k* single trees that were 279 constructed as described above.

281
$$\widehat{Y_T}(x) = \sum_{i=1}^n w_{Ti}(x)Y_i$$

280

282 with
$$w_{Ti}(x) = k^{-1} \sum_{t=1}^{k} w_{\theta i}(x, \theta)$$
 [6]

283

284 One could assume that the weighted observations deliver a good approximation not only of

[5]

the conditional mean but also of the full conditional distribution. This assumption is at the heart of the Quantile Regression Forest algorithm, which estimates the conditional distribution function of *Y* given *x* via:

288

289
$$\widehat{F}(y|x) = \sum_{i=1}^{n} w_i(x) \mathbf{1}_{\{Y_i \le y\}}$$
[7]

290

From this conditional distribution, it is possible to derive both the predicted value (the mean) and the bound of the 90% prediction interval that predicts the associated uncertainty (the 0.05 and 0.95 quantiles).

Numerous implementations of RF and QRF now exist. Ranger Package (Wright and Ziegler,
2017) was selected because it is a fast implementation of Random Forests that is suitable for
multiple model building.

297

298 3.1.2. Tuning Random Forest Parameters

299 The Random Forest Algorithm has several hyperparameters that must be set by the user. 300 Among them, three parameters may significantly impact the results and therefore should be 301 tuned to improve the predictions (Probst et al., 2018): i) the number of observations drawn 302 randomly for each tree, ii) the number of variables drawn randomly for each split and iii) the 303 minimum number of samples that a node must contain. These parameters were tuned using 304 one of the most established tuning strategies, sequential model-based optimization (Jones 305 et al., 1998; Hutter et al., 2011). This tuning algorithm iteratively uses the results of the 306 different already evaluated hyperparameter values and chooses future hyperparameters 307 based on these results. It is implemented in the TuneRanger Package (Probst et al., 2018). 308 After some trials, 100 iterations appeared to be a good compromise that ensured a fairly 309 good convergence towards an optimized solution while being acceptable in terms of 310 computing costs. 311 312 Insert figure 2 here 313 314 3.2. The numerical experiment 315 3.2.1. General approach 316 317 The workflow of the numerical experiment is presented in Figure 2. First, a master 318 evaluation set of 100,000 locations with pseudo values of clay content was randomly 319 selected from the total set of pixels. This master set served to determine the real 320 performances of the tested models through a set of indicators described further in 3.2.3. 321 The remaining locations were used to build and evaluate 12,000 models, i.e., 1,000 models 322 for each of the 12 considered sample sizes (100, 200, 300, 400, 500, 600, 800, 1,000, 2,000, 323 3,000, 5,000, and 10,000 locations), each corresponding to a given average spacing (1732 m, 324 1225 m, 1000 m, 866 m, 775 m, 707 m, 612 m, 548 m, 387 m, 316 m, 245 m and 173 m) 325 using the following equation:

326
$$average \ spacing = \sqrt{\frac{total \ area}{size}}$$
.

327

For a given average spacing, the soil inputs of the 1000 models were selected by a specific sampling procedure (see the next section) that mimicked the more or less uneven spatial distributions observed when using legacy data as soil inputs. The soil inputs were then randomly divided into two sets, keeping 75% of the locations to produce DSM models using the QRF algorithm and 25% to obtain a so-called independent evaluation set as currently

[8]

333 practised in DSM applications. The DSM models were obtained using QRF according to the 334 method presented above and then evaluated from the independent datasets. The same 335 performance indicators used for the master set were considered to enable statistical 336 comparisons.

337

338

Insert figure 3 here

- 339
- 340 3.2.2. The sampling procedure

The sampling procedure was designed to randomly produce spatial samplings with contrasting degrees of unevenness. The study area was first stratified into 25 geographical strata of equal area using a K-means classification of the locations (Walvoort et al., 2010). Then, the following algorithm was applied:

- 345 1) Define a given size of sampling N
- 346 2) Select at random an integer P between 1 and 25 (the number of strata) and select at
- random P strata among the 25
- 348 3) Select N/2 locations by a stratified random sampling, using the P strata selected in
 349 step 2
- 350 4) Complete the spatial sampling by N/2 locations selected at random over the entire351 study area

For a given size N, steps 2 through 4 were repeated 1,000 times to obtain 1,000 spatial sampling that differed in unevenness thanks to different random selections of P. The procedure was repeated for each selected sample size.

355 Figure 3 shows four examples of different spatial samplings provided by this procedure.

357 3.2.3. Model performance indicators

Four model performance indicators were considered. The first two were the Mean Square Error (MSE) and the 90% Prediction Interval Coverage probability (PICP90), which were calculated using the master evaluation set of 100,000 sites.

361
$$MSE_{ref} = \frac{1}{n} \cdot (\hat{y}_i - y_i)^2$$
[9]

362 with \hat{y}_i as the predicted value, y_i as the observed value of Clay, and n = 100,000

363

364 PICP90 =
$$\frac{1}{n}$$
 . card $(\{\hat{y}_i \ge y_{\text{pred05}} \text{ and } \hat{y}_i \le y_{\text{pred95}}\})^2$ [10]

with y_{pred05} and y_{pred95} as the lower and upper bounds of the predicted 90% confidence interval PICP90 expressing the probability that all observed values fit within the 90% prediction limits provided by the DSM model.

The last two indicators aimed to quantify the relative errors of Mean Square Error provided either by the QRF algorithm as a by-product (MSE_{mod}) or by removing 25% of the soil inputs taken as an independent evaluation set (MSE_{rmv}). To calculate these errors, the MSE calculated on the master evaluation (MSE_{ref}) set served as a reference.

$$372 \qquad \qquad Err_{mod} = \frac{MSE_{mod} - MSE_{ref}}{MSE_{ref}} \qquad [11]$$

373
$$Err_{rmv} = \frac{MSE_{rmv} - MSE_{ref}}{MSE_{ref}}$$
[12]

374

375 3.2.4. The Spatial sampling indicators

376 Several spatial sampling indicators quantifying the characteristics of the spatial distributions 377 of the tested spatial sampling were calculated as candidates to explain the performances of 378 the model summarized by the performance indicator presented above. The first three 379 indicators (Coverage Index, Kullback-Leibler Divergence and percentage of out of range) 380 were calculated in the covariate space, in the geographical space and with regard to the 381 target variable (Clay content). The last two (variance and spatially structured-Variance ratio) 382 were calculated for Clay content only. These indicators are detailed below.

383

384 Coverage index

The Coverage index (CI) (Gunzburer and Burkdart, 2004) expresses the degree of unevenness
of the spatial distribution of the locations of the spatial sampling.

387
$$CI = \sqrt{\frac{1}{\bar{d}} \left(\frac{1}{n} \sum_{i=1}^{n} (d_i - \bar{d})^2\right)}$$
 [13]

with d_i the distance of site *i* to its nearest neighbour and \overline{d} the mean value of the d_i

389 Note that, for a regular mesh, CI = 0. Then, a small value of CI means that the spatial 390 sampling has a spatial distribution close to that of a regular grid. The R package DiceDesign 391 (Dupuy et al., 2015) was used to calculate CI.

392

393 Kullback-Leibler Divergence (KLD)

The Kullback-Leibler divergence (KLD) (Kullback and Leibler, 1951) measures how close two probability distributions are. It was used here to measure the distance between the calibration or evaluation sets and the master validation set. It is a measurement of the representativeness of the calibration and validation sets with regard to the master validation set, which is assumed to represent the real distribution of the different variables across the study region.

400 For distributions P and Q defined in the same probability space, the Kullback–Leibler
401 divergence between P and Qis defined to be (Wikipedia,
402 https://fr.wikipedia.org/wiki/Divergence_de_Kullback-Leibler)

403
$$KLD(P||Q) = -\sum_{x \in X} P(x) \cdot \log\left(\frac{Q(x)}{P(x)}\right)$$
[14]

404 For distributions P and Q of continuous random variables, the Kullback–Leibler divergence is

405
$$KLD(P||Q) = \int_{-\infty}^{\infty} p(x) \log\left(\frac{q(x)}{p(x)}\right)$$
[15]

406 The KLDs are first calculated for each variable and then averaged to obtain a unique value407 for the geographical and the covariate spaces.

408

409 Percentage of out of range

The percentage of out of range measures the proportion of locations of the study region having values of variables (in the covariates space, the geographical space of Clay values) that are out of the range of those of the sites included in the calibration or evaluation sets. It is also a measurement of representativeness but differs from the former due to its focus on extreme values.

415

416
$$\%Out_of_Range = \frac{card(\{y_i < \min_p y \& y_i > \max_p y\})}{card(R)}$$
[16]

417 with *P* the calibration or evaluation sets and *R* the set of locations in the study region

418

419 Clay Variance and percentage of spatially structured variance ratio

420 Variance of clay is a measure of dispersion within the calibration or validation dataset with421 regard to clay values.

422 A spatially structured variance ratio (SSVR) was proposed by Vaysse and Lagacherie (2015) as

423 the complement to 1 of the nugget-to-sill ratio (Kerry and Oliver, 2008). It indicates the

424 proportion of the spatially structured variance that is captured by the model.

426 SSVR = variance – nugget / variance. [17]

| 428 | Because it was impossible to fit variograms on 12,000 trials, the nugget could not be |
|-----|--|
| 429 | calculated directly. It was therefore approximated by computing the semi-variances at lags |
| 430 | centred on the average spacing ([average spacing – 100 metres, average spacing + 100 |
| 431 | metres]) |
| 432 | |
| 433 | Insert figure 4 here |
| 434 | |
| 435 | 4. Results |
| 436 | 4.1. Impact of average spacing |
| 437 | Figures 4a through 4d show the evolution of the different indicators of DSM performances |
| 438 | with the average spacing (Equation 8). The Mean Square error on the predicted Clay value |
| 439 | (MSE $_{ref}$) covered a large range of values across the 12,000 models (Figure 4a). These values |
| 440 | increased regularly with the average spacing: from MSE = 7,911 g^2 .kg ⁻² (68% of explained |
| 441 | variance) to MSE = 18,882 $g^2 kg^{-2}$ (22% of explained variance). The amount of variation of |
| 442 | MSE _{ref} for a given size of sampling also increased regularly with the average spacing. |
| 443 | PICP90 exhibited a positive bias (overestimated uncertainty) with regard to the expected |
| 444 | 90% value for the smallest average spacings (below 612 m) and a negative one |
| 445 | (underestimated uncertainty) beyond this threshold (Figure 4b). However, the errors were |
| 446 | only important (more than 1%) for the largest average spacing (- 2.5% for 1732 m) and for |
| 447 | the smallest ones (between 1.2 and 1.7 for average spacing at and below 316 m). Apart from |
| 448 | the influence of the average sampling variations, great variabilities of performances for |

449 PICP90 estimations were observed for the largest average spacings (see the bars of Figure450 4b).

451 The bagging procedure of the QRF algorithm and the external evaluation using 25% of 452 removed sites both had a negative bias (Figures 4c and 4d) regardless of the average 453 spacing, which revealed systematic underestimations of the overall uncertainty of the DSM 454 models (e.g., -17% and -10% respectively for 1732-m spacing). This bias seemed not as 455 closely related to the average spacing of sites as was observed previously for the other 456 indicators, although slight decreases could be observed beyond 866-m spacing. The most 457 important variations were observed within each sampling size, as shown by the large bars of 458 Figures 4c and 4d.

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Insert figure 5 here

461

462 4.2. The impacts of the spatial distributions of sites

The matrices of Figures 5a through 5d show, for each average spacing (the columns of the matrices), the correlations between the spatial sampling indicators (lines of the matrices) and the indicators of DSM performance (one matrix per indicator). The last lines of the matrices show the coefficients of determination of the stepwise regressions between the indicator of performance of interest and the set of indicators of spatial sampling, which allowed the strength of the relation between these two types of indicators to be appreciated.

Whatever the considered DSM performance indicators, the correlation coefficients were highly variable with regard to the spatial sampling indicators and the average spacing (between 0.00 to 0.91). These coefficients tended to increase with the decrease of average

spacing, which is summarized by the increase in the strength of the relation between the
indicators of performance and the spatial sampling indicators (last lines of the matrices).
However, some noticeable exceptions occurred for some relations between performance
indicators and spatial sampling indicators.

477 MSE_{ref} (Figure 5a), which expressed the ability of the DSM models to predict the correct 478 value of clay content, was strongly positively correlated with the coverage_index and 479 Kullback-Leibler divergence calculated in the geographical space, which means that the 480 performances of the DSM models were better for evenly geographically distributed and 481 representative spatial samplings. These correlations increased greatly when average spacing 482 decreased (until - 0.87 for the two indicators) but were already substantial for the largest 483 spacing (-0.42 and -0.38). For all of the tested average spacings, MSE_{ref} was also moderately 484 correlated with Variance Clay and %-out-of-range Clay (between 0.27 and 0.40 and 485 between – 0.27 and -0.56, respectively). This means that the performances of the DSM 486 models tended to increase as the clay values included in the spatial sampling were largely 487 dispersed, and this well covered the range of clay values of the study region. The three 488 indicators calculated in the covariate space were only significantly correlated with MSE_{ref} for 489 the smallest average spacings. Furthermore, these correlations were always smaller than 490 those obtained by the same indicators calculated in the geographical space. Finally, the 491 spatially structured variance ratio (SSVR) exhibited moderate negative correlations for 492 intermediate values of average spacing (between -0.27 and -0.42), which means that, for 493 these values, the more the spatially structured variability (especially the short range one) 494 was captured by the spatial sampling, the better the performances were.

495 PICP90, Err_{mod} and Err_{rmv} (Figures 5b, 5c and 5d), which all expressed the ability to predict 496 the uncertainty associated with the predicted values given by the DSM models, behaved

497 similarly to each other with regard to the correlations with the spatial sampling indicators, 498 with however stronger overall correlations for Err_{rmv} than for PICP90 and for Err_{mod} than 499 for Err_{rmv} (see the stepwise regression coefficient, the last lines of the matrices in Figures 500 5b, 5c and 5d). Contrary to MSE_{ref}, clear differences of correlation rankings were observed 501 between the smallest and the largest average spacings. As far as the former are concerned, 502 PICP90, Err_{mod} and Err_{rmv} were predominantly correlated with Variance_Clay and %-out-503 of-range_Clay (between 0.46 and 0.76 and between -0.38 and -0.62, respectively, for 504 average spacing larger than or equal to 866 m). This means that the uncertainty was much 505 better predicted when the clay values included in the spatial sampling were highly dispersed 506 and covered well the range of clay values of the study region. At the smallest spacings, the 507 strongest correlations were observed with the coverage_index and Kullback-Leibler 508 divergence calculated in the geographical space (between -0.49 and -0.88 and between -0.48 509 and - 0.85, respectively, for average spacing smaller than or equal to 387 m), which means 510 that evenly geographically distributed and representative spatial samplings enabled an 511 accurate prediction of the DSM model uncertainty. The spatial sampling indicators 512 calculated on the covariate space only exhibited substantial correlations with PICP90, 513 Err_{mod} and Err_{rmv} at the smallest spacings. Finally, SSVR exhibited substantial correlations 514 only for PICP90 (between 0.33 and 0.45).

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Insert figure 6 here

517

518 5. Discussion

519 5.1. The impact of the average spacing

520 All of the results confirmed that the average spacing, related with the size of the calibration 521 data sets used as input for the DSM approach, strongly impacted the results of a DSM 522 approach. As already observed by Somarathna et al. (2017) and Wadoux et al. (2019), we 523 observed (Figure 4a) a clear decrease of prediction errors (MSE_{ref}) when the average spacing 524 is decreasing. It should be noticed that, thanks to the use of pseudo-values of clay content 525 given by the hyperspectral image, we explored a more complete range of average spacing, 526 which allowed us to analyse a larger range of model performances (from 22% to 68% of 527 explained variance) that covered fairly well the ones cited in the literature. Figure 4a 528 revealed that the decrease of prediction errors with average spacing was not linear. By 529 substituting the average spacing X axis of Figure 4a by the spatially structured variance ratio 530 (SSVR, see section 3.2.4), a new insight into this average proportion of clay variance was 531 revealed (Figure 6): for the largest average spacing, that captured the least spatially 532 structured variance (<= 800 sites, average spacing = 707 m), the average increase in 533 performances was perfectly linear, whereas further increases of this ratio provided gains 534 that were smaller and smaller than the previously observed linear trend. Therefore, this 535 observed threshold separated two contrasting situations: below the threshold of average 536 spacing of 707 m, the spacing of sampled sites was the only limiting factor, while beyond the 537 threshold, other limiting factors, such as the precision of the covariates, also played a role in 538 the quality of the results. This contrasting behaviour could explain why contradictory results 539 have been obtained recently regarding the impact of the spatially structured variance ratio 540 on DSM results, as observed by Vaysse and Lagacherie (2015) and not observed by 541 Nussbaum et al. (2017). It may also explain why improving a covariate dataset often do not significantly improve the DSM products when overly sparse test datasets are used to 542 543 calibrate the DSM model (Samuel-Rosa et al., 2015; Loiseau et al., 2019).

544 Apart from its influence on the prediction error, the average spacing of sites also had an 545 impact on the estimations of the associated uncertainty, which, to our knowledge, has not 546 been observed before. Decreasing the average spacing reduced the underestimation of the 547 overall uncertainty provided either by the bagging procedure of the Random Forest (Figure 548 4c) or the model-free evaluation process (Figure 4d), although these reductions were not as 549 clear and regular as the prediction error because larger variabilities of results were observed 550 within each tested spacing (see the error bars in Figures 4c and 4d). A more complex 551 behaviour was observed for the local estimation of the confidence interval by the model 552 tested by PICP90 (Figure 4b). For the largest spacings, PICP90 estimates converged towards 553 the nominal value of the confidence interval (90%) as the spacing decreased, whereas for 554 the smallest spacings, PICP90 moved away from this nominal value. This latter unexpected 555 result could be interpreted as the inclusion of outliers as the spacing decreased, which could 556 perturb the estimates of the confidence interval bounds. It must be noticed that, as for the 557 estimations of the overall uncertainty evoked before, a large variability in estimating PICP90 558 was observed within each tested spacing.

559 Finally, a final effect of the spatial sampling size is that it changes the amount and the drivers 560 of the variations of performances observed within each sampling size. This will be developed 561 in the next section.

562

563 5.2. The impact of the distribution of sites over the study region

The bars on Figures 4a through 4d show that the average spacing is not the only driver of DSM performance, especially with regard to the ability of DSM approaches to estimate overall (Figures 4 c and 4 d) and local uncertainties (Figure 4b). The matrices of Figure 5 confirmed many of the underlying hypotheses of the sampling strategies that have been 568 proposed in the literature while providing new insights on the relation between spatial 569 sampling and uncertainty estimation and nuancing the importance of some sampling 570 characteristics according to the size of the spatial sampling.

571 From the matrices of Figure 5, it clearly appeared that the regularity of sampling and the 572 representativeness in the geographical space improved the DSM results whatever the size of 573 the spatial sampling and the considered indicators of performances. Therefore, the legacy 574 soil data that are often characterized by both under-sampled and over-sampled sub-regions 575 should be ideally completed using sampling strategies that could mitigate this irregularity of 576 sampling in the geographical space (Brus et al., 2011; Adamchuk et al., 2011). This would 577 require harmonizing the legacy and the new dataset techniques for removing biases caused 578 by differences of dates, field protocols and laboratory methods (Baume et al., 2011; 579 Ciampalini et al., 2013). An alternative to adding samples should be to better take into 580 consideration in the DSM modelling the perturbing effects of the clusters of sites. This could 581 be done by assigning different weights to the input sites according to their degree of 582 remoteness (Bel et al., 2009), applying resampling techniques (Richer-de-Forges et al., 2017; 583 Taghizadeh-Merjadhi et al., 2020) or restricting the predictions inferred from each cluster of 584 sites to representative areas corresponding to well-identified and well-mapped soil systems 585 (Lagacherie et al., 2001).

The spread of the spatial sampling with regard to the values of the target soil property (%out-of-range and variance of Clay in Figure 5) also seemed crucial for improving both the predictions of the soil property and the predictions of the associated overall and local uncertainties. However, correcting the existing legacy sample with regard to this characteristic is an uneasy task because it requires additional knowledge to anticipate the locations of the extreme values of the targeted soil property that should be preferentially

592 sampled. A local pedological knowledge or a proxy of the soil property of interest593 (Adamchuk et al., 2011) could be mobilized for that.

594 It is interesting to note that the sampling characteristics that involved the soil covariates 595 only had an impact on the results for the smallest spacing of spatial sampling. In these cases, 596 this impact was increased by strong relationships established between the covariates and 597 the predicted soil property, whereas for the largest spacing, these relationships were too 598 weak, even if the most related covariates were selected (results not shown in this paper). 599 This means that the strategies of sampling based on the regularity of coverage of the spatial 600 sampling in the covariate spaces (Minasny and Mc Bratney, 2006; Carré et al., 2007; Zhang 601 and Zhu, 2019) could not be effective for correcting overly sparse legacy datasets. Conversely, for large datasets for which more covariates were involved in the model, a fair 602 603 distribution of the covariates values would be required. However, the coverages and KLD 604 indices in the covariate space and the geographical one were found to be highly correlated 605 for the smallest average spacing (r > 0.90 for average sampling >= 1225 m), which means 606 that taking into account the covariate space would be of little interest if the regularity of 607 sampling in the geographical space is already ensured. However, this result would not hold 608 in particular pedological contexts characterized by small inclusions of land with contrasted 609 values of covariates that could be missed by regular samplings in the geographical space.

Finally, the stepwise regression coefficients of determination given in the last lines of the matrices of Figure 4 clearly showed that the selected sampling characteristics could not alone explain the variations of performances that were observed across the 12,000 trials. This was particularly true for the sparsest spatial sampling when we considered the mean square error on predicted value (Figure 5a) or the biases of estimation of the latter (Figure

5c or 5d). The reverse tendency was observed for the error on PICP, for which the smallest
average spacing of sites obtained the lowest coefficient of determination.

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5.3. Uncertainty estimation biases

619 The two tested procedures of overall uncertainty estimation - the model-based and the 620 model-free ones - exhibited non-negligible biases on uncertainty of clay content predictions 621 (Figures 4c and 4d). Although the two procedures could be considered as intrinsically 622 unbiased, some specific characteristics of the legacy spatial sampling to which they were 623 applied were responsible of these biases. Although it could be observed (Figure 4) that the 624 sparse samplings were more prone to bias than the dense ones, the average spacing did not 625 seem to be a first-order driver because much more variability occurs within a given sampling 626 size (see the bars of Figures 4c and 4d).

627 The correlations matrices (Figures 5c and 5d) provided some insights on the causes of such 628 biases. As far as the largest spacing were concerned, biases were all the more great that the 629 sampling underestimated the real variations of clay content and thus left aside their extreme 630 values. This observation can be related with the general difficulty of the inference models, 631 such as Random Forest, to predict values that are out of the range of their learning sample 632 (Conn et al., 2014). Alternately, overly clustered datasets (see examples in Figure 3, left 633 column) resulted in selecting evaluation sites that could be too close from the calibration 634 sites for satisfying the condition of independence, which may induce underestimations of 635 the prediction errors. Therefore, to estimate the overall uncertainty as well, it is important 636 to mitigate the perturbing effects of the clusters of sites techniques cited above.

Finally, it is worth noting that the estimations of the local uncertainty through a confidenceinterval calculated by the QRF algorithm seemed to be more robust than the estimations of

the overall uncertainty (Figure 3b). Only the largest spacing (1732 m) and, to a lesser extent,
smallest ones gave unsatisfactory results. This confirmed the results obtained by Vaysse and
Lagacherie (2017) using the same algorithm.

642

643

5.4. Limitations and open questions.

644 Although some clear and coherent tendencies could be retrieved from the results of this 645 numerical experiment (see above), some open questions remain. First, the characteristics of 646 the spatial sampling that were considered in this paper did not explain the entire variability 647 of DSM performances. The weak statistical relations observed in Figure 5 for the largest 648 spacing suggest that some hidden factors should be evoked. Among others, we hypothesize 649 that the random process used for optimizing the hyperparameters of the Random Forest 650 generated a noise on DSM performances, the best possible combination of parameters not 651 always being reached because of local optimal solutions, especially when the size of the 652 learning sample is small. This hypothesis is supported by the fact that the average 653 variabilities of the optimal QRF parameters provided by the optimization process decreased 654 as the size of the sampling increased (average Coefficient of Variation from 35% to 21%).

655 Second, although a large range of soil sampling spacings were explored in this case study, 656 the size of the study areas limited the testing of the sparser soil datasets that fed the DSM 657 applications conducted at national (e.g. Mulder et al., 2016), continental (Ballabio et al., 658 2016) or global scale (Hengl et al., 2017). Whether or not the trends exhibited in Figures 4 659 and 5 can be extrapolated to these applications remains an open question. With the next 660 availability of hyperspectral VIS-NIR-SWIR satellite data (such as the French HYPerspectral X 661 Imagery –HYPXIM-, Briottet et al., 2013; the Spaceborne Hyperspectral Applicative Land and 662 Ocean Mission –SHALOM-, Bussoletti, 2012; the German Environmental Mapping and

Analysis Program –EnMAP-, Stuffler et al., 2007; Steinberg et al., 2016 and the Hyperspectral Infrared Imager -HyspIRI-, Lee et al., 2015), it could be envisaged to reproduce the same numerical experiment at a wider extent with, however, a loose spatial resolution. In the absence of such an experiment, the results obtained for the largest average spacing considered in this numerical experiment (1732 m) should help in orienting the future design of DSM approaches at these largest extents.

669

670 **6.** Conclusions

671 The main lessons of the numerical experiment are as follows

- User and producers of DSM products should be aware that the current methods of
 evaluation tend to underestimate the overall uncertainty, especially for sparse and
 unevenly distributed soil sampling
- Although decreasing the average spacing of soil inputs always brings improvements
 of DSM performances, one should be aware that, beyond a given threshold of
 average spacing, the improvement would need also to collect better soil covariates.
- The spatial distributions of the legacy data and the sampling strategies for correcting
 these distributions play a key role in reaching the best DSM performances. Sampling
 strategies that provide complete and even distributions in the geographical space
 and have as great a spread of the target soil property as possible should be
 privileged.
- Some hidden sampling characteristics that were not considered in this experiment
 seem to play a significant role, especially for sparse sampling. More research is
 required for identifying these characteristics.

686

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Figure 1: Location of the study area (a) and the spatial pattern of pseudo values of topsoil clay content (b) (after Lagacherie et al, 2009)

Figure 2: General approach for the numerical experiment

Figure 3: Examples of tested spatial sampling in the numerical experiment. Left column: Three clusters, right column: Fifteen clusters, top row : 75 calibration sites and 25 evaluation sites, bottom row : 750 calibration sites and 250 evaluation sites. Calibration sites are in black. Evaluation sites are in red.

Figure 4: Evaluation of DSM models (quantile Random Forests) using different size of soil input data (size is expressed by spacing):

a) Mean Square error on predicted Clay value (MSE_{ref}), (in g^2/kg^2). The green line is the total variance of Clay content over the study area

b) 90% Prediction Interval Coverage Index (PICP90) (in %). The green line is the expected value of 90%.

c) error on the QRF based estimation of MSEref (in % MSEref). The green line is 0 (no error)

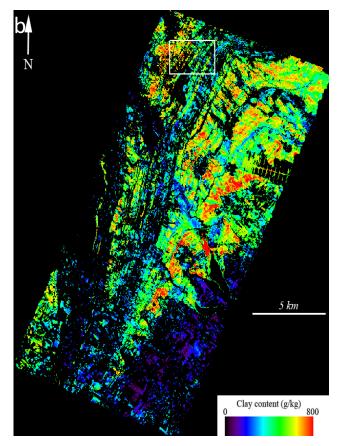
d) error on the model-free estimation of MSEref (removing 25% of the soil inputs for validation) (in % MSEref),). The green line is 0 (no error).

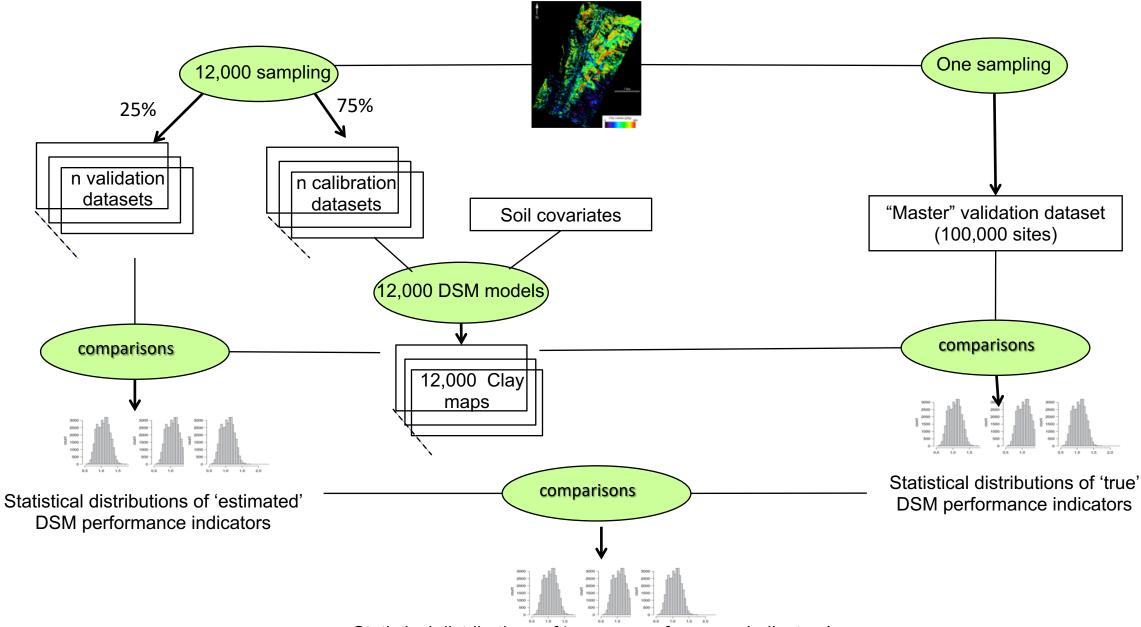
Red dots are averaged values per spacing and bars are +- the standard deviations (1000 models per spacing)

Figure 5: Correlation coefficients (CC) between the indicators of performances and the indicators of spatial distribution of sampling for different sizes of spatial sampling (1000 simulations per size): a) Mean Square error (MSE_{ref}), b) PICP90 c) error on MSE estimated by the random forest bagging procedure d) error on MSE estimated by removing 25% of sample.

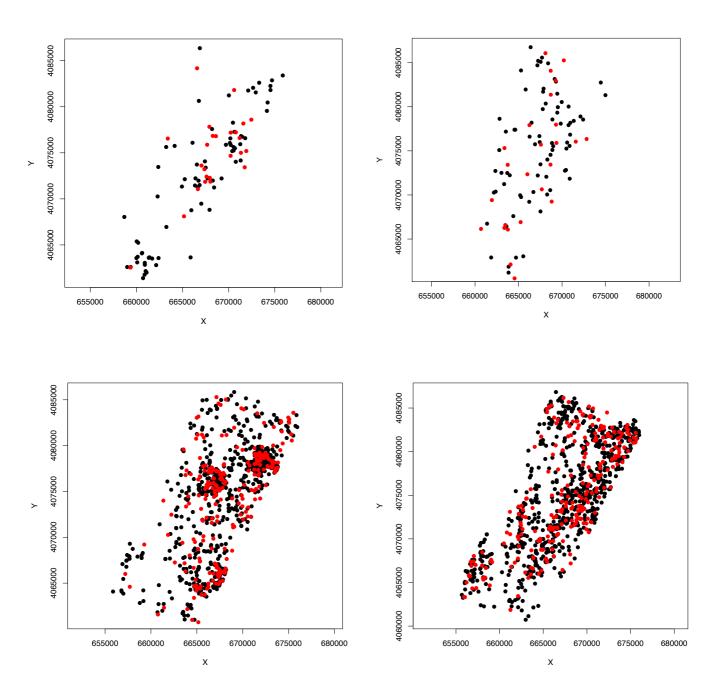
Figure 6 : Evolution of the average performances of predictions (mean MSEref) with the spatially-structured variance ratio (SSVR). The red line is the linear regression using the seven spatial sampling (out of 12) having the smallest values of SSVR.

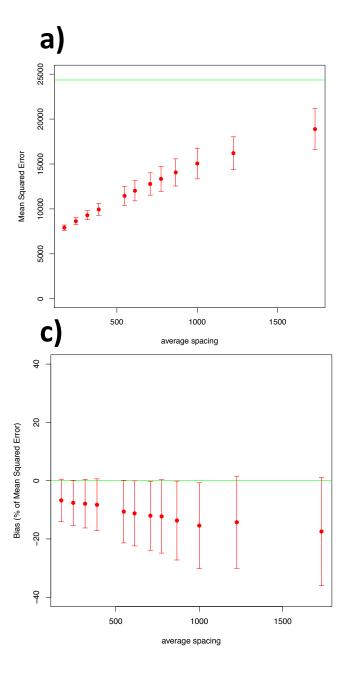


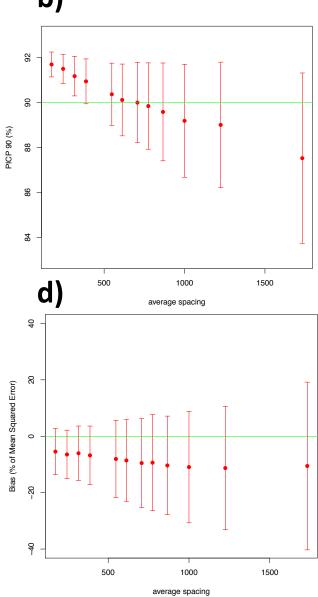




Statistical distributions of 'error on performance indicators'







b)

| - | | Average spacing (m) | | | | | | | | | | | |
|--|-------------------|---------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| space | Indicator | 1732 | 1225 | 1000 | 866 | 775 | 707 | 612 | 548 | 387 | 316 | 245 | 173 |
| | coverage | 0.11 | 0.17 | 0.15 | 0.16 | 0.23 | 0.24 | 0.38 | 0.39 | 0.58 | 0.67 | 0.79 | 0.84 |
| Covariates | KLD | 0.05 | 0.01 | 0.07 | 0.03 | 0.05 | 0.08 | 0.30 | 0.09 | 0.11 | 0.12 | 0.36 | 0.29 |
| geographical | %out of range | 0.29 | 0.32 | 0.40 | 0.40 | 0.40 | 0.42 | 0.47 | 0.46 | 0.54 | 0.53 | 0.64 | 0.60 |
| | coverage | 0.42 | 0.46 | 0.53 | 0.54 | 0.57 | 0.58 | 0.68 | 0.68 | 0.74 | 0.79 | 0.85 | 0.87 |
| geographical | KLD | 0.38 | 0.48 | 0.52 | 0.54 | 0.56 | 0.61 | 0.67 | 0.67 | 0.73 | 0.78 | 0.83 | 0.87 |
| Covariates geographical Clay | %out of range | 0.20 | 0.24 | 0.32 | 0.30 | 0.33 | 0.25 | 0.29 | 0.31 | 0.31 | 0.37 | 0.26 | 0.41 |
| | coverage | 0.06 | 0.10 | 0.23 | 0.12 | 0.18 | 0.17 | 0.17 | 0.08 | 0.18 | 0.05 | 0.04 | 0.02 |
| | KLD | 0.08 | 0.22 | 0.12 | 0.19 | 0.27 | 0.25 | 0.25 | 0.31 | 0.26 | 0.37 | 0.36 | 0.37 |
| Clay | %out of range | 0.34 | 0.37 | 0.36 | 0.38 | 0.35 | 0.39 | 0.36 | 0.36 | 0.27 | 0.40 | 0.34 | 0.29 |
| | variance | -0.38 | -0.47 | -0.53 | -0.54 | -0.53 | -0.41 | -0.56 | -0.38 | -0.40 | -0.25 | -0.33 | -0.42 |
| | Var/semiVar ratio | -0.18 | -0.31 | -0.33 | -0.38 | -0.37 | -0.28 | -0.42 | -0.30 | -0.27 | -0.13 | -0.14 | -0.28 |
| Stepwise multiple linear regression R ² | | 0.31 | 0.42 | 0.48 | 0.47 | 0.52 | 0.50 | 0.57 | 0.56 | 0.61 | 0.68 | 0.77 | 0.80 |

b)

| -1 | | Average spacing (m) | | | | | | | | | | | |
|------------------|------------------------------------|---------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| space | Indicator | 1732 | 1225 | 1000 | 866 | 775 | 707 | 612 | 548 | 387 | 316 | 245 | 173 |
| Covariates | coverage | -0.06 | -0.03 | -0.08 | -0.12 | -0.17 | -0.13 | -0.27 | -0.23 | -0.36 | -0.36 | -0.42 | -0.43 |
| | KLD | 0.04 | 0.12 | 0.02 | 0.00 | 0.02 | 0.13 | -0.24 | 0.07 | -0.06 | 0.06 | -0.16 | -0.16 |
| | %out of range | 0.20 | 0.25 | 0.34 | 0.32 | 0.30 | 0.29 | 0.37 | 0.33 | 0.33 | 0.42 | 0.39 | 0.38 |
| geographical | coverage | -0.27 | -0.26 | -0.42 | -0.41 | -0.36 | -0.33 | -0.50 | -0.44 | -0.51 | -0.49 | -0.49 | -0.51 |
| | KLD | -0.26 | -0.29 | -0.42 | -0.43 | -0.36 | -0.35 | -0.49 | -0.44 | -0.49 | -0.49 | -0.48 | -0.49 |
| | %out of range | 0.19 | 0.16 | 0.25 | 0.27 | 0.21 | 0.16 | 0.22 | 0.20 | 0.25 | 0.26 | 0.13 | 0.26 |
| | coverage | -0.11 | -0.16 | -0.22 | -0.09 | -0.15 | -0.19 | -0.15 | -0.14 | -0.15 | -0.04 | -0.05 | -0.08 |
| Clay | KLD | -0.10 | -0.09 | -0.12 | -0.11 | -0.14 | -0.09 | -0.15 | -0.17 | -0.16 | -0.18 | -0.12 | -0.17 |
| | %out of range | -0.62 | -0.55 | -0.52 | -0.53 | -0.44 | -0.47 | -0.47 | -0.44 | -0.38 | -0.38 | -0.34 | -0.25 |
| | variance | 0.76 | 0.71 | 0.68 | 0.68 | 0.64 | 0.62 | 0.65 | 0.57 | 0.54 | 0.49 | 0.41 | 0.54 |
| | Var/semiVar ratio | 0.34 | 0.33 | 0.35 | 0.41 | 0.38 | 0.38 | 0.40 | 0.41 | 0.35 | 0.34 | 0.30 | 0.45 |
| Stepwise multipl | e linear regression R ² | 0.31 | 0.42 | 0.48 | 0.47 | 0.52 | 0.50 | 0.57 | 0.56 | 0.61 | 0.68 | 0.79 | 0.85 |

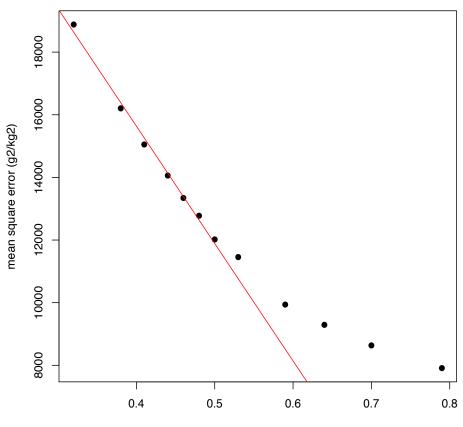
<u>c)</u>

| | | | | | | | Average s | pacing (m) | | | | | |
|------------------------------------|----------------------------------|-------|-------|-------|-------|-------|-----------|------------|-------|-------|-------|-------|-------|
| space | Indicator | 1732 | 1225 | 1000 | 866 | 775 | 707 | 612 | 548 | 387 | 316 | 245 | 173 |
| | coverage | -0.13 | -0.15 | -0.17 | -0.20 | -0.27 | -0.29 | -0.41 | -0.46 | -0.67 | -0.75 | -0.85 | -0.91 |
| Covariates | KLD | -0.05 | -0.01 | -0.12 | -0.07 | -0.07 | -0.12 | -0.30 | -0.12 | -0.15 | -0.15 | -0.37 | -0.24 |
| Covariates geographical Clay | %out of range | -0.29 | -0.37 | -0.44 | -0.43 | -0.43 | -0.42 | -0.49 | -0.47 | -0.51 | -0.51 | -0.58 | -0.55 |
| | coverage | -0.41 | -0.45 | -0.58 | -0.57 | -0.58 | -0.59 | -0.68 | -0.69 | -0.78 | -0.81 | -0.86 | -0.88 |
| geographical | KLD | -0.36 | -0.46 | -0.57 | -0.56 | -0.58 | -0.60 | -0.67 | -0.68 | -0.76 | -0.78 | -0.82 | -0.85 |
| geographical | %out of range | -0.21 | -0.21 | -0.32 | -0.28 | -0.29 | -0.25 | -0.28 | -0.31 | -0.31 | -0.34 | -0.22 | -0.33 |
| | coverage | -0.04 | -0.07 | -0.18 | -0.04 | -0.15 | -0.13 | -0.13 | -0.08 | -0.13 | -0.01 | -0.03 | 0.01 |
| | KLD | -0.12 | -0.25 | -0.22 | -0.24 | -0.32 | -0.26 | -0.30 | -0.36 | -0.29 | -0.45 | -0.50 | -0.42 |
| Clay | %out of range | -0.49 | -0.46 | -0.40 | -0.43 | -0.36 | -0.41 | -0.39 | -0.35 | -0.30 | -0.32 | -0.28 | -0.26 |
| | variance | 0.57 | 0.54 | 0.52 | 0.54 | 0.54 | 0.38 | 0.56 | 0.36 | 0.35 | 0.13 | 0.18 | 0.28 |
| | Var/semiVar ratio | 0.18 | 0.18 | 0.19 | 0.28 | 0.27 | 0.16 | 0.31 | 0.21 | 0.15 | -0.03 | -0.07 | 0.08 |
| Stepwise multiple | linear regression R ² | 0.49 | 0.50 | 0.52 | 0.52 | 0.55 | 0.51 | 0.60 | 0.58 | 0.67 | 0.73 | 0.83 | 0.87 |

d)

| | | | | | | | Average s | pacing (m) | | | | | |
|--|-------------------|-------|-------|-------|-------|-------|-----------|------------|-------|-------|-------|-------|-------|
| space | Indicator | 1732 | 1225 | 1000 | 866 | 775 | 707 | 612 | 548 | 387 | 316 | 245 | 173 |
| | coverage | -0.01 | -0.06 | -0.08 | -0.05 | -0.09 | -0.17 | -0.23 | -0.27 | -0.44 | -0.53 | -0.65 | -0.83 |
| <u>Covariates</u> | KLD | -0.02 | -0.03 | -0.02 | -0.02 | -0.06 | -0.08 | -0.07 | -0.07 | -0.13 | -0.14 | -0.45 | -0.38 |
| | %out of range | 0.13 | 0.26 | 0.28 | 0.32 | 0.33 | 0.39 | 0.36 | 0.40 | 0.41 | 0.44 | 0.44 | 0.47 |
| | coverage | -0.25 | -0.30 | -0.35 | -0.42 | -0.45 | -0.49 | -0.53 | -0.60 | -0.66 | -0.71 | -0.78 | -0.83 |
| geographical | KLD | -0.23 | -0.26 | -0.33 | -0.39 | -0.40 | -0.45 | -0.53 | -0.59 | -0.63 | -0.68 | -0.74 | -0.81 |
| | %out of range | 0.18 | 0.24 | 0.27 | 0.22 | 0.26 | 0.23 | 0.35 | 0.30 | 0.30 | 0.32 | 0.33 | 0.31 |
| | coverage | 0.08 | -0.02 | -0.02 | -0.03 | -0.03 | -0.05 | -0.16 | -0.10 | -0.07 | -0.07 | -0.03 | -0.01 |
| | KLD | -0.10 | -0.07 | -0.15 | -0.15 | -0.25 | -0.22 | -0.23 | -0.27 | -0.29 | -0.39 | -0.47 | -0.39 |
| Clay | %out of range | -0.46 | -0.43 | -0.38 | -0.46 | -0.40 | -0.38 | -0.35 | -0.34 | -0.35 | -0.23 | -0.19 | -0.26 |
| | variance | 0.56 | 0.51 | 0.46 | 0.50 | 0.49 | 0.39 | 0.51 | 0.34 | 0.33 | 0.14 | 0.16 | 0.26 |
| | Var/semiVar ratio | 0.11 | 0.11 | 0.12 | 0.16 | 0.12 | 0.07 | 0.16 | 0.09 | 0.12 | -0.05 | 0.05 | 0.04 |
| Stepwise multiple linear regression R ² | | 0.39 | 0.36 | 0.34 | 0.42 | 0.42 | 0.40 | 0.45 | 0.46 | 0.51 | 0.59 | 0.69 | 0.80 |

a)



Spatially-Structured Variance Ratio