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1 **Density of soil observations in digital soil mapping: A study in the Mayenne region,**  
2 **France**

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12

13 **Abstract**

14 The density of soil observations is a major determinant of digital soil mapping (DSM)  
15 prediction accuracy. In this study, we investigated the effect of soil sampling density on the  
16 performance of DSM to predict topsoil particle-size distribution in the Mayenne region of  
17 France. We tested two prediction algorithms, namely ordinary kriging (OK) and quantile  
18 random forest (QRF). The study area is a region of  $\sim 5000 \text{ km}^2$  with the highest density of  
19 field soil observations in France (1 profile per  $0.64 \text{ km}^2$ ). The number of training sites was  
20 progressively reduced (from  $n = 7500$  to  $n = 400$ , corresponding to 1 profile per  $0.7 \text{ km}^2$  to 1  
21 profile per  $13 \text{ km}^2$ ) to simulate the different density of observations. For OK and QRF, we  
22 tested random subsampling for splitting the data into training and testing datasets using k-fold  
23 cross validation. For QRF we also tested conditioned Latin hypercube sampling based on the  
24 point coordinates or the covariates. The results indicated that, with increasing density of  
25 observations, OK performed as well or even better than QRF, depending on the particle-size  
26 fraction. For silt prediction, OK was systematically better than QRF. However, the prediction  
27 intervals were much larger for OK than for QRF, and OK did not seem to estimate uncertainty  
28 correctly. Overall, the performance indicators increased with the density of observations with  
29 a threshold at about 1 profile per  $2 \text{ km}^2$  which suggests that the main limitation of DSM  
30 prediction accuracy using QRF is the amount of data collected in the field, not the type of  
31 calibration sampling strategy. Future DSM activities should focus on gathering more field  
32 observations.

33 **Keywords:** Digital Soil Mapping; topsoil particle-size distribution; sampling strategy;  
34 sampling density; prediction performance; Multiple soil classes; France

35

## 36 **1. Introduction**

37 It is generally accepted that a major limitation to Digital Soil Mapping (DSM) prediction  
38 performance is the density of soil observations that carry up-to-date information (e.g.,  
39 Arrouays et al., 2014a, 2017; Samuel-Rosa et al., 2020). Samuel-Rosa et al. (2015) evaluated  
40 whether investing in more spatially detailed environmental covariates improves the accuracy  
41 of digital soil maps. Their conclusions showed that more detailed covariates only result in a  
42 modest increase in prediction performance and it may be more useful to spend extra resources  
43 on collecting more soil observations. Indeed, substantial discrepancies in soil observations'  
44 density exist among, and even within, national soil databases (Morvan et al., 2008; Arrouays  
45 et al., 2017). Somarathna et al. (2017) tested various machine learning algorithms to predict  
46 soil carbon and found that the density of observations was more important than the type of  
47 machine learning models. While many DSM studies focused on comparing various machine  
48 learning models (Padarian et al., 2020), less work focused on the impact of the density of  
49 observations. By using a large dataset of pseudo values of clay content obtained from  
50 hyperspectral data, Lagacherie et al. (2020) confirmed the importance of sampling density on  
51 DSM performances but showed that this importance diminished as sampling densities  
52 increased and that other spatial characteristics of the soil sampling (completeness and  
53 evenness in space) also had a strong effect.

54 Even within harmonized soil conventional mapping programs, the methodology and spatial  
55 coverage are far from homogeneous, even at the national scale. This is the case in France,  
56 where a national program for mapping soil-scapes at 1:250,000 is finalised (Laroche et al.,  
57 2014; Richer-de-Forges et al., 2019). In their prospective analysis on the future of the French  
58 national soil-mapping program, Voltz et al. (2020) proposed to move from conventional soil  
59 mapping to DSM and to improve the density of observed soil profiles to homogenize and  
60 enhance the accuracy of 1:250,000 soil maps for France. In practice, the French program of

61 1:250,000 soil mapping has been done using conventional mapping by administrative units  
62 i.e., the French “Départements” the mean area of which being about 6,000 km<sup>2</sup>. Within these  
63 “Départements”, the density of soil observations is highly variable, from 1 observation per  
64 0.64 km<sup>2</sup> to 1 observation per 123 km<sup>2</sup>. Three thresholds were set to indicate the quality of the  
65 maps (InfoSol, 2005): (i) at least 1 profile per 60 km<sup>2</sup> as a minimum standard designated as  
66 “operational level”, (ii) more than 1 profile per 40 km<sup>2</sup> for a higher quality “advanced level”  
67 and (iii) more than 1 profile per 20 km<sup>2</sup> as “optimal level”. These thresholds were set by  
68 experts and used to deliver labels of quality by the Ministry in charge of Agriculture, but their  
69 relevance was never assessed quantitatively. In particular, we never tested if increasing the  
70 density of points substantially would increase the performance of the predictions when using  
71 DSM techniques to map a “Département”.

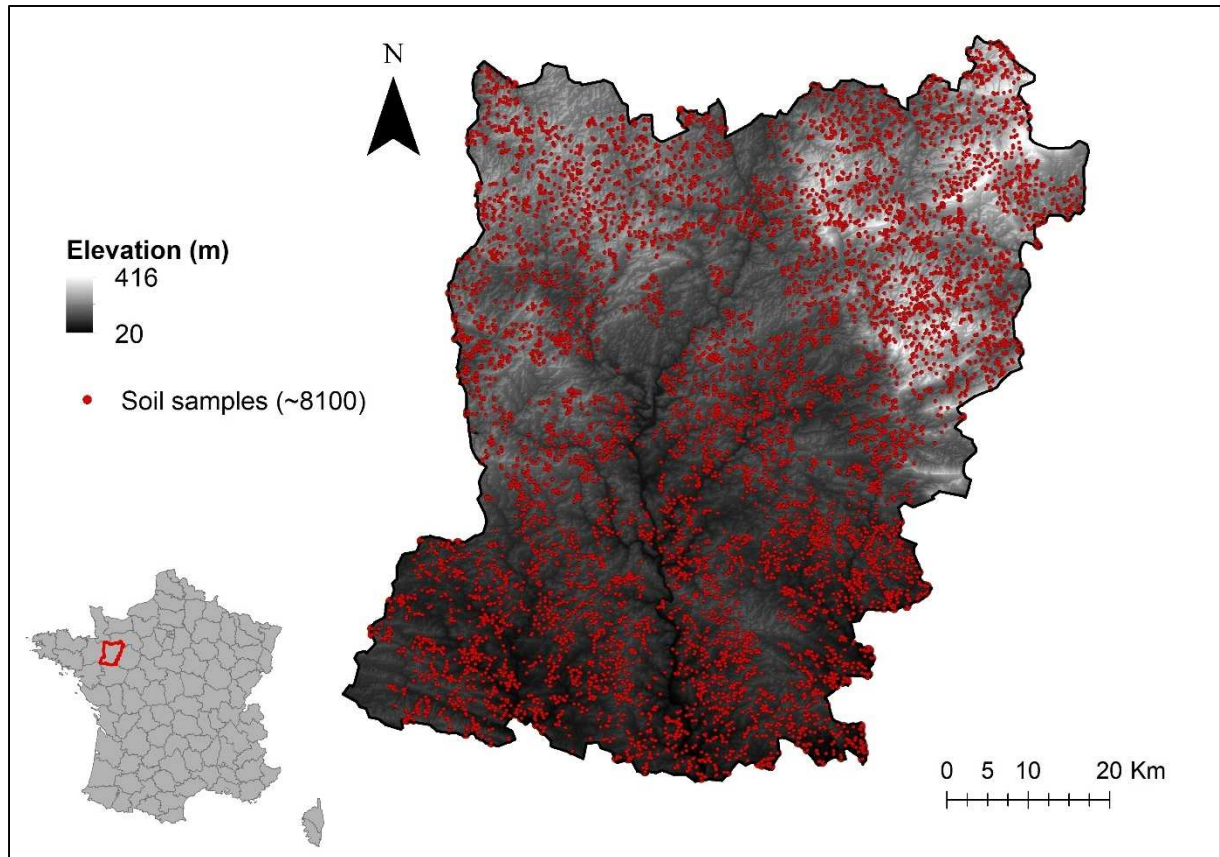
72 In this study, we chose the French “Département” with the highest soil profile density  
73 observations. We tested how the density of training profiles affects the prediction of topsoil  
74 particle size distribution, namely clay, silt, and sand contents. This paper has two objectives:  
75 i) to assess if we could identify thresholds of the density of soil profiles for prediction  
76 performances when applying DSM techniques to predict some basic soil properties and, ii) to  
77 compare the performances of a machine learning algorithm (quantile random forest) to pure  
78 spatial interpolation, ordinary kriging, as a function of the density of observations.

## 79 **2. Material and methods**

### 80 *2.1. Study area and general framework of the study*

81 We chose the “Mayenne” French “Département”. (~8,100 points for a total area of 5208 km<sup>2</sup>,  
82 corresponding to a density of one profile per 0.64 km<sup>2</sup>), which has the highest density of  
83 observations for a French department in the framework of the systematic conventional survey  
84 of soils at the scale of 1:250,000. Figure 1 shows the study area with the original sampling  
85 points from the soil surveyor and the elevation. Except for some urban areas, sampling points

86 are rather homogeneously distributed. Of course, the density of points is not regular, because  
87 conventional survey allows the surveyor to place the points for maximum information on the  
88 soil-landscape, but we can reasonably expect that most of the soil/landscape situations are  
89 represented in this sampling.



90

91 **Fig. 1.** Map of the study area with soil sampling points used for the conventional mapping and  
92 elevation (m).

93 The region is located at the boundary of sedimentary deposits (mainly calcareous and loess)  
94 and crystalline and metamorphic rocks. Thus, we expect that we would be able to see  
95 contrasting spatial structures of soil texture within this region. In addition, the area is covered  
96 by interesting spatial covariates, namely, (i) a harmonized and revised lithological map  
97 (1:50,000 scale; Vernhet, 2010, recoded by Bialkowski et al., 2019), and (ii) an airborne  
98 gamma-ray survey.

100 *2.2. Soil sampling and analysis*

101 Soil sampling was done in the framework of a conventional soil survey; its density was  
 102 adapted to the soil variations observed in the field by the soil surveyors. At each field  
 103 sampling location, the soils were sampled either by digging a soil pit or by augering. The  
 104 topsoil organo-mineral horizon (excluding O horizons when present) was sampled. For most  
 105 of the agricultural plots, the corresponding thickness was the ploughed layer (from 0-20 to 0-  
 106 30 cm, with an average thickness of 24 cm) whereas the thickness ranged from 0-5 to 0-30 cm  
 107 (with an average of 20 cm) and from 0-5 to 0-25 cm (with an average of 18 cm) under  
 108 permanent pastures and forest respectively. Samples were air-dried at 30°C to a constant mass  
 109 and then gently crushed to a 2 mm sieve. The particle-size analysis was performed using the  
 110 Robinson pipette method (Robinson, 1933).

111 As the fractions clay (< 2 µm), silt (2-50 µm), and sand (50-2000 µm) sum to 1000 g kg<sup>-1</sup>, the  
 112 data were transformed with the additive log-ratio (alr-transform, Aitchison, 1982) for the  
 113 spatial prediction of compositional data (Lark and Bishop, 2007). The alr-transformed  
 114 variables were calculated as follows (Eqs (1 and 2)):

115 
$$\mathbf{Clay}_{alr} = \ln\left(\frac{\mathbf{Clay}}{\mathbf{Sand}}\right) \quad (1)$$

116 
$$\mathbf{Silt}_{alr} = \ln\left(\frac{\mathbf{Silt}}{\mathbf{Sand}}\right) \quad (2)$$

117 The alr predicted variables were then back-transformed to sand, silt, and clay through the alr  
 118 inverse transformation (Eqs (3-5)):

119 
$$\mathbf{Clay} \text{ (g. kg}^{-1}\text{)} = \frac{e^{\mathbf{Clay}_{alr}}}{(1 + e^{\mathbf{Clay}_{alr}} + e^{\mathbf{Silt}_{alr}})} \times 1000 \quad (3)$$

120 
$$\mathbf{Silt} (g.kg^{-1}) = \frac{e^{Silt_{alr}}}{(1 + e^{Clay_{alr}} + e^{Silt_{alr}})} \times 1000 \quad (4)$$

121 
$$\mathbf{Sand} (g.kg^{-1}) = \frac{1}{(1 + e^{Clay_{alr}} + e^{Silt_{alr}})} \times 1000 \quad (5)$$

122 To assess the confidence interval of our predictions, we calculated the variance of the back-  
 123 transformed clay, sand, and silt fractions. Román Dobarco et al. (2019) showed that since the  
 124 prediction and variance are independent, the Taylor analysis method is more efficient than  
 125 using Monte Carlo simulation to estimate the prediction variance of each particle-size.  
 126 Utilising the first-order Taylor analysis, the variance of prediction can be derived as follow  
 127 (Eqs (6-8)):

128 • 
$$\mathbf{var}(\mathbf{Clay} (g.kg^{-1})) = \sigma_{Clay_{alr}}^2 \left( \frac{1000(e^{Clay_{alr}}(1+e^{Clay_{alr}}+e^{Silt_{alr}})-e^{2Clay_{alr}})}{(1+e^{Clay_{alr}}+e^{Silt_{alr}})^2} \right)^2 +$$
  
 129 
$$\sigma_{Silt_{alr}}^2 \left( \frac{-1000e^{Clay_{alr}}e^{Silt_{alr}}}{(1+e^{Clay_{alr}}+e^{Silt_{alr}})^2} \right)^2 + 2cov(Clays_{alr}, Silt_{alr}) \frac{-10^6 e^{2Clay_{alr}} e^{Silt_{alr}} (1+e^{Silt_{alr}})}{(1+e^{Clay_{alr}}+e^{Silt_{alr}})^2} \quad (6)$$

130 • 
$$\mathbf{var}(\mathbf{Silt}(g.kg^{-1})) = \sigma_{Silt_{alr}}^2 \left( \frac{1000(e^{Silt_{alr}}(1+e^{Clay_{alr}}+e^{Silt_{alr}})-e^{2Silt_{alr}})}{(1+e^{Clay_{alr}}+e^{Silt_{alr}})^2} \right)^2 +$$
  
 131 
$$\sigma_{Clay_{alr}}^2 \left( \frac{-1000e^{Clay_{alr}}e^{Silt_{alr}}}{(1+e^{Clay_{alr}}+e^{Silt_{alr}})^2} \right)^2 + 2cov(Clays_{alr}, Silt_{alr}) \frac{-10^6 e^{Clay_{alr}} e^{2Silt_{alr}} (1+e^{Clay_{alr}})}{(1+e^{Clay_{alr}}+e^{Silt_{alr}})^2}$$
  
 132 (7)

133 • 
$$\mathbf{var}(\mathbf{Sand}(g.kg^{-1})) = \sigma_{Clay_{alr}}^2 \left( \frac{-1000e^{Clay_{alr}}}{(1+e^{Clay_{alr}}+e^{Silt_{alr}})^2} \right)^2 +$$
  
 134 
$$\sigma_{Silt_{alr}}^2 \left( \frac{-1000e^{Silt_{alr}}}{(1+e^{Clay_{alr}}+e^{Silt_{alr}})^2} \right)^2 + 2cov(Clays_{alr}, Silt_{alr}) \frac{10^6 e^{Clay_{alr}} e^{Silt_{alr}}}{(1+e^{Clay_{alr}}+e^{Silt_{alr}})^2}$$
  
 135 (8)

136 For more detailed explanations on the use of first-order Taylor analysis in spatial models, we  
 137 refer to Heuvelink et al. (1989).



138

139

140

141

142 2.3. *Covariates*

143 The list of covariates used in this study is provided in Table 1.

**Table 1.** Spatially exhaustive co-variates used in the Mayenne department.

<b>Covariates</b>	<b>Resolution</b>	<b>Data type</b>	<b>Reference</b>
<b><i>Climate</i></b>			
Climate type	250 m	<i>Qualitative</i>	Joly et al., (2010)
<b><i>Vegetation</i></b>			
Forest type	1:25 K	<i>Qualitative</i>	Inventaire Forestier National (2006)
Land use 2016	10 m	<i>Qualitative</i>	CESBIO (2016)
Principal Component (N=3)	NDVI 500 m	<i>Quantitative</i>	Loiseau et al., (2019)
<b><i>Soil maps</i></b>			
Clay content France (%)	500 m	<i>Quantitative</i>	Ballabio et al., (2016)
Silt Content France (%)	500 m	<i>Quantitative</i>	Ballabio et al., (2016)
Sand content France (%)	500 m	<i>Quantitative</i>	Ballabio et al., (2016)
Rate of river network development and persistence (IDPR)	1:50 K	<i>Quantitative</i>	BRGM (2014)
<b><i>Topography</i></b>			
Elevation	25 m	<i>Quantitative</i>	IGN (2014)
Compound topographic index (CTI)	25 m	<i>Quantitative</i>	IGN (2014)
Multi-Resolution Valley Bottom Flatness (MRVBF)	25 m	<i>Quantitative</i>	IGN (2014)
Multi-Resolution Ridge Top Flatness (MRRTF)	25 m	<i>Quantitative</i>	IGN (2014)
Roughness	25 m	<i>Quantitative</i>	IGN (2014)
Curvature	25 m	<i>Quantitative</i>	IGN (2014)
Exposition	25 m	<i>Quantitative</i>	IGN (2014)
Slope position	25 m	<i>Quantitative</i>	IGN (2014)
Slope, cosines(slope)	25 m	<i>Quantitative</i>	IGN (2014)

### *Gamma ray data*

Thorium (Gamma) 250 m *Quantitative* Bonijoly et al., (1999)

Uranium (Gamma) 250 m *Quantitative* Bonijoly et al., (1999)

Potassium (Gamma) 250 m *Quantitative* Bonijoly et al., (1999)

Th/K ratio (Gamma) 250 m *Quantitative* Bonijoly et al., (1999)

Th/U ratio (Gamma) 250 m *Quantitative* Bonijoly et al., (1999)

### *Simplified Lithology*

1:50 K *Qualitative* Loiseau et al., (2020) from Vernhet (2010)

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144

145 All covariates were transformed to a 90 m resolution grid according to the *GlobalSoilMap*  
146 specifications (Arrouays et al., 2014b), either through downscaling for coarser-resolution  
147 layers, or upscaling for the finer ones. The upscaling was done in two ways: 1) by the average  
148 aggregation for quantitative data, 2) by a majority vote estimation for the qualitative  
149 covariates. In addition, we transformed the classes from the qualitative covariates to binary  
150 information (0: absence and 1: presence) to assess each class's importance in our model.

### 151 *2.4.Digital soil mapping modelling*

152 In order to assess the effect of point density on the performance of the predictions, we reduced  
153 the number of training samples progressively and adopted three different strategies to predict  
154 particle-size distribution over the “Département”. To keep comparable testing sizes for large  
155 and small datasets, we selected 8100 to 600 sample points with a 1000 to 200 increment  
156 (Table 2). We used 200 testing points for cross-validation when the number of training points  
157 was larger than 2000, and 500 testing points when the number of training points was smaller  
158 or equal to 2000. This strategy aimed at keeping enough testing points for each fold, and as  
159 many folds as possible. Each splitting procedure was repeated 100 times.

**Table 2.** Training and testing datasets used in this study.

<b>Total samples (n)</b>	<b>600</b>	<b>800</b>	<b>1000</b>	<b>1200</b>	<b>1400</b>	<b>1600</b>	<b>1800</b>	<b>2000</b>	<b>3000</b>	<b>4000</b>	<b>5000</b>	<b>6000</b>	<b>7000</b>	<b>8100</b>
<b>Training samples</b>	400	600	800	1000	1200	1400	1600	1800	2500	3500	4500	5500	6500	7600

<b>(n)</b>														
<b>Training points density (n/km<sup>2</sup>)</b>	0.08	0.12	0.15	0.19	0.23	0.27	0.31	0.35	0.48	0.67	0.86	1.06	1.25	1.46
<b>Training points density (1/a km<sup>2</sup>)</b>	13	8.7	6.5	5.2	4.3	3.7	3.3	2.9	2.1	1.5	1.2	0.9	0.8	0.7
<b>Number of points per-fold (n)</b>	200	200	200	200	200	200	200	200	500	500	500	500	500	500
<b>Number of k- fold</b>	3	4	5	6	7	8	9	10	6	8	10	12	14	16

160

161 We tested four different prediction methods, summarized as follows:

162 1) Ordinary Kriging (OK), to assess the prediction of soil texture, only using soil sample  
 163 location and measured particle-size values as information. Samples were randomly  
 164 selected to form various sizes of training data.

165 2) Quantile Regression Forest (QRF) using the R package quantregForest (Meinshausen,  
 166 2006) with covariates listed in Table 1. We chose this technique as it has been shown  
 167 to be robust, and it enabled us to derive quantile distributions instead of a single mean  
 168 value (Vaysse and Lagacherie, 2017). Samples were randomly selected as in OK.

169 3) QRF as previously, but we chose to sample the points using the conditional Latin  
 170 Hypercube Sampling (cLHS, Minasny and McBratney, 2006) method based on their  
 171 coordinates to reduce the clustering of samples.

172 4) QRF as previously, but we chose to sample the points using cLHS applied on the  
 173 covariates to ensure even coverage of the covariates.

#### 174 2.5. Assessing the performance of the predictions

175 The performance of the predictions was evaluated through a k-fold cross validation by  
 176 keeping a minimum of 200 to 500 samples apart for testing, depending on the strategy of

177 partitioning the data. We assessed the model performance through a 100 times replication of  
 178 the cross-validation method by reporting the medianvalue of the following indicators:

- 179 ➤ The coefficient of determination ( $R^2$ ), which measures the adequacy between our  
 180 model and our observed value.

$$181 \quad R^2 = 1 - (1 - R_{non-adjusted}^2) \frac{n - 1}{n - p - 1} \quad (9)$$

$$182 \quad \text{where } R_{non-adjusted}^2 = \frac{\sum_{i=1}^n (z_i^* - \bar{z})^2}{\sum_{i=1}^n (z_i - \bar{z})^2} \quad (10)$$

183 Here,  $z_i$  and  $\bar{z}$  are the value of the observation for point  $i$  and the mean of all  
 184 observations, respectively;  $z_i^*$  is the value of the prediction for point  $i$ .

- 185 ➤ The root-mean-square error (RMSE), which provides information on the statistical  
 186 dispersion of our predictions in relation to our observations.

$$187 \quad RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (z_i - z_i^*)^2} \quad (11)$$

- 188 ➤ The concordance coefficient (CC; Lin, 1989), which is given as

$$189 \quad CC = \frac{2\rho\sigma_{z^*}\sigma_z}{\sigma_z^2 + \sigma_{z^*}^2 + (\bar{z} - \bar{z}^*)^2} \times 100 \quad (12)$$

190 where  $\sigma_z^2$  and  $\sigma_{z^*}^2$  are the observation and prediction variances, respectively,  $\rho$   
 191 is their correlation coefficient, and  $\bar{z}^*$  is the mean of the prediction

- 192 ➤ The bias of the predictions, which is the difference between the mean predicted  
 193 and mean observed values.

$$194 \quad \text{Mean error} = \frac{1}{n} \sum_{i=1}^n (z_i^* - z_i) \quad (13)$$

- 195 ➤ The PICP (prediction interval coverage probability). This indicator assesses the  
 196 uncertainty between the observed and predicted distribution. The PICP is the

197 probability that the target of an input pattern lies within the prediction limits  
 198 (Shrestha and Solomatine, 2006). The PICP was calculated from the confidence  
 199 interval of 90% with the extreme quantile 5% and 95% of the model prediction.

200

$$201 \quad \mathbf{PICP} = \frac{\sum_{i=1}^n (z_{5\%}^* < z_i < z_{95\%}^*)}{n} \times 100 \quad (14)$$

202

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### 208 **3. Results and discussion**

#### 209 *3.1. Summary statistics*

210 The distribution of the particle-size fractions in g.kg<sup>-1</sup>, over the Mayenne department, is  
 211 shown in Table 3. We observed a large dominance of the silt fraction over the samples.  
 212 Moreover, testing the skewness and kurtosis indices, silt and sand seemed to follow a rather  
 213 symmetric distribution with fewer and less extreme outliers than the normal distribution. The  
 214 clay distribution was positively skewed and had a high kurtosis value, which shows its  
 215 asymmetry and more outliers in the right part of its distribution.

216 **Table 3.** *Summary statistics of particle-size distribution of the samples over the Mayenne*  
 217 *department.*

	<b>Clay</b>	<b>Silt</b>	<b>Sand</b>
<b>Min</b>	18,83	20	19,06
<b>Q1</b>	141	448	189
<b>Mean</b>	177,22	529,26	293,33
<b>Median</b>	164	540	267

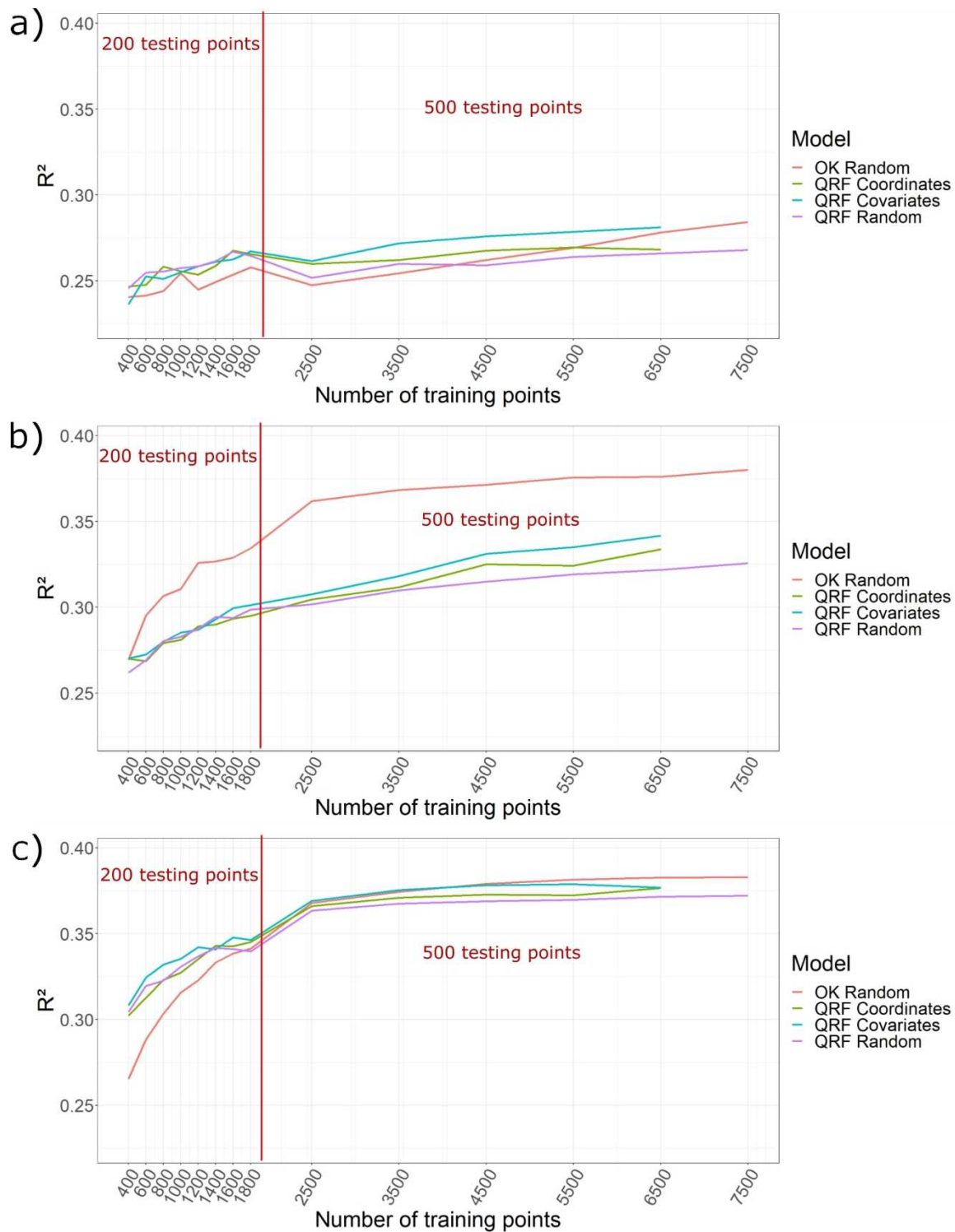
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<b>Q3</b>	200	624	374
<b>Max</b>	631	839	898
<b>Decile 1</b>	125,87	360,6	144
<b>Decile 9</b>	249	683	481,54
<b>Skewness</b>	1,76	-0,48	0,88
<b>Kurtosis</b>	6,07	-0,08	0,59

### 3.2. Performance of the predictions

In order to assess the performances of each sampling strategy, we compared the performance of the predictions for each sampling density and algorithms used. Figures 2 to 6 show the evolution of selected statistical indicators ( $R^2$ , RMSE, ME, CCC, and PICP) as a function of training sample densities.

The  $R^2$  for the QRF algorithms for silt and sand showed a sharp increase with an increasing number of training points until about 1800 and 2500 respectively, followed by a small increase (Fig 2). This shape is similar to those obtained by Lagacherie et al (2020). These threshold were less evident for clay. The three QRF algorithms gave quite similar results. Interestingly the  $R^2$  for silt was always higher when using OK than using QRF methods. This may be due to the fact that the covariates we used did not capture silt distribution effectively. Moreover, when the number of training samples was very large, OK  $R^2$  gave similar results compared to QRF for clay and slightly better results for sand. Note, however, that OK gave poorer results than QRF for clay and especially for sand at the lowest densities of sampling and that for these fractions, the decrease of  $R^2$  was more pronounced for low sampling densities.

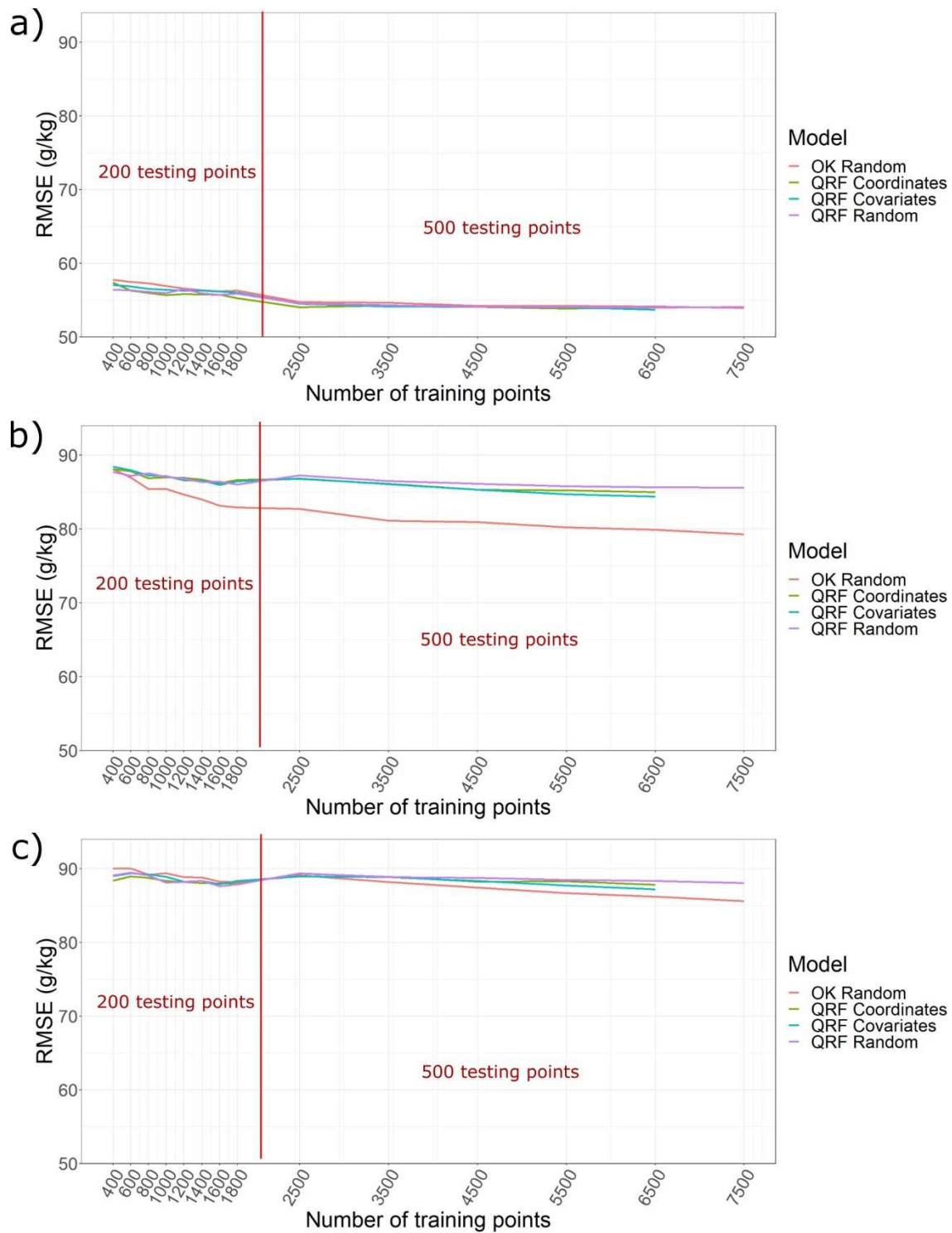


241 **Fig 2.** Median R<sup>2</sup> for testing: comparison for a) Clay, b) Silt and c) Sand fraction for each  
 242 sampling strategy with increasing training sample size over the Mayenne department. The red  
 243 line separates the strategies using 500 testing points from those using 200 testing points.  
 244 For clay, the RMSE (Fig 3) showed a substantial decrease with increasing training densities  
 245 until reaching a threshold of about 2500, followed by a slight decrease thereafter. No real

246 trend was observed for silt and sand. No substantial difference was observed between the  
247 algorithms (Fig. 3) except for silt, in which OK always performed slightly better than the QRF  
248 methods, especially at high sampling densities, which is consistent with the results of  $R^2$ . Note  
249 that the RMSE values are always lower than the interquartile range (see Table 3), suggesting  
250 that the mapping is effective.

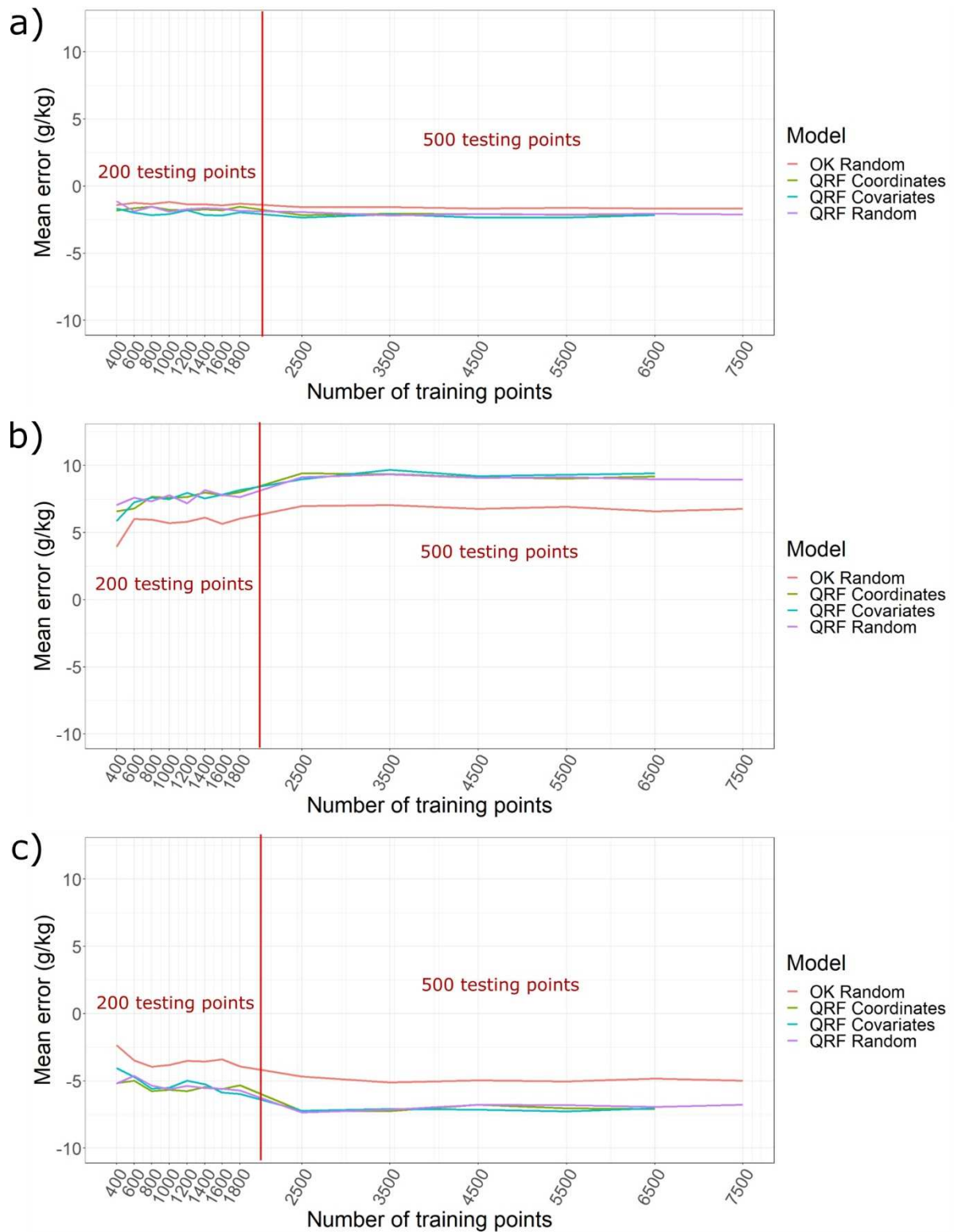
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252 **Fig 3.** Median RMSE for testing: comparison for a) Clay, b) Silt and c) Sand fractions for  
 253 each sampling strategy with increasing training sample size over the Mayenne department.  
 254 The red line separates the strategies using 500 testing points from those using 200 testing  
 255 points.

256 The mean error for clay seemed to be constant for all models at a very low value for clay  
257 (around  $-2 \text{ g.kg}^{-1}$ ). Silt and sand exhibited much larger ME, even if the OK presented better  
258 results for these fractions. For all QRF models, the ME median value stayed somewhat  
259 similar. Interestingly, silt and sand showed opposite trends, increasing ME for silt until about  
260 2500 points and a decreasing one for sand until the same threshold.



261

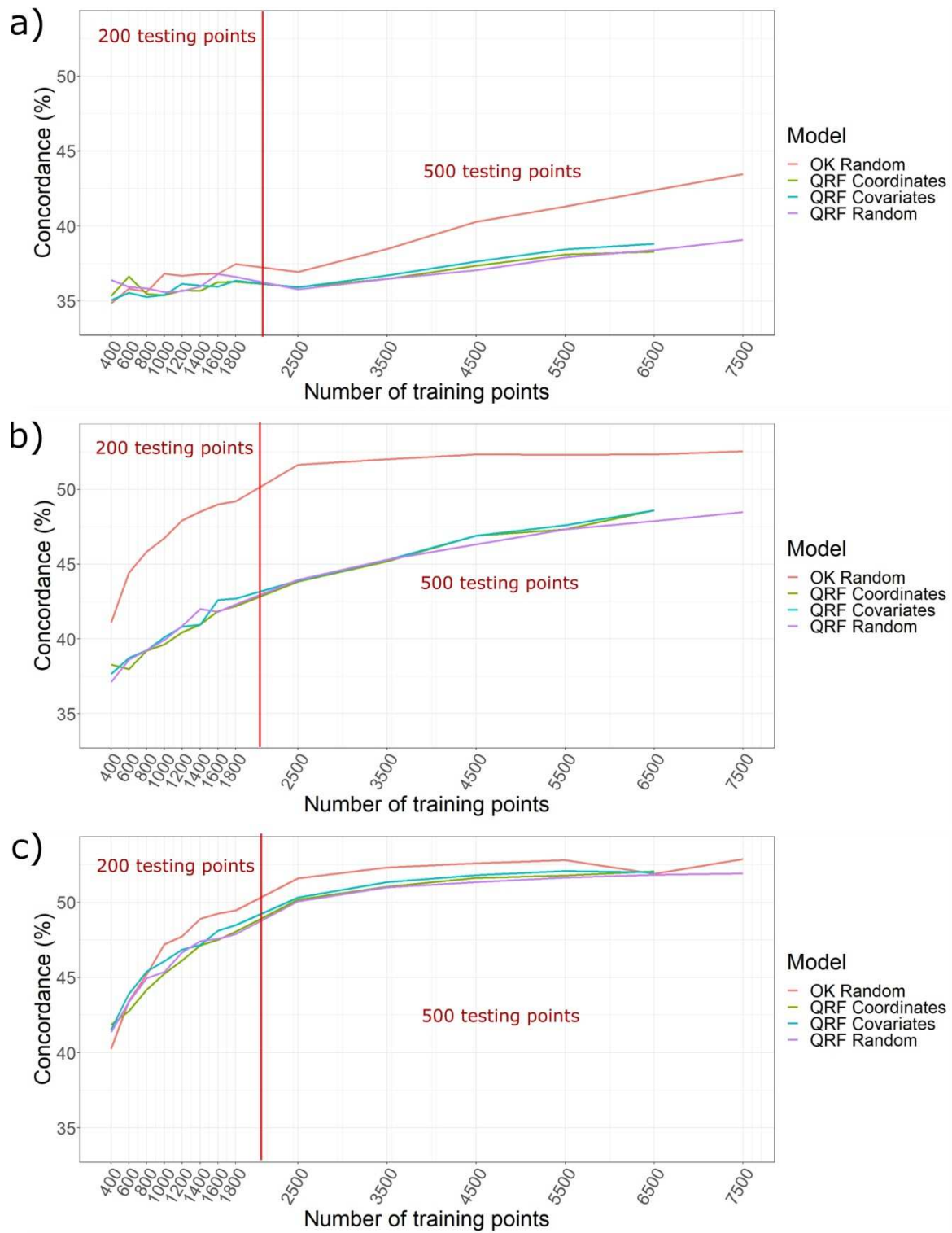
262 **Fig 4.** Median error for testing: comparison for a) Clay, b) Silt and c) Sand fraction for each

263 sampling strategy with increasing training sample size over the Mayenne department. The red

264 line separates the strategies using 500 testing points from those using 200 testing points.

265

266 The CCC indicator increased with increasing density for all fractions (Fig. 5). Interestingly,  
267 OK worked better than QRF for large sampling densities, and even for all densities for silt.  
268 For sand, the CCC trend was similar to  $R^2$ , with a sharp increase with the increasing density  
269 of training points and a lower increase when the number of training points became higher  
270 (> 2500). For the highest training densities, it was higher for OK than for QRF, especially for  
271 silt. On the contrary, for the lowest densities, it became lower for OK than for QRF.



272

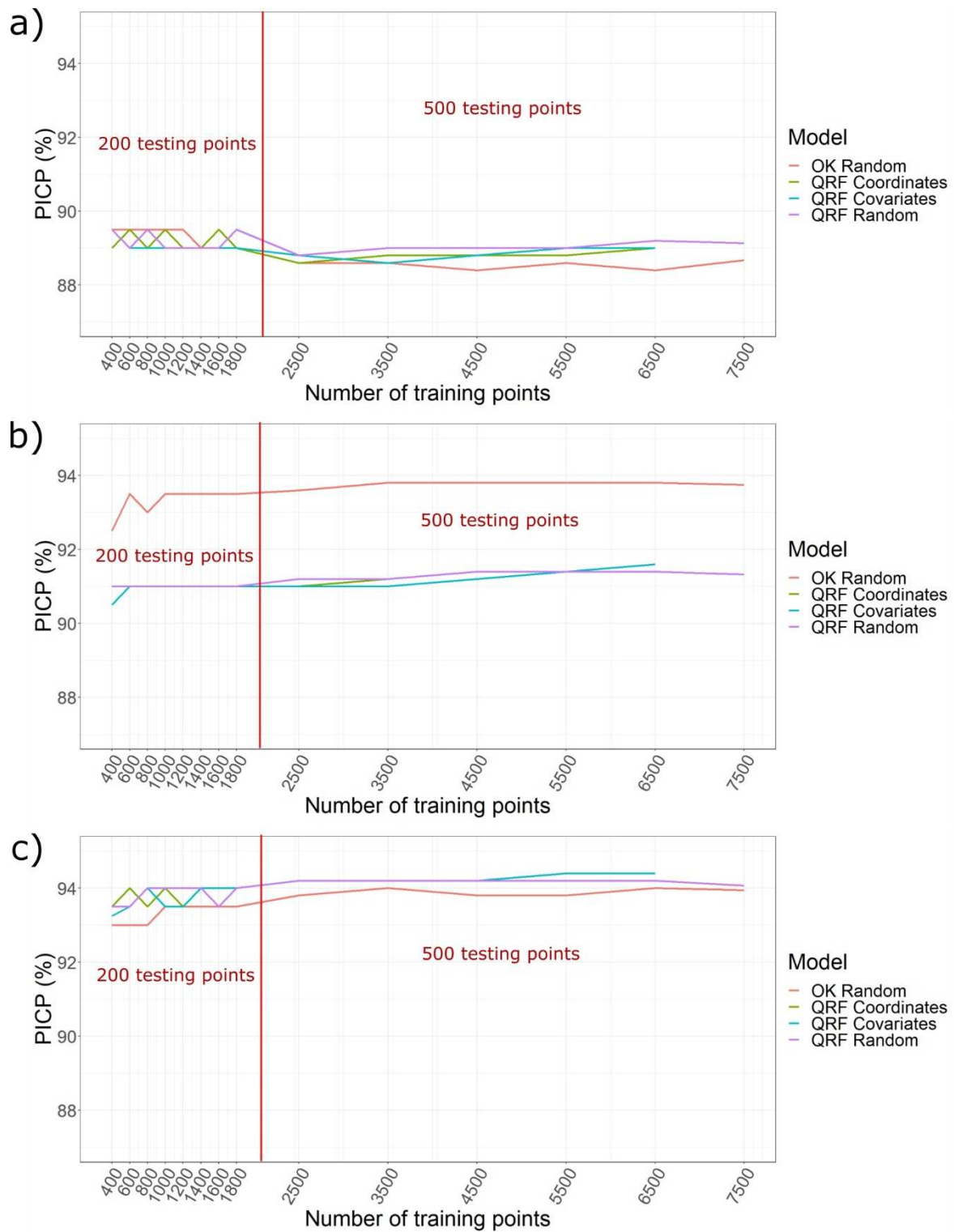
273 **Fig 5.** Median Concordance for testing: comparison for a) Clay, b) Silt and c) Sand fractions  
 274 for each sampling strategy with increasing training sample size over the Mayenne department.  
 275 The red line separates the strategies using 500 testing points from those using 200 testing  
 276 points.

277

278 For clay (Fig. 6), the PICP was always lower than 90%, which shows that the 90% prediction  
279 intervals were slightly under-estimated. This was more evident for OK. From a practical point  
280 of view, this shows that kriging smoothed out high/low values, thus under-estimated the  
281 prediction intervals. The PICP is mostly over 90% for the prediction of silt by OK, although it  
282 shows acceptable values (close to 90%) for the QRF models. This shows that contrary to clay,  
283 OK over-estimated PIs for silt prediction, which counter-balanced the better prediction results  
284 obtained by OK. For sand prediction, all PICPs were larger than 90%. The contrast between  
285 the trends observed for clay and sand could be due to the negative correlation between these  
286 two fractions. We observed a rather erratic behavior of the PICP for the lowest calibration  
287 sample values. This is likely due to the low number of training and testing samples and the  
288 small number of k-fold cross-validations. This is consistent with the findings of Lagacherie et  
289 al. (2019), who showed that a small number of validation samples is not robust enough to  
290 assess the performance of the model predictions. However, this erratic behavior remains in a  
291 narrow range and we should recall here that we replicated 100 times the splitting between  
292 training and testing samples.

293

294



295

296 **Fig 6.** Median PICP for testing: comparison for a) Clay, b) Silt and c) Sand fraction for each  
 297 sampling strategy with increasing training sample size over the Mayenne department. The red  
 298 line separates the strategies using 500 testing points from those using 200 testing points.

299

300 There were no substantial differences between the 3 different sampling strategies for the QRF  
301 algorithms. This may be because all subsampling strategies that we tested were denser than  
302 the sampling strategies commonly used in France. Moreover, when the number of selected  
303 samples is large, cLHS has no advantage over other sampling designs (Wadoux et al., 2019).

304 When the number of training samples was equal or larger than 2500, some QRF performance  
305 indicators were slightly improved with increasing sampling density. This suggests that  
306 collecting new data or rescuing more legacy data should further improve the prediction  
307 accuracy, as indicated by Arrouays et al. (2017) and Samuel-Rosa et al. (2015; 2020). When  
308 the sampling density was very high, OK performed as well, or even better than machine  
309 learning methods, which validates the general framework proposed by Minasny and  
310 McBratney (2010) for global digital soil mapping, that was thereafter adopted by the  
311 *GlobalSoilMap* initiative (Arrouays et al., 2014b). Interestingly, the silt fraction had a  
312 particular behavior compared to other fractions, i.e., except for PICP, the performance was  
313 better when using OK for most sampling densities. This may be due to the fact that the  
314 covariates that we selected were less responsive for silt than for the other fractions. A  
315 threshold of the number of points (around 2500) was identified, under which most of the  
316 performance indicators performed worse. Over this threshold, the performance indicators  
317 remained stable or increased more slowly with the density of points, suggesting that the main  
318 limitation of the goodness of DSM predictions is the amount of data collected in the field. We  
319 note that the number of testing points was changed from 200 to 500 at 2500 training points,  
320 which may affect the results. To keep a minimum number of k-fold the same time, we needed  
321 to change the number of testing points. But we assessed the model performance through a 100  
322 times replication of the cross-validation method. This avoids a random chance of under- or  
323 over-estimation of error. Moreover, our results are consistent with those obtained recently by  
324 Lagacherie et al. (2020).



325 It is worth noting that this threshold of 2500 points (about 1 profile per 2 km<sup>2</sup>) corresponds to  
326 a nearly ten times larger density than the density recommended in the traditional 1:250,000  
327 soil mapping programs, even for those considered as optimal (1 profile per 20 km<sup>2</sup>). The  
328 conventional survey recommendation at 1:250,000 may be adequate if applied by a skilled  
329 soil surveyor, but certainly not for fine resolution DSM applications. The large majority of the  
330 French departments have a number of profile observations much less than this threshold of 1  
331 profile per 2 km<sup>2</sup>. One can, therefore, assess the enormous efforts needed if the objective is to  
332 produce fine resolution DSM products with an acceptable level of quality at the department  
333 level using only training points and available covariates. This is even more critical if we  
334 consider that the most important covariates in our case (airborne gamma-ray, Loiseau et al.,  
335 2020) are not available for the entire French territory.

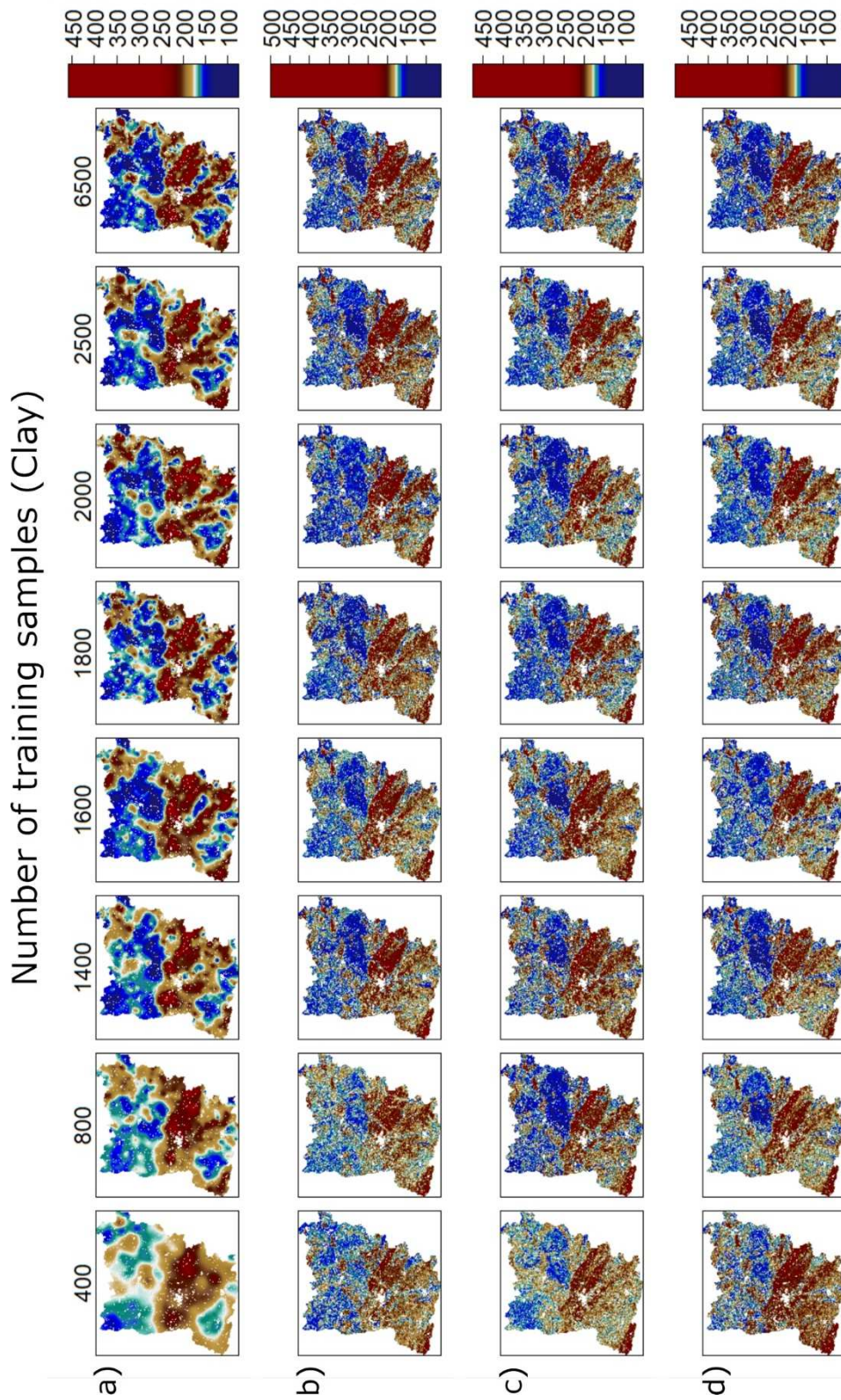
### 336 *3.3. Maps of predictions*

337 To assess the influence of increasing the number of calibration points on mapping predictions,  
338 we mapped several examples for the four trials that we tested for each particle-size fraction  
339 (Figures 7 to 9).

340 The trend showed in these figures is a stabilization of the spatial prediction with the  
341 increasing number of training points. This trend is also more pronounced when we focus on  
342 OK. The increasing number of calibration points allowed the models to describe more  
343 detailed spatial structures, and decreased the smoothing effect of the kriging.

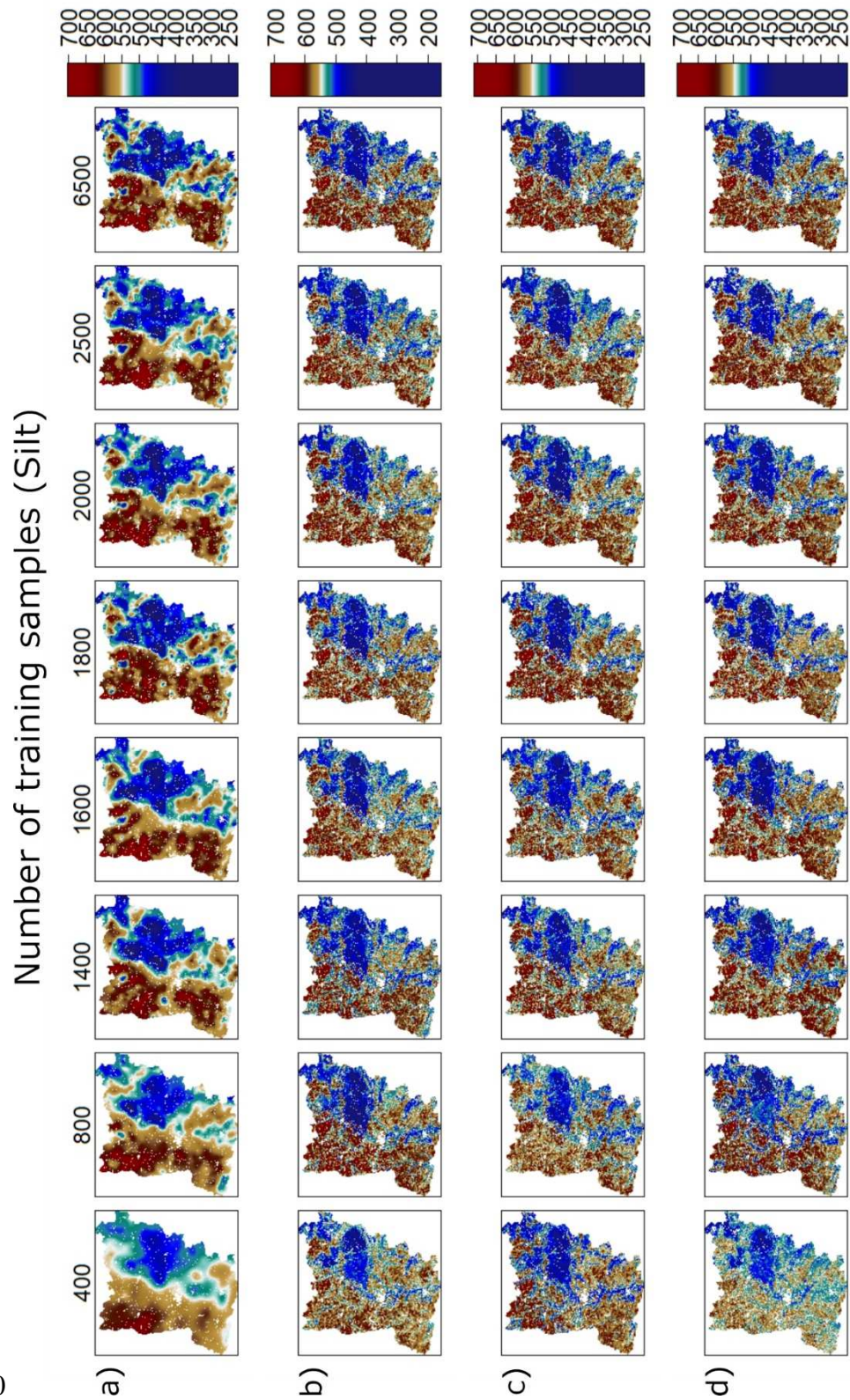
344 When comparing QRF methodologies sampling, few differences were observed between  
345 sampling densities. However, for the lowest training densities, the predictions were more  
346 pixelated and some spatial patterns were less visible on the maps. At thresholds ranging from  
347 1800 to 2500 training points, the general patterns seemed to remain stable for clay, silt, and  
348 sand.

349 For clay (figure 7), the spatial patterns with high values (over 200 g.kg<sup>-1</sup>) seemed to remain  
350 stable from 1800 training points in the middle part of the department.



352 **Fig 7.** Clay predictions comparison for the four maps a) OK, b) QRF random, c) QRF  
353 coordinates and d) QRF covariates, when the number of training data increases.

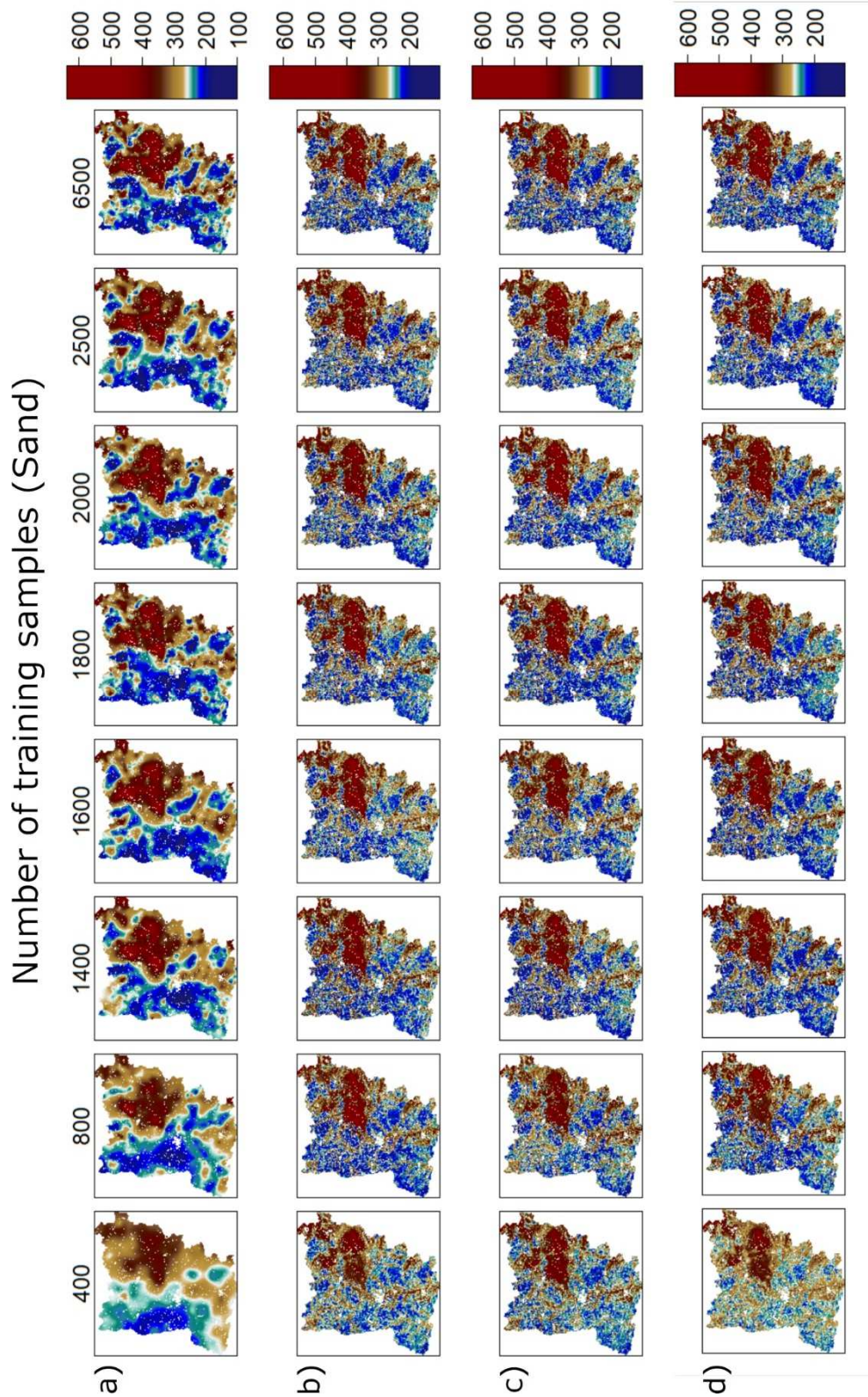
354 For silt, (figure 8), the spatial patterns remained more stable with the integration of more  
355 training data and produced more detailed patches when the number of training points



356 exceeded 2000

357 **Fig 8.** Silt predictions comparison for the four maps a) OK, b) QRF random, c) QRF  
358 coordinates and d) QRF covariates, when the number of training data increases.

359 The predictions of sand (figure 9) presented also similar variations, with a quite similar  
360 stabilization of the predictions, for all QRF models, over a threshold close to 1800 points.



361

362 **Fig 9.** Sand predictions comparison for the four maps a) OK, b) QRF random, c) QRF

363 coordinates and d) QRF covariates, when the number of training data increases.

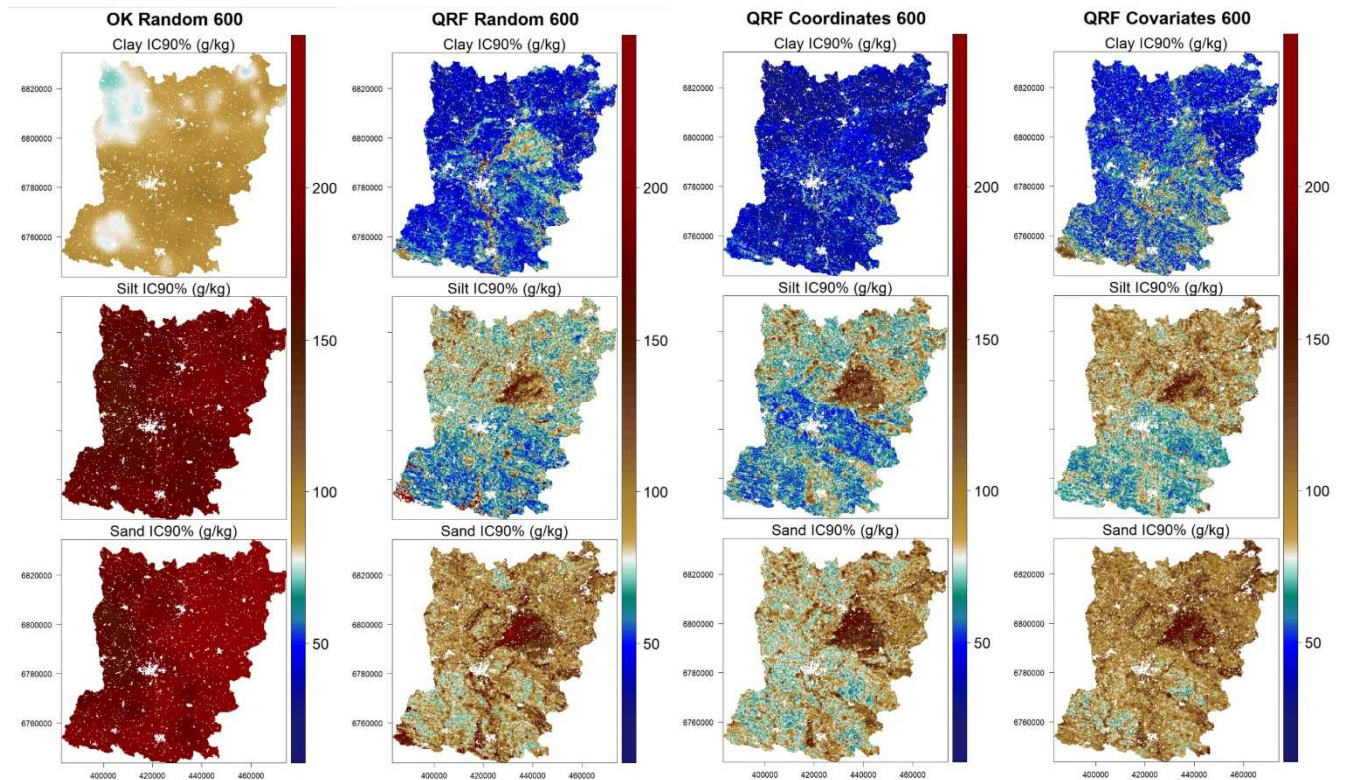
364

365 Several thresholds, ranging from 1800 to 2500 training points, can be observed for the  
366 prediction maps of particle-size over the Mayenne department. Indeed, the sampling strategies  
367 did not impact the prediction maps compared to the number of training points. However, as  
368 shown in the precedent observations, the particle size variability was not entirely explained by  
369 our selected covariates. In complex regions, more observations could explain the spatial  
370 variation of the soil in more detail. Moreover, using good quality covariates increased a lot in  
371 the details of the spatial prediction. In comparison to OK, QRF seemed to indicate the  
372 variability of the predictions closer to the observed soil properties variability and produced  
373 less smoothed predictions. There are limitations in this study; we still missed some crucial  
374 covariates and that our selection of training samples was based on observations collected by a  
375 traditional soil survey, which may not be statistically optimal.

376

#### 377 *3.4.Interval of predictions and mapping*

378 To assess the influence of the training dataset size over our textural predictions, we  
379 estimated and mapped their 90% prediction interval (PI). Figures 10 and 11 show the PI of  
380 each sampling strategy for training sets of 400 and 2500 points. We observed for each  
381 sampling, a decrease of the PI with the increase of the number of training points, except for  
382 coordinates sampling where the PI seemed relatively stable or better, depending on the  
383 particle size, with a smaller dataset (Figure 9).

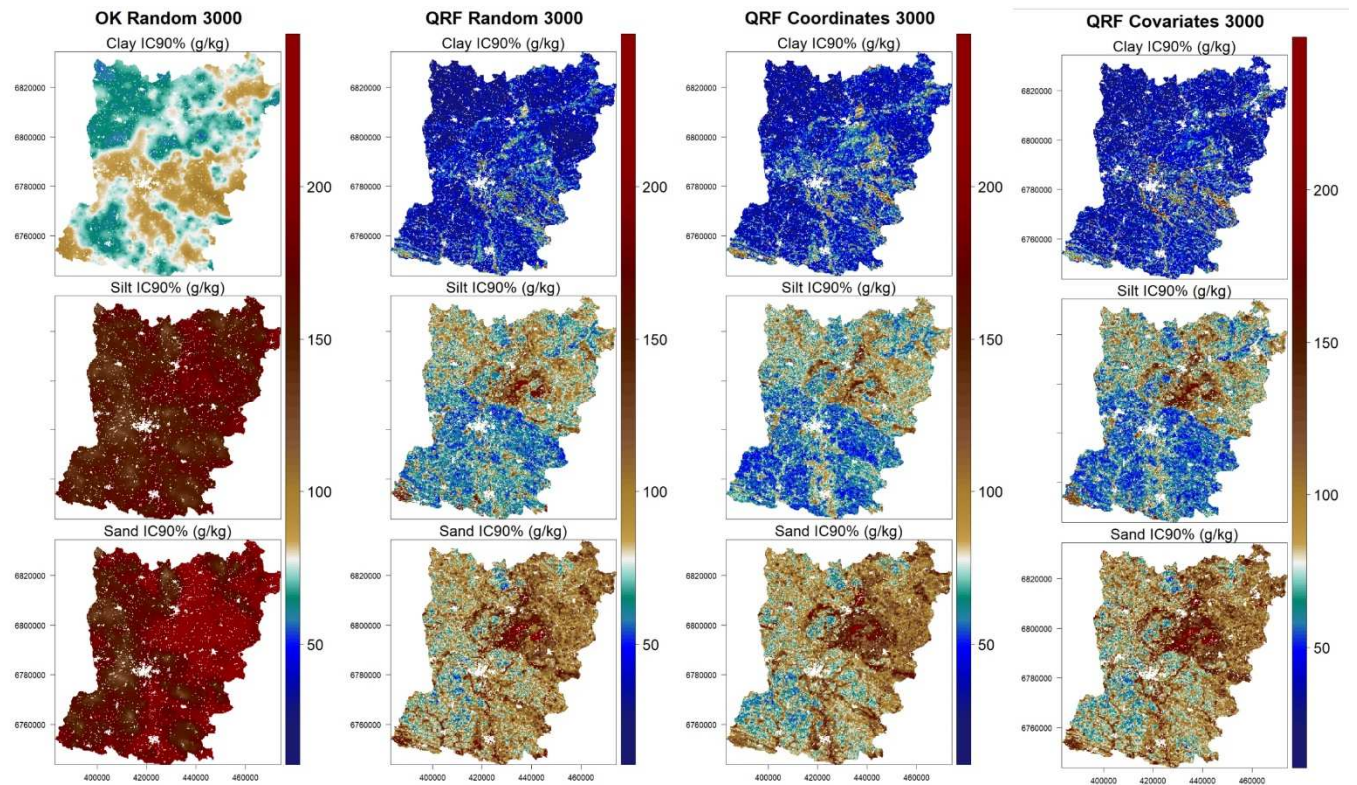


384

385 **Fig 10.** Particle-size prediction interval (90%) for the four maps using 600 points (400 for  
 386 training and 200 for testing).

387 For clay, PIs were lower and showed the most extensive variations over the metamorphic  
 388 area, whereas the uncertainty was much larger with a few points for each sampling strategy.  
 389 Silt showed large variations in the North, but also in the South-Est. This can be due to its  
 390 variability and the fact that complex deposition processes could not be captured by our model  
 391 and covariates, even with a large set of training points (Figure 11). The global variation of  
 392 sand over the department resulted from the cumulative error from the back transformation and  
 393 presented the largest variation compared to clay and silt. Note that the PIs were always much  
 394 larger for OK than for QRF models and that, as expected, the PI intervals strongly decreased  
 395 when going from a small number to a large number of training points. The spatial patterns of  
 396 PIs were very different from OK to QRF as already observed by Vaysse and Lagacherie  
 397 (2017). Note also that the PI maps were very similar for all the QRF models, suggesting that  
 398 the sampling strategy is not important at this high number of sampling points.





399

400 **Fig 11.** Particle-size prediction interval (90%) for the four maps using 3000 sampling points  
 401 (2500 for training and 500 for testing)

402 These results were expected and supported environmental information integration in DSM  
 403 models for mapping against pure geostatistical interpolation. With a large set of data, the QRF  
 404 sampling strategies were indifferent, and the variability of prediction was more affected by  
 405 the number of calibration samples. However, for small size of training points, cLHS appeared  
 406 to be useful (i.e., for QRF, sampling capturing the maximum combinations of the values of  
 407 relevant covariates). We suggest that for planning soil sampling for DSM, the use of sampling  
 408 design that aims to capture the maximum of information is required. There are still  
 409 discussions about the best sampling strategy for a small number of samples: it is beneficial to  
 410 use methods such as cLHS or k-means clustering based on covariates when covariates exhibit  
 411 contrasted values, which is the case in the present study. However, if the contrast of  
 412 covariates is smoother, then it may be more important to get a rather regular coverage of the  
 413 geographical space. Overall, increasing the number of training points to more than 2500 led to

414 a relatively small increase in prediction performances, which suggests that acquiring more  
415 points may not be worth considering the gain in accuracy that can be achieved. This  
416 observation might be different if we consider more complex models such as deep learning  
417 (Padarian et al., 2019; Ng et al., 2020) or new (or finer resolution) covariates that can explain  
418 soil texture variability better. This proposal will be tested in future work.

#### 419 **4. Conclusions**

420 We evaluated the effect of soil observations density on the digital soil mapping model's  
421 performance for topsoil particle-size distribution with four sampling strategies and with a  
422 decreasing number of training points. We demonstrated a threshold of sampling density, and  
423 that sampling with a density less than about 1 profile per 2 km<sup>2</sup> could lead to a substantial  
424 decrease in the performance accuracy. This result is significant, considering that the density  
425 recommended for conventional soil mapping at 1:250,000 is 1 profile per 20 km<sup>2</sup>, which is 10  
426 times smaller. We showed that sampling strategies based on covariates or coordinates with  
427 cLHS did not produce different results from random sampling when the number of training  
428 samples was large. We showed that increasing the number of training samples produced  
429 better improvements in the predictions maps when using QRF models compared to ordinary  
430 kriging. We conclude that the main limitations of DSM prediction accuracy are the amount of  
431 data collected in the field and high-quality covariates. Future DSM activities should focus on  
432 gathering more field observations. However, increasing the number of training points may in  
433 some cases not be worth considering the gain in accuracy that can be achieved.

434

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#### 457 **Authors’ contribution**

458 D.A. and A.R-d-F conceptualized and supervised the work and obtained the funding for the  
459 project. T.L. did the majority of the data treatment and modelling. P.L., C.D., and B.M.,  
460 substantially improved several early drafts of the paper especially for methods considerations,  
461 comments on the results and discussion. C.D. provided point data and his expertise of soil  
462 mapping in this region. T.L., D.A. and A.R-d-F wrote the final draft of the paper with a

463 substantial contribution from B.M., P.L., and C.D. All authors contributed equally to the  
464 revision of the paper.

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