

Some considerations on aggregate sample supports for soil inventory and monitoring

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Short title: *Sample support*

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1 **Summary**

2 Soil monitoring and inventory require a sampling strategy. One component of this strategy
3 is the support of the basic soil observation: the size and shape of the volume of material
4 that is collected and then analysed to return a single soil datum. Many, but not all, soil
5 sampling schemes use aggregate supports in which material from a set of more than one
6 soil cores, arranged in a given configuration, is aggregated and thoroughly mixed prior to
7 analysis. In this paper it is shown how the spatial statistics of soil information, collected on
8 an aggregate support, can be computed from the covariance function of the soil variable on
9 a core support (treated as point support). This is done via what is called here the discrete
10 regularization of the core-support function. It is shown how discrete regularization can
11 be used to compute the variance of soil sample means, and to quantify the consistency of
12 estimates made by sampling then re-sampling a monitoring network, given uncertainty in
13 the precision with which sample sites are relocated. These methods are illustrated using
14 data on soil organic carbon content from a transect in central England. Two aggregate
15 supports, both based on a 20-m \times 20-m square, are compared with core support. It is
16 shown that both the precision and the consistency of data collected on an aggregate
17 support are better than data on a core support. This has implications for the design of
18 sampling schemes for soil inventory and monitoring.

19 Introduction

20 There is a growing interest in how to sample the soil most efficiently for purposes of
21 inventory and monitoring, spurred by concerns about the impact of human activities on
22 soils and their functions (Arrouays *et al.*, 2009). Among the questions that have been
23 discussed is the choice of sampling design (Papritz & Webster, 1995) and the sources of
24 uncertainty in the resulting estimates (Goidts *et al.*, 2009). Less attention has been paid
25 to the question of what should constitute the support of the basic soil observation.

26 ‘Support’ is a term from geostatistics. It denotes the size and shape of the volume
27 of material which is analysed to return a single observation in a sample, so the support for
28 a soil observation may be, for example, a vertical cylindrical core of diameter 5 cm and
29 depth 0–15cm. A change of support will result in a change in the statistical properties of
30 soil observations. In practice a support such as a soil core in the example above is so small
31 in comparison to the region of interest that it can be regarded as a point support. The
32 covariance function or variogram of observations on an (effective) point support can be
33 used to compute the statistical properties of observations on a larger support. This process
34 is known as regularization, and is described in standard geostatistical texts (Journel &
35 Huijbregts, 1978; Webster & Oliver, 2009). The question of sample support is discussed
36 briefly by de Gruijter *et al.* (2006). In general increasing the extent of the sample support
37 reduces the contribution of fine-scale variation to our data, this is the regularization effect.
38 It is most readily achieved in soil sampling by bulking.

39 When we sample soil, and other materials such as water or grain, it may be possible
40 to mix thoroughly a number of specimens (aliquots) from within a specified region, such
41 as an experimental plot, so that the properties of the aggregated material correspond to
42 the average value of the original individual aliquots. This is known as aggregate, bulk
43 or composite sampling. Composite sampling is appropriate for compositional properties
44 of the soil such as its clay or water content or concentrations of elements such as carbon
45 determined by a total element analysis. Exchangeable species can also be determined

46 from a bulk sample (it is common practice for nutrients) if it can be assumed that the
47 adsorption isotherm is effectively linear over the range of concentrations in the aliquots.
48 Bulk sampling is not generally suitable for soil pH in conditions where significant frag-
49 ments of carbonate are present in some of the aliquots (Webster & Oliver, 1990), and
50 obviously is not applicable to soil properties that require the structural integrity of soil
51 below some representative elementary volume for laboratory determination (for example,
52 for hydraulic conductivity or parameters of the soil water characteristic curve). De Gruij-
53 jter *et al.* (2006) discuss sample support and composite sampling separately, but in the
54 case of soil sampling it seems appropriate to define the sample support both in terms
55 of the size and shape of the aliquots, and their spatial distribution. I refer to this as
56 the ‘aggregate sample support’. In the case of the National Soil Inventory (England and
57 Wales)(NSI), for example, the aggregate support of the analytical data is 25 cores, each
58 2.5 cm in diameter and extracted from depth 0–15 cm, collected from a nodes of a square
59 grid of interval 5 m in a 20-m square centred at the nominal sample location (SNIFFER,
60 2007).

61 The aggregate sample support varies between different soil sampling schemes. In
62 the United Kingdom we have already seen that the NSI (England and Wales) uses one
63 particular aggregate support. The Geochemical Baseline Survey (G-BASE) of the British
64 Geological survey uses a similar aggregate support for soil: 5 cores (depth 0–15 cm) are
65 collected at the centre and vertices of a 20-m square centred at the nominal sample loca-
66 tion and then aggregated (SNIFFER, 2007). The Representative Soil Sampling Scheme
67 (England and Wales) aggregates 20–25 cores collected in a ‘W’-pattern across a sample
68 field of no larger than 10 ha. By contrast the Countryside Survey of Great Britain does
69 not undertake aggregate sampling and the sample support for analytical data is a single
70 core (Emmett *et al.*, 2008). Similarly, any analytical datum from the National Soil In-
71 ventory of Scotland corresponds to a horizon in a single soil pit (SNIFFER, 2007). The
72 implications of the differences in sample support between these schemes, and the question

73 of what support is most appropriate, has received little attention.

74 One reason for this is that, as De Gruijter *et al.* (2006) point out, there is no general
75 theory of composite sampling. Webster & Burgess (1984) considered the use of a single
76 composite sample across a small region to estimate the mean value of soil properties across
77 that region, and gave expressions for the error variance. In this case the aggregate support
78 of a single composite specimen consists of cores drawn from across the region of interest,
79 which might be a field or experimental plot. This does not describe the situation we are
80 concerned with here, in which the region represented by the aggregate support of a single
81 sample is small compared to the overall domain of interest, which may be very large in
82 regional, national or even supra-national soil inventory and monitoring.

83 Aggregate sample support influences the variability of our basic soil data when we
84 conduct inventory and monitoring across a region, and therefore determines the precision
85 with which we can estimate regional means. It is also likely that sample support will
86 affect the contribution of spatial variation to the sampling error for estimates of temporal
87 change in the soil when monitoring by revisiting a sample network. The aim of this paper
88 is therefore to develop some theory for comparing different aggregate sample supports
89 (including supports in which a single aliquot is collected). Sample supports are compared
90 with respect to the variability of the basic observations made on the support, and so the
91 precision of estimates that we draw from them. They are also compared with respect
92 to the repeatability, site-by-site, of estimates made by re-sampling the soil with error in
93 relocation of the sites, and so the confidence with which we can detect change. Having
94 shown how this can be done, the methods will be applied in order to compare some
95 sampling supports for the measurement of soil organic carbon content, using data collected
96 across a region of lowland England in mixed land-use.

97 **Theory**

98 In this section I first show how one can derive the spatial covariance function of a variable
99 measured on an aggregate support from the covariance function on core-support. This is

100 a necessary preamble to a demonstration of the effect of sample support on the precision
101 of sampling estimates, and on their site-by-site repeatability.

102 When we fit covariance functions (or, comparably, variograms) to data on soil and
103 then use these to predict by kriging we are undertaking model-based statistical analysis, in
104 which the random variation of our target variable is assumed to come from an underlying
105 stochastic process, and our data are treated as a realization of a random function which
106 is modelled. This is in contrast to design-based analysis in which we have sampled the
107 soil according to a probability sample design (such as stratified random sampling) and it
108 is this randomized sampling scheme that allows us to analyse our observations as random
109 variables (de Gruijter *et al.*, 2006). However, having fitted a model for a random function
110 we can compute its variance over some region, and can then treat this as the expected
111 value of the variance of the population of values in that region when it is sampled according
112 to a randomized design (Cochran, 1977). This approach was taken by Papritz & Webster
113 (1995) to compare the variances of model and design-based estimates in soil monitoring,
114 and I follow it here. The covariance function on an aggregate support can be used to
115 compute both the variance of observations on that support across a region, and, from this
116 variance, the standard errors of the estimates made from design-based samples of such
117 observations.

118 I then consider the problem of how repeatable our observations of soil are, site-by-
119 site, in the presence of relocation error. I quantify this by presenting a calculation of the
120 correlation between an observation of the soil, and a repeat observation with relocation
121 error, assuming no underlying change in the soil.

122 Note that in this paper I assume that all samples are drawn from a two-dimensional
123 space and aggregate sample supports are defined over two-dimensional regions, although
124 the individual aliquots are defined in three dimensions (as with cylindrical cores). The
125 principles, however, would extend simply to aggregation of cores on a transect in one
126 dimension or over volumes in three dimensions.

127 *The covariance function.*

128 In the following sections the observations of a soil variable on a point support are modelled
129 as realizations of a random function, $Z(\mathbf{x})$. We assume that this random function consists
130 of a mean (fixed effect) and a random effect. The mean may be the overall mean of Z
131 across the region of interest, in which case the random effect represents the variation of
132 Z about that mean. Alternatively, we may have divided the region of interest into classes
133 such as soil map units or land-use classes. In this case the mean for $Z(\mathbf{x})$ could be the
134 mean value of Z for the class that occurs at location \mathbf{x} , and the random effect is the
135 within-class variation. For simplicity in this section the overall mean is the fixed effect.
136 The random effect is assumed to be a second-order stationary random function which
137 means that it has finite variance and so the spatial covariance function exists:

$$C(\mathbf{h}) = \text{E} [\{Z(\mathbf{x}) - \text{E}[Z(\mathbf{x})]\} \{Z(\mathbf{x} + \mathbf{h}) - \text{E}[Z(\mathbf{x} + \mathbf{h})]\}], \quad (1)$$

138 where \mathbf{h} denotes a separation (lag) in space. The covariance declines as the lag distance,
139 $|\mathbf{h}|$, increases and equals zero at lag distances larger than or equal to the range of the
140 covariance function. The *a priori* variance of the random effect is equal to the covariance
141 at lag zero. This is the variance of the variable in a region which is large in comparison with
142 the range of the covariance function. In practice we must fit some appropriate function to
143 describe the covariance of data, and the range (or a related distance parameter) and the
144 *a priori* variance are parameters of this function. One complication that often arises in
145 practice is the nugget effect. There is always some minimum separation, larger than zero,
146 between observations in a real data set and variation that is not spatially dependent at
147 lags larger than this minimum distance cannot be distinguished from spatially correlated
148 variation. As a result the covariance function will appear to converge to some value less
149 than the *a priori* variance as the lag distance decreases, the spatially correlated variance,
150 c_1 . The difference between the *a priori* variance and c_1 is the nugget variance, c_0 which
151 is the variance of all components of the random function with spatial dependence over
152 distances smaller than the minimum lag between our observations. A general form of a

153 model for the covariance function, fitted to data, is therefore

$$\begin{aligned}
 C(\mathbf{h}) &= c_0 + c_1, \quad |\mathbf{h}| = 0, \\
 &= c_1 \rho(\mathbf{h}), \quad |\mathbf{h}| > 0,
 \end{aligned}
 \tag{2}$$

154 where $\rho(\mathbf{h})$ is a spatial correlation function such as the spherical

$$\begin{aligned}
 \rho_{\text{sp}}(\mathbf{h}|a) &= 1 - \left\{ \frac{3|\mathbf{h}|}{2a} - \frac{1}{2} \left(\frac{|\mathbf{h}|}{a} \right)^3 \right\} \quad \text{for } |\mathbf{h}| < a \\
 &= 0 \quad \text{for } |\mathbf{h}| \geq a,
 \end{aligned}
 \tag{3}$$

155 where a is presented after the vertical bar because it is a parameter of the correlation
 156 function, the range.

157 *The covariances of bulk samples: discrete regularization.*

158 Let \mathbf{x}_i denote the i th sample location, for which a single composite sample is to be
 159 formed on an aggregate support. A total of n_i cores is collected at a local array of sites
 160 $X_i = \{\mathbf{x}_{i,1}, \mathbf{x}_{i,2}, \dots, \mathbf{x}_{i,n_i}\}$. I assume that the aggregate support is fixed for all sites so
 161 $n_i = n_j = n \forall i, j$ and $(\mathbf{x}_{i,m} - \mathbf{x}_i) = (\mathbf{x}_{j,m} - \mathbf{x}_j) = \mathbf{a}_m \forall i, j; 1 < m \leq n$. I denote the
 162 aggregate support by $\mathcal{A} = \{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n | \boldsymbol{\kappa}\}$ where the vector $\boldsymbol{\kappa}$ characterizes the size
 163 and shape of a single aliquot.

164 Let $\check{Z}_{\mathcal{A}}(\mathbf{x}_i)$ denote a random function, the value of soil property z determined on
 165 the material collected on aggregate support \mathcal{A} at location \mathbf{x}_i . Note that I follow the usual
 166 convention here of putting random functions in upper case and their realizations in lower
 167 case. An actual observation of property z on this aggregate support would be written
 168 $\check{z}_{\mathcal{A}}(\mathbf{x}_i)$. I assume that $\check{Z}_{\mathcal{A}}(\mathbf{x}_i)$ is equal to the arithmetic mean of Z at the locations in the
 169 aggregate support

$$\check{Z}_{\mathcal{A}}(\mathbf{x}_i) = \frac{1}{n} \sum_{m=1}^n Z(\mathbf{x}_{i,m}).
 \tag{4}$$

170 This ignores any sub-sampling error in extracting material for analysis from the aggregated
 171 material, but this error is present in all analysis of field soil samples, regardless of their
 172 basic support, and so is not relevant to a comparison between sample supports.

173 The implication of Equation (4) is that the expectation (mean) of the variable Z
 174 within our domain is independent of the aggregate support. This requires that there is
 175 nothing in the process of aggregation that introduces bias. We now require a spatial
 176 covariance function for the variable on an aggregate support, $\check{Z}_{\mathcal{A}}$, that is

$$C_{\mathcal{A}}(\mathbf{h}) = \text{Cov} \left[\check{Z}_{\mathcal{A}}(\mathbf{x}_i), \check{Z}_{\mathcal{A}}(\mathbf{x}_i + \mathbf{h}) \right], \quad (5)$$

177 where \mathbf{h} is a lag vector. On the assumption that the variable on point support is stationary
 178 in the variance, it is clear from the covariance of two sample means that this expression
 179 is given by

$$\begin{aligned} C_{\mathcal{A}}(\mathbf{h}) &= \frac{1}{n^2} \sum_{\mathbf{x} \in X_i} \sum_{\mathbf{x}' \in X_{i+\mathbf{h}}} \text{Cov} [Z(\mathbf{x}), Z(\mathbf{x}')], \\ &= \frac{1}{n^2} \sum_{\mathbf{x} \in X_i} \sum_{\mathbf{x}' \in X_{i+\mathbf{h}}} C(\mathbf{x} - \mathbf{x}'), \end{aligned} \quad (6)$$

180 where $X_{i+\mathbf{h}} = \{\mathbf{x}_{i,1} + \mathbf{h}, \mathbf{x}_{i,2} + \mathbf{h}, \dots, \mathbf{x}_{i,n} + \mathbf{h}\}$ and $C(\mathbf{h})$ denotes the covariance function
 181 of the point-support variable Z . In practice we will use a suitable function of the form of
 182 Equation (2), fitted to available data on a small enough support (e.g. cores) to be treated
 183 as point support.

184 Equation (6) is directly analogous to the expression for the regularization of the
 185 covariance function to a continuous support (Jupp *et al.* 1988). Let \mathcal{B} denote some such
 186 support (it might be a square raster pixel in a GIS, for example, that takes the mean value
 187 of some variable, such as vegetation cover, over its extent). If $C(\mathbf{h})$ denotes the point-
 188 support covariance function of the variable of interest, then the regularized covariance
 189 function on support \mathcal{B} is given by

$$C_{\mathcal{B}}(\mathbf{h}) = \frac{1}{|\mathcal{B}_{\mathbf{s}}| |\mathcal{B}_{\mathbf{s}+\mathbf{h}}|} \int_{\mathbf{x} \in \mathcal{B}_{\mathbf{s}}} \int_{\mathbf{x}' \in \mathcal{B}_{\mathbf{s}+\mathbf{h}}} C(\mathbf{x} - \mathbf{x}') \, dx dx' \quad (7)$$

190 where $\mathcal{B}_{\mathbf{s}}$ denotes the sample support centred at location \mathbf{s} and $\mathcal{B}_{\mathbf{s}+\mathbf{h}}$ denotes the support
 191 with the same size and shape translated to location $\mathbf{s} + \mathbf{h}$; and $|\mathcal{B}|$ denotes the Lebesgue
 192 measure of the support (equivalent to its area in two dimensions) and the integrals are
 193 over the dimensions of \mathcal{B} . The difference between the regularized covariance function and

194 the expression in Equation (6) is that the former is the covariance of the mean of some
195 variable over a continuous region while the latter is the covariance of the average value
196 of a specific set of discrete observations of the variable on some sample array. For this
197 reason I call Equation (6) the ‘discretely regularized covariance function’ of the variable,
198 for the specified aggregate support.

199 The discretely regularized covariance function must be computed from Equation (6)
200 using an available covariance function on a point support, that is one fitted to available
201 data. There may be bias in the regularized function if the lag distances between the
202 individual locations that comprise the support, $|\mathbf{a}_1|, |\mathbf{a}_2|, \dots, |\mathbf{a}_n|$, are smaller than the
203 shortest distance in the data set from which the point-support covariance function, $C(\mathbf{h})$
204 is estimated, $|\mathbf{h}_{\min}|$. This is because the fitted model may underestimate or overestimate
205 the covariance at lags shorter than $|\mathbf{h}_{\min}|$. If we wish to evaluate possible aggregate
206 supports then we require covariance functions based on data which include lag intervals
207 shorter than the distances between the aliquots that comprise the aggregate supports of
208 interest. Stein (1999) (page 220) showed that adding a small number of additional points
209 to a regular sample array can substantially improve the modelling of spatial dependence
210 at short distances, and Haskard (2007) showed dramatic improvements in the modelling of
211 short range variation by placing just 10 (out of 100) sample locations at short separations
212 within a sample grid.

213 *Variances of discretely regularized variables.*

214 We have obtained a discretely regularized covariance function for soil data on an aggregate
215 support. Our next objective is to show how we can compute variances of variables
216 measured on this aggregate support. Consider a region \mathcal{R} which we intend to sample on
217 the aggregate support \mathcal{A} at sites selected by simple random sampling. To compute the
218 variance of the resulting sample mean of variable $Z_{\mathcal{A}}$, we require the variance of $Z_{\mathcal{A}}$ in \mathcal{R}
219 according to the covariance model, which we treat as the expected population variance
220 for random sampling. In geostatistics this is called the dispersion variance (Journal &

221 Huijbregts, 1978) and it can be calculated from the covariance function as:

$$\sigma_{\mathcal{A},\mathcal{R}}^2 = C_{\mathcal{A}}(0) - \frac{1}{|\mathcal{R}|^2} \int_{\mathbf{x} \in \mathcal{R}} \int_{\mathbf{x}' \in \mathcal{R}} C_{\mathcal{A}}(\mathbf{x} - \mathbf{x}') \, d\mathbf{x}d\mathbf{x}'. \quad (8)$$

222 If the linear extent of \mathcal{R} is large in comparison with the range of the covariance function
223 then the double integral in Equation (8) is negligible and the dispersion variance and the
224 *a priori* variance can be assumed to be equal (Journel & Huijbregts, 1978). Otherwise the
225 second term on the right-hand side of Equation (8) can be calculated most conveniently
226 by a Monte Carlo double integration in which random pairs of locations are drawn from
227 within \mathcal{R} and the average value of the covariance function for the lag interval between
228 them is computed.

229 It may be that region \mathcal{R} is to be sampled by stratified random sampling. In this case
230 the within-stratum variance is required to compute the standard errors of our estimates.
231 We may distinguish two situations here. In the first, geometrical stratification, the strata
232 are formed by dividing \mathcal{R} into equal subregions, within each of which samples are drawn
233 independently and at random. If one stratum can be represented by region \mathcal{S} then the
234 expectation of the within stratum variance can be computed by substituting \mathcal{S} for \mathcal{R} in
235 Equation (8). Provided that the dimensions of \mathcal{S} are not large relative to the range of $C_{\mathcal{A}}$
236 the within-stratum variance will be smaller than the dispersion variance for \mathcal{R} , wherein lies
237 the benefit of stratification. In the second situation our strata may be categories such as
238 land-use, or soil map units. To obtain the within-stratum variance in this case we require
239 the point-support covariance function for the within-stratum variation. The discretely
240 regularized covariance function of the within-class variation can then be computed, and
241 the expected within-stratum variance is then obtained using Equation (8) evaluating the
242 double integral over the region \mathcal{R} .

243 Some hypothetical examples are presented in Figure 1. Here I considered variables
244 which, on a point support, have a spherical covariance function with range 100 or 500
245 m and an *a priori* variance of 1.0, of which some varying proportion from 0 to 0.75
246 corresponds to the nugget variance. I then computed the dispersion variance for these

247 variables within a 1×1-km block. The calculation was then repeated for the discretely
248 regularized variable, with the support being five aliquots collected at the centre and
249 vertices of a 20-m square then bulked. Note that the dispersion variance on the point
250 support is very close to the *a priori* variance when the range of the covariance function is
251 100 m, since this is small relative to the dimensions of the block. The dispersion variance
252 is smaller when the range is larger, but the discrepancy decreases as the proportion of the
253 nugget variance increases. In all cases the dispersion variance on the aggregate support is
254 smaller than on the core support. The extent of this reduction in variance by aggregation
255 depends in part on the range of the covariance function, but most dramatically on the
256 relative importance of the nugget variance since this very short-range variation is most
257 susceptible to the regularizing effect of aggregation. If we consider the dispersion variance
258 as the expected population variance for a random sample of the region, it is clear that
259 substantial reductions in the variances of sample means can be achieved by use of an
260 aggregate support. For example, with a nugget variance of 0.25 and a range of 100 m, the
261 variance of the sample mean is reduced by 37% by use of the aggregate support rather
262 than the core support. To achieve this reduction in variance while retaining the core
263 support would require an increase in the number of sample sites of 270%.

264 *Re-sampling and location error.*

265 When monitoring the soil we estimate the change that has occurred in the value of some
266 property over the time period between successive samplings. When our interest is in the
267 change in the spatial mean, then the most efficient sampling design entails revisiting the
268 original sample sites (de Gruijter *et al.*, 2006; Lark, 2009). At the limit the exact sample
269 site cannot be revisited since soil properties are almost always determined destructively
270 by the removal of material for analysis. In practice there is error in the relocation of the
271 sample site, the magnitude of which depends on whether the site is permanently marked
272 or whether it must be relocated by survey from local landmarks or with a GPS. Defra
273 (2003) report studies on the error in locating sample sites for soil monitoring.

274 A surveyor has visited a site at time t_1 and recorded its location. Let the true
 275 location be \mathbf{x}_1 . At time t_2 the site is relocated as carefully as possible. Let the true
 276 location of the identified position be \mathbf{x}_2 , so the location error is $\mathbf{d} = \mathbf{x}_1 - \mathbf{x}_2$. In practice
 277 the surveyor may collect soil at time t_2 from $\mathbf{x}_2 + \boldsymbol{\delta}$ where $\boldsymbol{\delta}$ is a deliberate offset to avoid
 278 sampling disturbed ground. I assume that the location error is isotropic (the surveyor is
 279 no more likely to err in one direction than another) and that relocation is unbiased, so on
 280 average $|\mathbf{d}| = 0$. I assume that the additive effects of sources of location error result in a
 281 normal distribution, so that the relocation error is a bivariate normal random variate \mathbf{D}
 282 with probability density function $f(\mathbf{D})$ and distribution

$$\mathbf{D} \sim \mathcal{N}(0, \sigma_l^2 \mathbf{I}), \quad (9)$$

283 where the mean of zero indicates the lack of bias, and the form of the covariance matrix,
 284 with \mathbf{I} the identity matrix, shows that the errors are isotropic, they are uncorrelated and
 285 their standard deviation in any dimension is equal to σ_l .

286 We may characterize the repeatability of a soil monitoring scheme given location
 287 error and sampling on a particular aggregate support, \mathcal{A} , by calculating the expected cor-
 288 relation between determinations of a soil property on sampling on the aggregate support,
 289 and then independently re-sampling on the same support, with location error in each case.
 290 We assume that no change occurs between the two samplings, so the differences between
 291 the determinations simply reflect spatial variability on the aggregate support. The mean
 292 covariance between the determinations is $C^{1,2}$

$$C^{1,2} = \int_{-\infty}^{\infty} f(\mathbf{D}) C_{\mathcal{A}}(\mathbf{D} + \boldsymbol{\delta}) d\mathbf{D}, \quad (10)$$

293 where the integral is over both dimensions of the variate \mathbf{D} . This can be scaled to a
 294 correlation, $\rho^{1,2}$ by

$$\rho^{1,2} = \frac{C^{1,2}}{C_{\mathcal{A}}(0)}. \quad (11)$$

295 The stronger this correlation the greater the repeatability of our observations of the soil,
 296 site-by-site, on the specified aggregate support.

297 If there is a substantial nugget effect in the point-support covariance function model
 298 which is largely attributable to fine-scale soil variation, then Equation (11) may under-
 299 estimate the correlation between successive re-samplings of a site because the correlation
 300 of the variable over very short distances is underestimated. To compute an upper bound
 301 on the correlation $\rho^{1,2}$ I propose that the empirical covariance function in Equation (2) is
 302 replaced by

$$\begin{aligned}
 C'(\mathbf{h}) &= c_0 + c_1, \quad |\mathbf{h}| = 0, \\
 &= c_0 \rho_{\text{sp}}(\mathbf{h}||\mathbf{h}_{\text{min}}|) + c_1 \rho(\mathbf{h}), \quad |\mathbf{h}| > 0,
 \end{aligned}
 \tag{12}$$

303 where $\rho(\mathbf{h})$ is the fitted correlation function and $\rho_{\text{sp}}(\mathbf{h}||\mathbf{h}_{\text{min}}|)$ is a spherical correlation
 304 function with range equal to $|\mathbf{h}_{\text{min}}|$, the shortest distance between observations in the data
 305 set from which the empirical model is obtained. Since the spherical correlation function is
 306 zero at distances greater than the range this modified covariance function and the fitted
 307 one are identical over lag distances larger than $|\mathbf{h}_{\text{min}}|$, and it is assumed that all the
 308 variation attributed to the nugget is spatially correlated at distances up to $|\mathbf{h}_{\text{min}}|$. I used
 309 a spherical correlation function here because its correlation goes exactly to zero at the
 310 range. Other functions with this property (e.g. the circular model) could be used and the
 311 choice of function will have a small effect on the computed upper bound.

312 If it is possible to estimate the independent measurement error for the soil variable
 313 of interest, σ_{m}^2 , which is a component of the nugget variance, c_0 , then Equation (12) may
 314 be replaced by

$$\begin{aligned}
 C'(\mathbf{h}) &= c_0 + c_1, \quad |\mathbf{h}| = 0, \\
 &= (c_0 - \sigma_{\text{m}}^2) \rho_{\text{sp}}(\mathbf{h}||\mathbf{h}_{\text{min}}|) + c_1 \rho(\mathbf{h}), \quad |\mathbf{h}| > 0,
 \end{aligned}
 \tag{13}$$

315 I propose that $\rho^{1,2}$ is estimated initially with the discretely regularized form of the
 316 fitted covariance function for the target soil property, but that the modified covariance
 317 function, Equation (12) or (13) is also used to indicate how much stronger the correlation
 318 between site-by-site repeated observations might be if the fine-scale variation is spatially

319 dependent up to lag $|\mathbf{h}_{\min}|$.

320 **Case study**

321 It has been shown above how the covariance function of a soil property on a point support
322 (approximated in practice by a soil core) can be used to compute the discretely regularized
323 covariance function for observations on an aggregate support. This, in turn, can be used to
324 compute expected values of the variances of the variable on an aggregate support, and to
325 assess the susceptibility of repeated observations of the soil property at a site to relocation
326 error. In this case study I use these methods to calculate, for different sample supports,
327 the variances of means for topsoil organic carbon, obtained by stratified random sampling
328 with land-use classes as strata. I also compute the correlation of repeat samplings of this
329 variable given possible distributions of location errors.

330 *Data and Analyses*

331 The data used here were collected on core support in an agricultural landscape in Bed-
332 fordshire, eastern England. The collection of the data is described in detail elsewhere
333 (Haskard *et al.*, 2010, Milne *et al.*, 2011). In summary, the transect was approximately
334 7.5 km long. The transect started at 508329, 237450 on the UK Ordnance Survey grid
335 (units in metres) and was on a line of bearing 173.5 degrees from grid north, ending at
336 OS grid reference 509182, 229991. There were 256 sample locations at regular intervals
337 (29.45 m) along the transect. To allow analysis of spatial dependence at short distances
338 an additional ten pairs of points were added, each pair comprising one point at 3 m and
339 and one at 6 m along the transect from one of the regular sites. Any variation spatially
340 correlated at distances less than 3 m would therefore contribute to the nugget variance
341 of fitted covariance functions. The soil was sampled at each of the 276 locations to depth
342 150 mm with a cylindrical gouge auger of internal diameter 44 mm. Milne *et al.* (2011)
343 describe the soils of the transect in more detail. The northernmost point was over the
344 Lower Greensand and the transect intersected the boundary between this formation and

345 outcrops of the Gault Clay and the Chalk. The southernmost point was at the top of the
346 Chalk escarpment. The soil on the transect is formed in parent materials derived directly
347 from the country rock, and from varied superficial material including alluvium, drift of
348 varied texture and calcareous colluvium below the scarp of the Chalk. Milne *et al.* (2011)
349 also describe land-use along the transect. For purposes of this paper we describe three
350 land-use classes, and assume that these would be used as strata in stratified random sam-
351 pling of the soil. The classes are arable land (including some land recently set aside, but
352 still under stubble from a recent crop) with 176 observations, woodland (predominantly
353 broadleaf) with 39 observations and uncultivated land (permanent grass, paddock, some
354 waste ground on field margins and some sports grass) with 60 observations.

355 One sub-sample of the soil from each location was oven-dried to a constant weight
356 to determine the gravimetric water content. Another sub-sample of the soil from each
357 location was air-dried and sieved to pass 2 mm. A sub-sample of the air-dried material
358 was then analysed to determine the total carbon content by combustion in a LECO
359 analyser (LECO CNS 2000 combustion analyser, LECO, St Joseph, Michigan, USA).
360 The carbonate content was determined by the water-filled calcimeter method of Williams
361 (1949) and the organic carbon content (OC) was calculated by subtracting this value
362 from the total carbon content. Soil organic carbon content was then expressed in units
363 of grammes of organic carbon per 100 g dry soil.

364 One outlying observation was removed from the data set (19 g OC 100 g⁻¹ soil).
365 It was very different from the remaining data (the next-largest value was 8.5 g 100g⁻¹)
366 and would have an undue influence on estimated covariances. Table 1 provides sum-
367 mary statistics on the remaining 275 observations, and on the residuals from the land-use
368 means. These include the octile skewness coefficient (Brys *et al.*, 2003). It was clear that
369 the residuals were reasonably symmetrically distributed, and can plausibly be treated
370 as a realization of a normal random function. The empirical covariance function of the
371 residuals, estimated by the standard methods of moments estimator described by Box &

372 Jenkins (1976), is shown by the solid symbols in Figure 2. This shows continuity of the
373 covariance down to the shortest lag distance (3 m), and a substantial nugget effect.

374 A linear mixed model was then fitted to the data (Stein, 1999) by residual maximum
375 likelihood using the `lme` procedure from the `nlme` library (Pinheiro *et al.*, 2010) for the R
376 statistical platform (R Development Core Team, 2010). In this model, the land-use was
377 treated as a fixed effect. The empirical covariance function of the residuals suggested that
378 a covariance model with a spatially correlated component (spherical or exponential) and
379 a nugget effect would be appropriate. Both spherical and exponential models were fitted.
380 These can be compared directly with respect to their residual log likelihoods. The log
381 likelihood for the exponential model (-338.5) was larger than that for the spherical model
382 (-341.7) so the exponential model was selected. The estimated fixed and random effects
383 for this mixed model are presented in Table 2. Since the data were on a transect it had to
384 be assumed that the random effect was isotropic. Figure 2 shows the covariance function
385 for the random effects (the covariance of the residuals from the land-use means) with the
386 covariance parameters given in Table 2 (solid line). The modelled covariance is smaller
387 than the empirical covariance function at longer lag distances and the modelled *a priori*
388 variance is larger than the empirical estimate, which is consistent with theory, indicating
389 the bias entailed by estimating the covariance from ordinary least squares residuals (Lark
390 *et al.*, 2006).

391 I then computed discretely regularized covariance functions for soil organic carbon
392 on different supports, treating the estimated covariance function given in Table 2 as the
393 point-support function. Functions were computed for the NSI (England and Wales) and
394 the British Geological Survey G-BASE soil sample aggregate supports that are described
395 earlier. In both cases the shortest distance between aliquots in the sample support (5 m in
396 NSI and 14 m in G-BASE) is larger than the shortest distance between observations from
397 which the covariance parameters have been estimated (3 m). The difference between the
398 discretely regularized covariance function for these two aggregate supports was negligible

399 (the *a priori* variances differed by 0.13%). This is of interest because it suggests that
400 collecting as many as 25 individual cores from a 20-m square may not be justified (unless
401 it is necessary to ensure sufficient soil for the planned analyses). To investigate this further
402 I computed the *a priori* variance for data on an aggregate support based on a 20-m square
403 with varying numbers of cores. The variances are plotted against the number of cores in
404 Figure 3, which also shows the disposition of cores within a single square. This confirms
405 that the variance drops rapidly as the number of aliquots is increased to five, but adding
406 further aliquots has little effect.

407 I then computed dispersion variances by Monte Carlo integration for soil organic
408 carbon on the point support and G-BASE aggregate support within square domains with
409 sides of various lengths between 1 and 10 km. These are plotted on Figure 4, including
410 the *a priori* variances which are very close to the dispersion variances for regions length 5
411 km or more. The *a priori* variance of the variable on an aggregate support is 32% of that
412 on the point support. The dispersion variances on the aggregate support within a 1-km
413 square block is 36% of that on the point support.

414 Assume that a sample is drawn from a region of 10-km×10-km or larger, with soil
415 variability comparable to the landscape investigated here. Stratified random sampling
416 is used with the land-use classes as strata. The *a priori* variances of the point-support
417 and aggregate support covariance functions computed from the estimated parameters in
418 Table 2 would be the expected pooled within-stratum variance, σ_w^2 (there are not sufficient
419 data here to estimate separate variance parameters for the different classes). The standard
420 error of the mean SOC estimated from N observations distributed in proportion to the
421 areas of the different strata would be $\sqrt{\frac{\sigma_w^2}{N}}$. If we wanted the 95% confidence interval on
422 an estimate of the mean to be approximately $\pm 10\%$ of the mean (which is 2.7 g 100g⁻¹
423 soil) then calculations show that we would require about 62 samples on a core support,
424 but because of the smaller variance on the aggregate support only 42 aggregate samples
425 would be required. This would be a substantial saving of field effort and analytical costs.

426 I used Equations (10) and (11) to compute the expected correlation between data
427 obtained by two samplings of the same set of locations, assuming that the location error
428 \mathbf{D} is normally distributed with mean zero and different standard deviations, and that
429 the offset δ to avoid re-sampling disturbed sites is 10 cm. The point-support covariance
430 function with parameters in Table 2 was used. The results are plotted in Figure 5 for
431 point, G-BASE and NSI support. An upper bound for the correlation was also obtained
432 by substituting a spherical covariance function for the nugget as in Equation (12) with
433 $|\mathbf{h}_{\min}| = 3$ m, and this is also shown in Figure 5.

434 Defra (2003) reports estimates of relocation error in revisiting soil sampling sites.
435 On enclosed land it was estimated that the relocation error was less than 10 m in 61%
436 of trials. If the relocation error is assumed to be bivariate normal then this implies a
437 standard deviation in any one dimension of about 7 m. On open land it was estimated
438 that the error was less than 10 m in 33% of cases, which implies a standard deviation in
439 any one dimension of about 11 m. When the standard deviations of the location error
440 are of this magnitude the difference between the calculated correlation of the sampled
441 and re-sampled observations and the upper bound of this correlation are negligible. The
442 calculated correlations with the standard deviation (one dimension) of 7 m were 0.62,
443 0.89 and 0.89 for the core, G-BASE and NSI supports respectively, and were very little
444 different for a standard deviation of 11 m (0.61, 0.87, 0.88).

445 Discussion

446 A geostatistical analysis allows us to make some plausible inferences about the relative
447 merits of different sample supports for soil inventory and monitoring, provided that we
448 have robust spatial covariance functions for the soil variable of interest from data sets
449 which allow us to model spatial dependence over distances less than the intervals between
450 aliquots of any proposed aggregate support. There is a general awareness that robust
451 planning of soil inventory and sampling requires some exploratory data on soil variability,
452 and this paper shows that information on fine-scale variation is also needed. This should

453 be a priority for future work on soil variability for planning soil surveys. Short-range
454 variability of soil properties may differ markedly between soils on different parent materials
455 and with different histories of land-use. It is therefore unrealistic to expect that a general
456 purpose covariance model will describe the effects of aggregation on the statistics of soil
457 data across a country or even a large region. This is true of any decisions on sampling
458 strategy based on observed statistics, some degree of generalization is unavoidable. In
459 practice two options are possible. One could identify areas where the fine-scale variation
460 of the soil is likely to be largest, and sample that region to obtain a covariance function
461 at fine scales to plan the sampling support. This would ensure that the precision of
462 measurements in the most variable regions was adequate. Alternatively, one might obtain
463 covariance functions for general regions which are expected to differ in their variability (for
464 example, lowland arable soils and upland grassland) and plan different sample supports
465 for these regions so that the precision in each is similar.

466 There are potentially large differences between the *a priori* variances of soil data on
467 point and aggregate supports, since in the latter case short-range variation is removed by
468 the process of bulking. The extent of this advantage depends on the spatial covariance
469 function of the variable on the point support. Nonetheless, it is clear that there are
470 potential advantages in using an aggregate support when the objective is to sample to
471 characterize a large region. While we cannot generalize from the results presented here on
472 soil organic carbon, from one particular data set, it is notable that the *a priori* variance
473 on the aggregate support is some 30% less than that on a core support, and about 30%
474 fewer samples were required to meet a reasonable quality standard for estimating regional
475 mean soil carbon content by stratified random sampling.

476 Given the interest in soil monitoring, the results on the effect of sample support on
477 the repeatability of sampling are important. These show considerable improvements in
478 the correlation between independent determinations of soil properties over sites when an
479 aggregate support is used. This is plausible since, with even quite large relocation errors,

480 the region of the aggregate support for the baseline and re-sampled observations will often
481 overlap, and aggregation reduces the short-range variation which contributes most to the
482 uncertainty in site-by-site comparisons over time. Figure 5 shows that the differences
483 in correlation can be large even when the relocation standard deviation is small, which
484 suggests that this is an significant consideration even as the performance of GPS or other
485 technology to aid relocation improves.

486 The aggregate sample requires more effort to collect at the local site than a single
487 core. The local grid must be marked out, and the samples collected, physically mixed and
488 sub-sampled. However, it is likely that the additional cost of these operations within each
489 sampling site will be less than that of adding additional sites to a randomized scheme,
490 with the administrative overheads, travel and analytical costs that each additional site
491 entails. It is also of interest in this case that the benefits of increasing the number of
492 aliquots within a 20-m square beyond five were negligible. By calculating the *a priori*
493 variance of observations on aggregate supports with different numbers of aliquots we can
494 make a rational decision as to how many are required to achieve target precision (although
495 there must also be enough to provide sufficient material for the planned analyses and for
496 archiving).

497 As noted earlier, there is considerable variation in the sample support used in differ-
498 ent schemes for soil inventory and monitoring, even within the United Kingdom. These
499 results suggest that it is advantageous to use an aggregate support where this is possible
500 for the soil properties of interest. Is it appropriate for existing surveys to change the sup-
501 port that they use? A change in the support of soil data can, in principle, influence all its
502 statistics. It would clearly be undesirable to change the support of soil data if this would
503 change the mean. If the depth in the soil from which individual aliquots are extracted
504 remains unchanged then a change of support should not affect the mean of a compo-
505 sitional property expressed gravimetrically such as organic carbon content or available
506 nutrients. Provided that the size and shape of the aliquots (as determined by sampling

507 tins or augers) as well as sample depth are unchanged then introducing an aggregate
508 support would have no effect on the mean of volumetric properties such as porosity or
509 bulk density. A change in the variance of soil data caused by a change in support need
510 not cause problems for the statistical analysis of the resulting data and their comparison
511 with earlier observations on a different support. There are quite standard expressions, for
512 example, to compute a standard error on the difference between two independent samples
513 of a variable when the samples cannot be assumed to have the same variance (Snedecor
514 & Cochran, 1989).

515 **Conclusions**

516 To conclude, provided that we have a sound model of the spatial covariance of a soil
517 property on point support, it is possible to compute the discretely regularized covariance
518 function for that same property on a range of aggregate supports. This function can be
519 used to compute the variance of the soil property on those supports within regions of
520 any size or shape, and to calculate how consistently the soil can be re-sampled on the
521 particular support, given relocation error.

522 In the case of soil organic carbon in a lowland environment, it was shown that the
523 variance of observations on the aggregate supports used by the National Soil Inventory
524 (NSI) of England and Wales, and the British Geological Survey's Geochemical Baseline
525 Survey (soils) is substantially smaller than on a single core support, and that the con-
526 sistency of re-sampling is also greater. To form robust conclusions across a range of
527 conditions and soil properties would require further sampling to allow us to model the
528 spatial covariances of these properties at fine (within-support) scales.

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534 **References**

- 535 Arrouays, D., Bellamy, P.H & Paustian, K. 2009. Soil inventory and monitoring: current
536 issues and gaps. *European Journal of Soil Science*, **60**, 721–722.
- 537 Box, G.E.P. & Jenkins, G.M. 1976. *Time Series Analysis: Forecasting and Control*.
538 Holden-Day, San Francisco.
- 539 Brys, G., Hubert, M. & Struyf, A. 2003. A comparison of some new measures of skewness.
540 In: *Developments in Robust Statistics* (eds R. Dutter, P. Filzmoser, U. Gather and
541 P.J. Rousseeuw), pp. 98–113. Physica-Verlag, Heidelberg.
- 542 Cochran, W.G. 1977. *Sampling Techniques*. 3rd Edition. John Wiley & Sons, New York.
- 543 de Gruijter, J., Brus, D., Bierkens, M.F.P. & Knotters, M. 2006. *Sampling for Natural*
544 *Resource Monitoring*. Springer, Heidelberg.
- 545 Defra. 2003. *Sampling strategies and soil monitoring: Report SP0514*. Defra, London.
- 546 Emmett, B. A., Frogbrook, Z. L., Chamberlain, P. M., Griffiths, R., Pickup, R., Poskitt,
547 J. *et al.* 2008. *Soils manual. Countryside Survey Technical Report no 03/07*. Centre
548 for Ecology and Hydrology, Lancaster.
- 549 Goidts, E., van Wesemael, B. & Crucifix, M. 2009. Magnitude and uncertainties in soil
550 organic carbon (SOC) stock assessments at various scales. *European Journal of Soil*
551 *Science*, **60**, 723–739.
- 552 Haskard, K.A. 2007. *An anisotropic Matérn spatial covariance model: REML estimation*
553 *and properties*. Ph.D. Thesis, University of Adelaide. <http://hdl.handle.net/2440/47972>
- 554 Haskard, K.A., Welham, S.J., Lark, R.M. 2010. A linear mixed model with spectral
555 tempering of the variance parameters for nitrous oxide emission rates from soil
556 across an agricultural landscape. *Geoderma*, **159**, 358–370.

- 557 Journal, A.G. & Huijbregts, C.J. 1978. *Mining Geostatistics*. Academic Press, London.
- 558 Jupp, D.L.B., Strahler, A.H. & Woodcock, C.E. 1988. Autocorrelation and regular-
559 ization in digital images. I. Basic theory. *IEEE Transactions on Geoscience and*
560 *Remote Sensing*, **26**, 463–473.
- 561 Lark, R.M. 2009. Estimating the regional mean status and change of soil properties: two
562 distinct objectives for soil survey *European Journal of Soil Science* **60**, 748–756.
- 563 Lark, R.M., Cullis, B.R. & Welham, S.J. 2006. On spatial prediction of soil properties
564 in the presence of a spatial trend:— the empirical best linear unbiased predictor
565 (E-BLUP) with REML. *European Journal of Soil Science*. **57**, 787–799.
- 566 Milne, A.E., Haskard, K.A., Webster, C.P., Truan, I.A. Goulding, K.W.T. & Lark, R.M.
567 2011. Wavelet analysis of the correlations between soil properties and potential
568 nitrous oxide emission at farm and landscape scales. *European Journal of Soil*
569 *Science* **62**, 467–478.
- 570 Papritz, A. & Webster, R. 1995. Estimating temporal change in soil monitoring: I.
571 Statistical theory. *European Journal of Soil Science*, **46**, 1–12.
- 572 Pinheiro, J., Bates, D., DebRoy, S., Sarkar, D & the R Development Core Team.
573 2010. *nlme: Linear and Nonlinear Mixed Effects Models*. R package version 3.1-
574 97.<http://www.R-project.org/>.
- 575 R Development Core Team. 2010. *R: A language and environment for statistical comput-*
576 *ing*. R Foundation for Statistical Computing, Vienna, Austria. <http://www.R-project.org/>.
- 577 SNIFFER, 2007. *National Soil Monitoring Network: Review and Assessment Study*.
578 SNIFFER, Edinburgh, UK. LQ09, June 2007.
- 579 Snedecor, G.W., Cochran, W.G., 1989. *Statistical Methods*. 8th Edition. Iowa State
580 University Press, Ames, Iowa.

- 581 Stein, M.L. 1999. *Interpolation of Spatial Data: some Theory for Kriging*. Springer,
582 New York.
- 583 Webster, R. & Burgess, T.M. 1984. Sampling and bulking strategies for estimating soil
584 properties in small regions. *Journal of Soil Science*, **35**, 127–140.
- 585 Webster, R. & Oliver, M.A. 1990. *Statistical Methods in Soil and Land Resource Survey*.
586 Oxford University Press, Oxford.
- 587 Webster, R. & Oliver, M.A. 2009. *Geostatistics for Environmental Scientists*. 2nd Edi-
588 tion John Wiley & Sons, Chichester.
- 589 Williams, D.E. 1949. A rapid manometric method for the determination of carbonate in
590 soil. *Soil Science Society of America Proceedings*, **25**, 248–250.

Table 1. Summary statistics for data on soil organic carbon from the Bedfordshire transect (after removal of one outlier).

	Soil organic carbon /g carbon 100g ⁻¹ soil.	Residual from land-use mean /g carbon 100g ⁻¹ soil.
Mean	2.66	0.00
Median	2.39	0.00
Standard deviation	1.30	1.02
Skewness	1.84	0.27
Octile skew	0.17	0.004
Minimum	0.12	-2.89
Maximum	8.52	3.97

Table 2. Estimated parameters for a linear mixed model fitted to data on soil organic carbon from the Bedfordshire transect.

Fixed effects	Mean soil organic carbon content /g 100g ⁻¹ soil
Arable	2.20
Wood	4.11
Uncultivated	3.04
Random effects	Parameter values
Correlation function type.	Exponential
c_0	0.392 g ² 100 g ⁻² .
c_1	0.738 g ² 100 g ⁻² .
a	215.8 m

Figure Captions.

1. Dispersion variances within a 1×1 -km block for data with point support (solid symbol) or aggregate support (open symbol) on random functions with a spherical variogram, *a priori* variance 1.0, differing nugget variances (abscissa) and a range of 100 or 500 m.
2. Empirical covariance function (solid symbols) of soil organic carbon residuals from land-use mean. The solid line is the (point-support) exponential covariance function with parameters estimated by REML for the linear mixed model for soil organic carbon with land-use as a fixed effect.
3. Expected *a priori* variances of measurements of soil carbon for measurements on seven different sample supports (illustrated). Each support is based on a 20×20 -m square and has differing numbers of aliquots (indicated by solid symbols).
4. Dispersion variances for soil organic carbon (within land-use) on point support or aggregate support (G-BASE) within square blocks with differing lengths.
5. Correlation between two independent re-samplings of soil carbon on point and aggregate supports plotted against standard deviation (in any one dimension) of the relocation error. For each support the lower line is the correlation calculated from the fitted covariance function, and the upper line is an upper bound on the correlation calculated with the covariance function given in Equation (12).









