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Farm-scale soil carbon auditing

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ABSTRACT

A novel method for soil carbon auditing at farm scale based on data value is presented. Using a map of carbon content with associated uncertainty, it optimizes stratified random sampling: number of strata, stratum boundaries, total sample size and sample sizes within strata. The optimization maximizes the expected profit for the farmer on the basis of sequestered carbon price, sampling costs, and a trading parameter that balances farmer's and buyer's risks due to uncertainty of the estimated amount of sequestered carbon. The stratification is optimized by a novel method (*Ospats*), an iterative procedure that re-allocates grid points to strata on the basis of pairwise differences between predictions and covariances of prediction errors. Optimal sample sizes are calculated from variance predictions by *Ospats*. An application on an Australian farm has shown that soil carbon changes across farms and regions can be audited effectively using the proposed method. It is concluded that sample bulking and returning to the same sites in subsequent sampling rounds are not recommendable.

1. Introduction

The soil system is recognized as a significant terrestrial sink of carbon. Estimates for the top meter of soil in the world, range between 1200 and 2500 petagrams for organic C (Batjes, 1996; Lal, 2004). The reliable assessment and monitoring of soil carbon stocks are of key importance for soil conservation and in mitigation strategies for increased atmospheric carbon (Stockmann et al., 2013). Carbon credits are the heart of a cap-and-trade scheme, by offering a way to quantify carbon sequestered from the atmosphere; carbon credits gain a monetary value to offset a given amount of carbon dioxide releases (Paustian et al., 2009). The agricultural industry worldwide has the capacity to capture and store carbon emissions in soil (Paustian et al., 2000). However there is still a debate on how soil can benefit for the offsets in the carbon economy because there is no good and efficient way of measuring soil carbon storage with appropriate statistical confidence (Post et al., 2001; Smith, 2004b). A scheme that can measure and monitor soil carbon storage on a farm, which is crucial to the participation of the agricultural sector in the carbon economy is essential.

There is a win–win position for increased carbon storage in soil. Soil organic carbon (SOC) provides benefits of enhanced soil fertility through improved soil structure, by promoting the agents and mechanisms of aggregation, and increased cation exchange capacity (Stockmann et al., 2013). Studies of Australian soil systems have shown that conversion of forested and grassland areas into cultivated agriculture has led to an overall decline in SOC stock in those soils (Dalal and Chan, 2001; Luo et al., 2010). Conservation tillage, reforestation, and sustainable development practices are recognized methods to promote carbon storage. One mechanism that can facilitate the effective management of the soil carbon is to treat it as a tradeable resource or commodity. A monetary value has been assigned to carbon, in all its states and forms, which can allow for the trading and offsetting of carbon budgets. The development of carbon credit markets accessible to the private sector would allow for incentives such as government payments, tax credits, and/or emissions trading, which can aid in overcoming farmer reluctance to adopting management strategies that increase soil carbon (Rosenberg and Izaurralde, 2001).

There are two distinct approaches recognized to establishing SOC stock with Tier 3 method (IPCC, 2006) including, i.e. process-based models and inventory measurement systems. The choice between each approach depends largely on applicability to the situation, data availability and cost-effectiveness. When considering the costs and low sequestration rates process-based models may be favored (Conant and Paustian, 2002; Smith, 2004b), however it is also challenging considering the diverse combinations of climate, soil type and managements (Rabotyagov, 2010). It is inevitable that not all combinations will be covered or parameterized and support for emerging managements will have a temporal lag in incorporation as data over time is required. Added to this, there are several other reasons to also develop Tier 3 direct measurement methods including:

1) providing an independent verification tool applicable to emerging managements at the farm scale; 2) encompassing adaptive land management through independence from established management assumptions; 3) provision of site-specific feedback to landholders as

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well as data generation for wider purposes; 4) continual improvement of sample design efficiency through time.

One of the biggest problems in direct measurement of soil carbon is the expense of verification as we are dealing with the inherent variability of soil in the landscape (Allen et al., 2010; Smith, 2004b). The amount of carbon stored in the soil per unit of land area is highly variable and depends on annual inputs, soil type and the degradation rate of the soil C (Jandl et al., 2013). Current methods for measuring, mapping, and quantifying soil carbon within an area are expensive and inefficient (Miklos et al., 2010). Furthermore, it is still not established how we can monitor changes in soil carbon efficiently and effectively with sufficient statistical confidence. A scheme that recognizes the whole farm as a system that can store carbon is crucial to the agricultural industry, particularly in the carbon economy. The applicability of direct measurement will likely expand with more efficient sampling and increasing analytical volumes through time.

Typically, repeat direct measurement of soil C for trend assessment has been carried out by revisiting intensively sampled plots (Bowman et al., 2002; Chappell et al., 2013) largely to reduce short range variability and maximize change detection from repeat visits (Lark, 2009). However, the optimal sample design for trend assessment of soil C due to management differences and establishing the soil C status of an area are two different objectives (de Gruijter et al., 2006; Lark, 2009).

Traditionally, soil carbon stock inventory has been based on performing direct measurement of soil C content for a number of sampling sites within an area, then extrapolating the data to the desired extent. In Australia, the standard sampling unit for soil organic carbon is recommended as a 25 m by 25 m square (McKenzie et al., 2000). The NSW Department of Environment, Climate Change and Water (DECCW) proposed that for a given unit of land, a 25 m by 25 m subarea is chosen and divided into 10 by 10 equal sized quadrats. Ten samples are chosen at random from these 100 quadrats and the carbon concentration and soil bulk density estimated to a fixed depth of usually 50 cm. At some later date the process is repeated in the same subarea. The difference in carbon content is calculated. The quadrat method has two drawbacks. First, the sampling area (that is, the subarea) is known, which potentially can lead to dishonest practices where carbon may be deliberately sequestered in the known sampling area. More importantly, the extrapolation of the average carbon content from the smaller subarea to the larger unit of land under sequestration management leads to a large sampling variance resulting in an uncertain estimate of the change in carbon content (Singh et al., 2012).

Such limitations inherent with conventional methods of soil C stock assessment have prompted the development of new technologies that provide alternative methods of data acquisition. Technologies such as remote sensing hyperspectral imagery (Denis et al., 2014; Stevens et al., 2010) and proximal sensing (Cremers et al., 2001; Gomez et al., 2008) have been proposed for estimating surface carbon content over large areas. However such imagery only provides measurement on or near the soil surface, moreover the high cost of acquiring such data and the need for laboratory calibration limit its application in a routine auditing process. Field near infrared spectroscopy can give estimates of carbon, however sampling is also required, and infrared estimation is based on calibration to standard analytical techniques (Stevens et al., 2010). Field prediction of SOC using NIR is still too uncertain, with a standard error of prediction ranging from 1.3 to 5.8 g/kg (Bellon-Maurel and McBratney, 2011). In addition correction of soil moisture from field-acquired spectra can also reduce the prediction accuracy. A precise and cost-effective means of carbon storage measurement needs to be developed urgently in order to be able to credit farmers and land holders for their beneficial inputs in improving both our air and soil. This paper will review various aspects on soil carbon auditing along with a case study on a farm in New South Wales, Australia.

2. Sampling objective

Before designing an effective auditing scheme, the primary step needed is detailing the objectives in statistical terms (de Gruijter et al., 2006). Generally there has been not enough effort put into this part in order to design a cost-effective scheme. Most effort is directed into finding a cheaper analytical measurement for soil carbon, however soil sampling is the largest cost in this activity. As a comparison, the analytical cost of total C by dry combustion is A$10 per sample, while sampling cost is on average A$100 per soil profile. Thus a careful definition of the sampling objectives will allow effective and efficient sampling design and auditing process. The details of the objective that must be clearly defined in this work are (de Gruijter et al., 2006, p.29):

1. *Target universe*: boundaries of the universe in space and in time.
   In our case, the target universe in space is a farm, and along the time-axis the universe spans 3–7 years, the auditor will monitor the target variable at a particular time and repeat the same measure after 3–7 years to establish the change in the measure.
2. *Target variable*: the soil property to be measured on the sampling units.
   We take as target variable the soil organic carbon stock, in ton per ha, denoted by C. The C stock is measured to a fixed depth (up to a maximum depth of 1 m), or better to a fixed cumulative mass of soil, which deals with compaction/tillage issues (Wendt and Hauser, 2013).
3. *Target parameter*: the statistic to be estimated from the sample data.
   In our case, the target parameter is the change in mean C stock between time t_1 and t_2, defined as:

$$\Delta := \bar{C}_{t_1} - \bar{C}_{t_2}, \tag{1}$$

   where $\bar{C}_t$ is the spatially averaged C stock at time t, defined as:

$$\bar{C}_t := \frac{1}{A}\int_{\mathbf{x}\in\mathcal{A}} C_t(\mathbf{x})\mathrm{d}\mathbf{x}, \tag{2}$$

   where $C_t(\mathbf{x})$ is C stock up to 1 m, or to a fixed cumulative mass of soil, at location $\mathbf{x}$ at time t, $\mathcal{A}$ is the project area (the farm), and A is the surface-area of the farm in ha.
   In this study we discretize the area by superimposing a fine grid, with N grid points serving as sampling units. The mean C stock is then re-defined as the average over the grid points:

$$\bar{C}_t := \frac{1}{N}\sum_{i=1}^{N} C_{i,t} \tag{3}$$

   where $C_{i,t}$ is the measured C stock at the i-th grid point at time t.

3. Major design decisions

Three major design decisions are to be made: the sampling approach, the type of sampling design, and whether to bulk samples or not.

3.1. Sampling approach

As repeated many times in the literature, there are two primary approaches in sampling: design-based and model-based. Their ideal applications are for global estimates of a target variable and mapping the target variable respectively (Brus and de Gruijter, 1997). The design-based approach is therefore the most appropriate for C stock auditing. It implies that sampling locations are selected by probability sampling, and that inference (e.g. estimation) is based on the sampling design used to select the sampling locations. A strong advantage in the context

of carbon auditing is that there is no need to make model-assumptions, which always remain questionable.

3.2. Type of sampling design

The simplest method in probability sampling is by Simple Random Sampling (SRS): a fixed number of sample points is drawn at random and independently from each other within the target area. However, the efficiency of SRS can often be markedly improved by Stratified Simple Random Sampling (StSRS). This divides an area into sub-areas called strata, and SRS is applied in each stratum.

Appropriate stratification and allocation of sample sizes to the strata will usually lead to higher precision and lower cost of estimation (Cochran, 1977). For a single sampling round, the precision can be expressed as the sampling variance of the estimated mean:

$$V\left(\hat{\bar{z}}\right) = \sum_{h=1}^{H} \left(\frac{N_h}{N}\right)^2 \frac{S_h^2}{n_h}, \tag{4}$$

where H is the number of strata, N_h is the size (number of grid points) of stratum h, S_h is the standard deviation of z in stratum h., and n_h is the sample size allocated to stratum h.

Given a stratification and a total sample size n, optimal allocation of sample sizes to the strata, in the sense of minimal sampling variance of the mean, can be realized by so-called Neyman allocation (Dalenius and Hodges, 1959; Cochran, 1977). The optimal sample size for stratum h is then given by:

$$n'_h = n \frac{N_h S_h}{\sum_{h=1}^{H} N_h S_h}. \tag{5}$$

The change in total soil carbon between time t_1 and t_2, Δ, can be estimated as the difference between the estimates at time t_1 and t_2:

$$\hat{\Delta} = \hat{\bar{C}}_{t_1} - \hat{\bar{C}}_{t_1}. \tag{6}$$

If measurement is based on sampling at the same locations in both rounds, then the variance of the estimated difference is given by:

$$V\left(\hat{\Delta}\right) = V\left(\hat{\bar{C}}_{t_1} - \hat{\bar{C}}_{t_1}\right) = V\left(\hat{\bar{C}}_{t_1}\right) + V\left(\hat{\bar{C}}_{t_2}\right) - 2\rho\sqrt{V\left(\hat{\bar{C}}_{t_1}\right)V\left(\hat{\bar{C}}_{t_2}\right)}, \tag{7}$$

where ρ is the temporal auto-correlation coefficient of the measurements at t_1 and t_2. However, to avoid the risk of fraudulent practices, it is prudent to sample at the second round at random locations that are selected independently from the first round. This is what we propose to do. So in our case the covariance term in Eq. (7) equals zero, so

$$V\left(\hat{\Delta}\right) = V\left(\hat{\bar{C}}_{t_1}\right) + V\left(\hat{\bar{C}}_{t_2}\right). \tag{8}$$

Clearly, the certainty thus achieved may have a price. No advantage is taken from a possibly positive temporal auto-correlation, which would render a higher precision. On the other hand, improving the stratification for the second round by using new prior information (at least the first round sample data), will reduce $V(\hat{\Delta})$. This advantage would be lost if the sample sites are re-visited, because then the stratification must be kept as it is.

3.3. Method of measurement

There are various methods to determine the C stock of a core sample, each having its own pros and cons in terms of costs and accuracy. The choice has consequences for the cost-effectiveness of the monitoring scheme as a whole, and should be considered in relation with the decision on bulking (Section 3.4).

The C stock of a core is usually measured indirectly, by taking subsamples and measuring their water content and C concentration. The C stock is then calculated from C concentration (kg/kg) × bulk density (kg/m^3) × depth of core (m). Clearly, subsampling errors add to the analytical errors, thus increasing the total measurement error. To address this problem, Pallasser et al. (2015) developed a carbon determination system for whole soil cores. Their method seems promising for routine application in soil carbon auditing. It has the additional advantage of a direct measurement of both C stock and C concentration.

3.4. Sample compositing

Stratified random sampling allows sample bulking or compositing in order to reduce laboratory costs. Soil materials sampled at the locations (aliquots) during a sampling round can be bulked and mixed thoroughly to form a composite or bulk sample. Each composite is formed by bulking a random selection of a pre-chosen number of aliquots, either within or across strata. Bulking is a common practice in sampling for soil testing. The basic assumption is that soil carbon is additive and analyzing a bulk sample gives the same result as averaging the values of the individual aliquots (de Gruijter et al., 2006). Bulking across evenly sized strata has been successfully applied in estimation of mean soil P concentration in The Netherlands (Brus and Noij, 2008), and was proposed for probability sampling in C stock estimation (Chappell et al., 2013).

The one and only advantage of compositing is cost reduction, however there are four disadvantages. First, the cost reduction is due to a smaller number of measurements, which increases the contribution of measurement errors to the total estimation error of the mean. Second, sample sizes (total and within strata) can no longer be chosen freely, as there have to be multiples of 2, 3 or higher factors, depending on how many aliquots are bulked. (For instance, with compositing across 10 strata, the sample size has to be a multiple of 10). This implies that the sampling variance cannot be minimized as effectively as in non-composite sampling. Third, as composites are larger than single aliquots, mixing and/or sub-sampling error will generally have a larger effect on the total estimation error than in non-composite sampling. Fourth, updating the prediction field using data from the first sampling round will be problematic because the geographical coordinates of the sample points are related only with averages over points. Local compositing (i.e. using an aggregate sample support) is a different matter and may be advantageous where there is substantial local variability (Lark, 2012).

We carried out a preliminary analysis (not reported here) on the cost-effectiveness of compositing in our circumstances, based on assumed values of sampling costs, measurement costs, measurement and mixing error and spatial variability of SOC. Our temporary conclusion is that the advantage of compositing will not outweigh its disadvantages for monitoring SOC at farm scale.

4. Stratification methods

There are various ways to stratify a farm, which includes: compact geographical stratification, stratification by ancillary variables, or stratification by a map of predictions of the target variable. A novel method is stratification by a map of predictions with uncertainties.

4.1. Compact geographical stratification

Compact geographical stratification works best when no information on the farm is available. It is just stratification on the basis of spatial coordinates to ensure that the target area is fully covered spatially. Typically a farm is represented by a regular grid. The spatial coordinates of

the grid points can be stratified into compact geographical strata by minimizing the within stratum sum of squared distances:

$$O_{\mathrm{MSSD}} = \sum_{i=1}^{N} \sum_{h=1}^{H} d_{ih}^2, \tag{9}$$

where d_{ih} is the Euclidean distance between location i (x_i, y_i) and the mean of stratum h (b_h, c_h):

$$d_{ih}^2 = (x_i - b_h)^2 + (y_i - c_h)^2. \tag{10}$$

The assumption is that the variable is spatially correlated so that the variation within each sub-region is smaller than the global variation. An example of the compact geographical stratification for a farm (details in Section 7) is given in Fig. 1.

4.2. Stratification by ancillary variables

In most situations ancillary variables will be available for the farm. Here we can recognize the readily (and cheaply) available information: digital elevation models and aerial photography or satellite imagery. The second option is to survey the area using proximal soil sensors, such as electromagnetic induction and gamma radiometrics. Land use is particularly important in auditing soil carbon, and needs to be incorporated in the stratification. We can perform k-means or fuzzy k-means clustering (McBratney and de Gruijter, 1992) of the ancillary variables to come up with the strata. Miklos et al. (2010) utilized radiometric surveys to stratify the study area (farm) to estimate soil carbon stock. Similarly Simbahan et al. (2006) used ancillary variables to target sampling for digital soil mapping. However, both of these studies used model-based sampling strategy for the purpose of mapping soil carbon stock. In addition, collection of high-resolution ancillary variables using proximal soil sensing is expensive and would not be feasible for C stock auditing. k-means clustering minimizes the mean squared distance between the grid of ancillary multi-variables and their nearest centroid. The clusters are represented by their centroids or means. In k-means the objective function is:

$$O_{\mathrm{KM}} = \sum_{i=1}^{N} \sum_{h=1}^{H} d_{ih}^2. \tag{11}$$

This is similar to Eq. (9), except that d here is the component of a distance matrix, calculated as:

$$d_{ih}^2 = (\mathbf{x}_i - \mathbf{c}_h)' \mathbf{A} (\mathbf{x}_i - \mathbf{c}_h), \tag{12}$$

where $\mathbf{c}_h$ is the class centre (centroid) of class h, and $\mathbf{A}$ is the distance norm matrix, which can be the inverse of variance–covariance matrix of $\mathbf{X}$' or called Mahalanobis distance. An example in Fig. 2 shows the farm stratified in 12 clusters based on ancillary variables: elevation and total gamma radiometric counts for the farm in the case study. The assumption is that the selected ancillary variables are known to control the distribution of soil carbon, and the weights of these variables are equal.

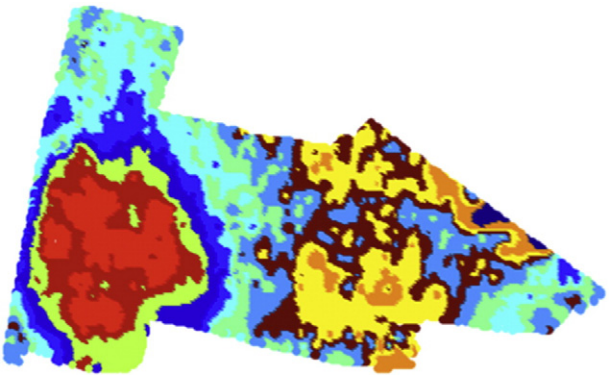

Fig. 2. Stratification by k-means clustering of ancillary variables of Nowley farm.

4.3. Stratification by a map of predictions

SOC prediction fields generated from digital soil mapping can be used as a source of univariate information for stratification (McBratney et al., 2011; Wheeler et al., 2012; Wheeler, 2014). This approach uses the available quantitative knowledge, the relationships between the covariates (ancillary variables) and soil carbon, the knowledge being embodied in the model used to generate the spatial distribution of estimated carbon content. Effective stratification involves locating stratum boundaries along its target variable distribution and allocation of sample sizes to each stratum in a manner that increases the efficiency of the survey leading to higher precision or lower costs (de Gruijter et al., 2006).

An approximate solution to the problem is provided by the cumulative square root of the frequency (cum-root-f) method of Dalenius and Hodges (1959). To deal with the frequency distribution of skewed variables, the geometric stratification method (Gunning and Horgan, 2004) or the method of Lavallee and Hidiroglou (1988) can be used to determine optimal stratum boundaries. This method attempts to minimize the sampling variance of the mean $V(\hat{z})$. However, a disadvantage is that it assumes implicitly that the predictions have only negligible errors. An example in Fig. 3 shows the farm stratified in 12 strata by the cum-root-f method.

4.4. Stratification by a map of predictions with uncertainties

The cum-root-f method and its variants on the one hand and the compact geographic stratification method on the other hand represent two

Fig. 1. Compact geographical stratification of Nowley farm.

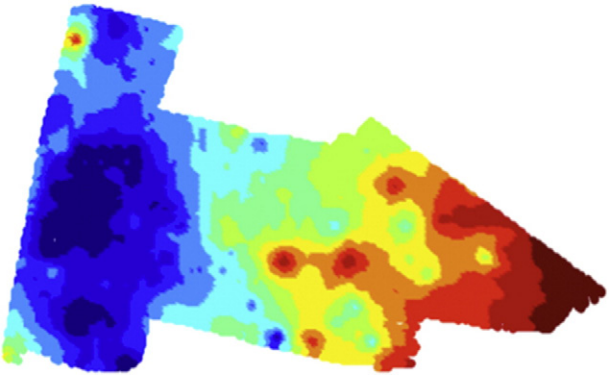

Fig. 3. Stratification of the carbon map of Nowley farm.

extreme solutions in the sense that they assume errorless predictions and absence of useful prediction, respectively. Realizing the limitations of the current methods de Gruijter et al. (2015) proposed a new stratification method (*Ospats*), which uses a raster of predicted values with associated error variances. By taking prediction errors into account this method can produce stratifications that represent transitions between the two extremes. The resulting stratification is optimized by minimizing the expected sampling variance, assuming optimal (Neyman) allocation of sample sizes to strata. This is implemented by minimizing:

$$O = \sum_{h=1}^{H} \left\{ \sum_{i=1}^{N_h - 1} \sum_{j=i+1}^{N_h} d_{ij}^2 \right\}^{1/2}, \tag{13}$$

where d_{ij}^2 here is the squared difference between the true values of the target variable C, which are unknown. However, d_{ij}^2 can be predicted using the predictions and their error variances. The prediction of d_{ij}^2 is obtained by taking its expectation, conditional on $\widetilde{C}_1 \cdots \widetilde{C}_N$:

$$D_{ij}^2 := \mathrm{E}_\xi \left(d_{ij}^2 | \widetilde{C}_i : i = 1, \ldots, N \right), \tag{14}$$

which can be written out as

$$D_{ij}^2 = \left(\widetilde{C}_i - \widetilde{C}_j \right)^2 + V(e_i) + V(e_j) - 2\mathrm{Cov}(e_i, e_j), \tag{15}$$

where $\widetilde{C}_i$ is the prediction of C_i, with prediction error e_i.

The objective function O is minimized by an iterative re-allocation algorithm similar to those for k-means, except that here mutual distances are taken between grid points instead of distances between grid points and centroids. See de Gruijter et al. (2015) for further details.

The value of O resulting after minimization can be used to predict the sampling variance of the estimated mean under Neyman allocation, for a given total sample size n (cf. Formula 18 in de Gruijter et al. (2015))

$$\widetilde{V}\left(\widehat{\overline{C}}\right) = \frac{\overline{O}^2}{n}, \tag{16}$$

where $\overline{O} = O/N$.

5. Optimization criterion

The total sample size is usually determined, either as the maximum affordable, or via a targeted Minimum Detectable Difference (MDD, the smallest detectable difference between means when the variation, significance level, statistical power, and sample size are specified) based on a prior estimate of the spatial variability of SOC (Garten and Wullschleger, 1999; Saby et al., 2008; Singh et al., 2012; Smith, 2004a). As a step towards further rationalization, we follow a Value Of Information (VOI) approach, not a statistical one. The sample size will be determined so as to maximize the expected profit for the farmer, by financial quantification of the value of the sample data and the costs to collect the data. The VOI approach to decide rationally on the level of research investment is generally considered as superior to more-or-less arbitrary statistical criteria such as variance, power or MDD. See Morgan et al. (1990) for a discussion of the VOI approach.

In the early seventies many quantitative studies have been devoted to the relation between quality and production costs of soil maps, notably by Philip Beckett et al. (Beckett and Burrough, 1971). However, the problem is often too complex to apply the VOI approach, mainly because the financial consequences of differences in data quality are hard to quantify. This is probably the reason why the VOI approach has found little application in soil survey so far. See Bie and Ulph (1972) for an early application, and more recently Giasson et al. (2000) and Knotters et al. (2010). As explained below, we can apply the VOI approach here, because we can quantify the value of sample data before they are collected.

The data value (*DV*) of a set of SOC sample data depends on the precision of the estimated sequestration $\hat{\Delta}$. This is because the farmer will not be able to trade his sequestration on the basis of $\hat{\Delta}$ alone, without accounting for uncertainty of the estimate. Therefore we wish to determine a tradeable amount of sequestration *tp*, such that there is large probability γ (say 95%) that the future sequestration will amount to *tp* or more. To that order we define *tp* as the lower boundary of a one-sided prediction interval around the predicted difference in estimated mean carbon contents, $\hat{\Delta} = \hat{\overline{C}}_{t_1} - \hat{\overline{C}}_{t_1}$:

$$tp := \hat{\Delta} - Z_\gamma \sqrt{\widetilde{V}\left(\hat{\overline{C}}_{t_1}\right) + \widetilde{V}\left(\hat{\overline{C}}_{t_2}\right)}, \tag{17}$$

where Z_γ is the γ quantile of the standard normal distribution.

Of course, after the second round *tp* will be calculated from the sample data as the lower boundary of the one-sided confidence interval:

$$tp = \hat{\Delta} - t_{\alpha,\nu} \sqrt{\widehat{V}\left(\hat{\overline{C}}_{t_1}\right) + \widehat{V}\left(\hat{\overline{C}}_{t_2}\right)}, \tag{18}$$

where $t_{\alpha,\nu}$ is the $(1\text{-}\alpha)$ quantile of the Student distribution with $\alpha = \gamma$ and $\nu = n_1\text{-}H_1 + n_2\text{-}H_2$ degrees of freedom (from both rounds).

Optimized stratification by *Ospats* and Value Of Information as optimization criterion are core elements of the auditing process that we propose. The process as a whole is schematically presented in Table 1.

6. Optimization of the first sampling round design

Using *Ospats* means that, for a given number of strata, the resulting stratification is optimized for any sample size, assuming optimal (Neyman) allocation of sample sizes to the strata. Thus there are two design parameters left that are still to be optimized: the number of strata, and the total sample size for that number.

First we optimize the sample size for a given number of strata. To do this we need to make an assumption about the sampling variance from the second round relative to the first round, because the data value *DV* depends on the sum of these variances; see Eq. (17). For

Table 1
Schematic overview of the auditing procedure.

Step	Action
1	**Preparation**:
1a	Delineate the area.
1b	Superimpose a grid with predictions and error variances.
1c	Determine cost per grid point and carbon offset price.
2	**Optimize design for the first sampling round**:
2a	Choose allowed minimum sample size within strata (e.g. 3).
2b	Choose a feasible range of stratum numbers.
2c	For each stratum number in the range, calculate stratification (*Ospats*), total sample size (Eq. (21)) and sample sizes within strata (Eq. (5)).
2d	Select the design with the largest stratum number that still fulfills the condition of step 2a.
2e	Draw a stratified random sample according to the design from step 2d.
3	**Execute the first sampling round**:
3a	Collect samples at the locations from step 2e, and take laboratory measurements to determine the carbon stock for each location.
3b	Estimate the total carbon stock (Eq. (6)) and its variance (Eq. (8)).
4	**Optimize design for the second sampling round**:
4a	Update the predictions and error variances using the sample data from the first round.
4b	Repeat step 2.
5	**Execute the second sampling round**: repeat step 3.
6	**Finish**: calculate the confidence interval for the total amount of sequestered carbon (Eq. (18)).

simplicity we assume that both variances will be equal. (This will happen, for instance, when the same stratification and the same sample size are used for both rounds, and the spatial variances within the strata do not change.) Under this assumption Eq. (17) simplifies to:

$$tp = \widehat{\Delta} - Z_\gamma \sqrt{2\widetilde{V}\left(\widehat{\overline{C}}_t\right)}, \tag{19}$$

where $\widetilde{V}(\widehat{\overline{C}}_t)$ follows from Eq. (16) and depends now only on n.

We define the expected financial gain (G) as the data value DV minus the data costs DC, so $G = DV - DC$. In order to maximize G, we need a cost function for DC. We assume that a simple linear function for the variable costs of field and laboratory work suffices here, so $DC = f \cdot n$, where f is the average cost of obtaining the data per grid point. (The average traveling time between sample sites will decrease with increasing sample size. However, we expect that this will have only a minor effect, at least at farm-scale.)

For the data value we have $DV = CP \cdot A \cdot tp$, where CP is the price of sequestered carbon per mass unit, and A is the surface area of the farm. So we wish to find the optimal sample size n' that maximizes G, using Eqs. (19) and (16):

$$\begin{aligned} G &= DV - DC = CP \cdot A \cdot tp - f \cdot n \\ &= CP\left\{A \cdot \widehat{\Delta} - A \cdot Z_\gamma \sqrt{2\widetilde{V}\left(\widehat{\overline{C}}_t\right)}\right\} - f \cdot n \\ &= CP \cdot A \cdot \widehat{\Delta} - CP \cdot A \cdot Z_\gamma \cdot \overline{O}\sqrt{\frac{2}{n}} - f \cdot n \end{aligned} \tag{20}$$

Equating the derivative dG/dn to zero, renders

$$n' = \left(\frac{CP \cdot A \cdot Z_\gamma \cdot \overline{O}}{f\sqrt{2}}\right)^{2/3}, \tag{21}$$

a real which should be rounded to the nearest integer. The optimal sample sizes for the strata follow by imputing n' in Eq. (5) and rounding to the nearest integer. Note that the underlying assumption here is that tp will not exceed the sequestration capacity of the farm during the contract period, or a possible limit set in advance by the auditor or a regulator.

To see how, for a given number of strata, the gain changes with increasing sample size, we cannot use G as in Eq. (20) because that depends on $\widehat{\Delta}$, which is unknown before sampling. Therefore we use an incremental gain, relative to $n = 1$:

$$G_{\text{inc}}(n) := G(n) - G(1). \tag{22}$$

Applying Eq. (20), this boils down to

$$G_{\text{inc}}(n) = CP \cdot A \cdot Z_\gamma \cdot \overline{O}\sqrt{2}\left(1 - \sqrt{\frac{1}{n}}\right) - f(n-1). \tag{23}$$

As $G(1)$ is negligible, $G_{\text{inc}}(n)$ is practically equal to $G(n)$.

Having analyzed above how the sample size can be optimized given the number of strata, we turn now to the optimization of the number of strata itself, where we assume that for each possible number of strata the optimal sample size will be chosen. Here we have the inconvenience that Eq. (23) cannot be used for gain comparisons between design alternatives with different numbers of strata, as O differs between stratifications. To enable these comparisons, we re-define the incremental gain as a function of H, relative to $H = 1$ (i.e. no stratification), while standardizing the sample size on the optimal size for the given number of strata, n'_H:

$$G_{\text{inc}}(H) := G(H, n'_H) - G(1, n'_1), \tag{24}$$

where $G(H, n'_H)$ is the gain with H strata and the optimal sample size for H. Again applying Eq. (20), this boils down to

$$G_{\text{inc}}(H) = CP \cdot A \cdot Z_\gamma \sqrt{2}\left(\overline{O}_1\sqrt{\frac{1}{n'_1}} - \overline{O}_H\sqrt{\frac{1}{n'_H}}\right) + f(n'_1 - n'_H), \tag{25}$$

where $\overline{O}_H$ is the value of $\overline{O}$ for the *Ospats* stratification with H strata. (Note that $\overline{O}_1$ follows from Eq. (13) without the need for iteration.)

7. Optimization of the second sampling round design

Optimization of the sampling design for the second round is similar to the first round, with one exception. The sample data from the first round are used to estimate the mean carbon content *and* the variance of that estimate. So the predicted sampling variance $\widetilde{V}(\widehat{\overline{C}}_{t_1})$ in the trading point Eq. (17) is replaced by the estimated sampling variance $\widehat{V}(\widehat{\overline{C}}_{t_1})$. So Eq. (17) is updated as

$$tp := \widehat{\Delta} - Z_\gamma \sqrt{\widehat{V}\left(\widehat{\overline{C}}_{t_1}\right) + \widetilde{V}\left(\widehat{\overline{C}}_{t_2}\right)}, \tag{26}$$

where the first variance is a fixed quantity, and the second is the result of optimizing H and n. As these variances cannot be assumed equal as for the first round, the gain Eq. (20) is updated as

$$\begin{aligned} G &= DV - DC = CP \cdot A \cdot tp - f \cdot n_2 \\ &= CP \cdot A\left\{\widehat{\Delta} - Z_\gamma \sqrt{V_1 + \widetilde{V}\left(\widehat{\overline{C}}_{t_2}\right)}\right\} - f \cdot n_2 \\ &= CP \cdot A \cdot \widehat{\Delta} - CP \cdot A \cdot Z_\gamma \sqrt{V_1 + \frac{\overline{O}_2^2}{n_2}} - f \cdot n_2 \end{aligned} \tag{27}$$

where n_2 is the sample size in the second round, $\overline{O}_2$ is the objective function value from the *Ospats* stratification used for the second round, and V_1 is shorthand for $\widehat{V}(\widehat{\overline{C}}_{t_1})$.

The optimal sample size is again found by equating the derivative of G with respect to n_2 to zero:

$$G' = \frac{CP \cdot A \cdot Z_\gamma \cdot \overline{O}_2^2}{2n_2^2\sqrt{V_1 + \overline{O}_2^2/n_2}} - f = 0 \tag{28}$$

which can be solved numerically by evaluation of G' for a range of n_2.

Eq. (25) for the incremental gain as function of H is updated as:

$$G_{\text{inc}}(H) = CP \cdot A \cdot Z_\gamma\left(\sqrt{V_1 + \overline{O}_1^2/n'_1} - \sqrt{V_1 + \overline{O}_H^2/n'_H}\right) + f(n'_1 - n'_H) \tag{29}$$

8. Case study

A study was performed at the University of Sydney E. J. Holtsbaum Agricultural Research property also known as the Nowley farm, located in North West Slopes and Plains of NSW, with an area of 23 km^2. Due to budget constraints we could only afford to take 50 samples. Within this limitation we wanted to maximize the number of strata, which led to 10 strata with 5 samples in each. Although the first round sampling design that we realized in this case study was pre-defined by the available budget, we still can demonstrate our data value approach to optimization, because this only needs a grid with predictions and a grid with associated uncertainties.

8.1. Optimizing the first round sampling

A digital map of C stock in the upper 7.5 cm was generated for the whole farm at a grid spacing of 10 m × 10 m, along with its uncertainty (Fig. 4). The map was made using stepwise multiple linear regression, with covariates: elevation, terrain wetness index, gamma radiometrics K, gamma radiometrics Th, Landsat Bands 2, 4 and 5.

$$C = 4.34 + 0.09 \times \text{Elevation} - 4.56 \times \text{GammaK} + 1.22 \times \text{GammaTh} - 1.62 \times \text{LSBand2} + 0.17 \times \text{LSBand4} + 0.37 \times \text{LSBand5} - 1.1 \times \text{WetnessIndex} \quad (30)$$

The model was calibrated with data from 80 samples collected in 2014 in the same area. Model residuals showed no spatial autocorrelation. Leave-one-out cross validation gives RMSE = 5.1 and R^2 = 0.42.

As indicated above, in this case study we used sample data to calibrate a prediction model, which was then used to generate a carbon map. However, we expect that in practice our optimization system will be bootstrapped directly from a carbon map, so that there will be no need to collect data. Carbon maps at reasonably high resolution are becoming available. These have associated uncertainty, and could be down-scaled if necessary. For instance: Soil and Landscape Grid of Australia (Grundy et al., 2015), http://www.clw.csiro.au/aclep/soilandlandscapegrid. See also Fig. 9 in Kidd et al. (2015) and Fig. 5 in Liddicoat et al. (2015).

The map of C stock and its uncertainty was used for stratifications with *Ospats*. Fig. 5 shows the *Ospats* stratification with 10 strata. Because of the current computational limit of the *Ospats* algorithm on grid size, the maps were coarse-gridded to 30 m × 30 m. The resulting 25,955 grid data were used to optimize the number of strata, the total sample size and the allocation of sample sizes to the strata.

In order to demonstrate the data value approach to optimization of the sample size for a given number of strata, we used the following parameters.

- Carbon offset price: CP = A$2.7 per Mg CO_2 = A$10 $Mg^{-1}C$
- Cost of obtaining data per grid point: f = A$120
- Surface area of the farm: A = 2336 ha
- Number of grid points: N = 25,955

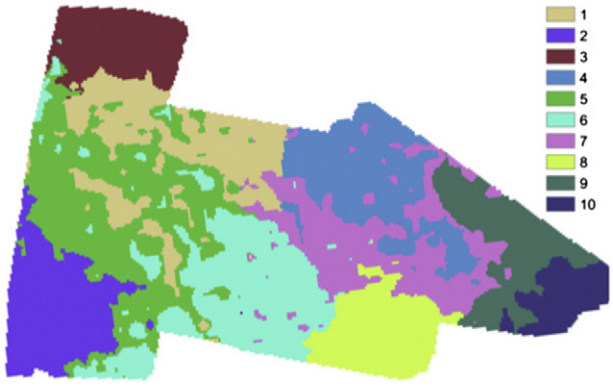

Fig. 5. Stratification based on predictions and error variances in Fig. 4.

- 95% quantile of the standard normal distribution: Z_γ = 1.645
- Objective function value resulting from *Ospats*: depends on the number of strata. For instance, in the first round as realized (Section 8.2) we used 10 strata, resulting in: $\overline{O}$ = 6.33 Mg · ha^{-1}

The optimal sample size, assuming Neyman allocation, follows from Eq. (21) and turns out to be 127. To see how the gain varies with sample size, we calculated the incremental gain G_{inc} using Eq. (23) for a range of sample sizes; see Fig. 6. The figure shows that the net-return from sampling investments declines somewhat beyond n = 127, but the curve is surprisingly flat between n = 50 and 250. Table 2 shows the Neyman allocation for n = 127. The variation of the allocated sample sizes is largely due to the variation in surface areas between the strata, as their standard deviations are fairly even.

To optimize the number of strata, we maximize the predicted gain, under the condition that none of the sample sizes in the strata as determined by Neyman allocation is smaller than a pre-chosen minimum. The bare minimum is 2, to enable estimation of the sampling variance. However, in view of the possible loss of a sample, it is prudent to maintain a higher minimum, for instance 3 or 4. So for a range of possible stratum number we calculate both the predicted incremental gain and the minimum sample size per stratum, given the optimal total sample size. Fig. 7 shows how the optimal total sample size and the maximum

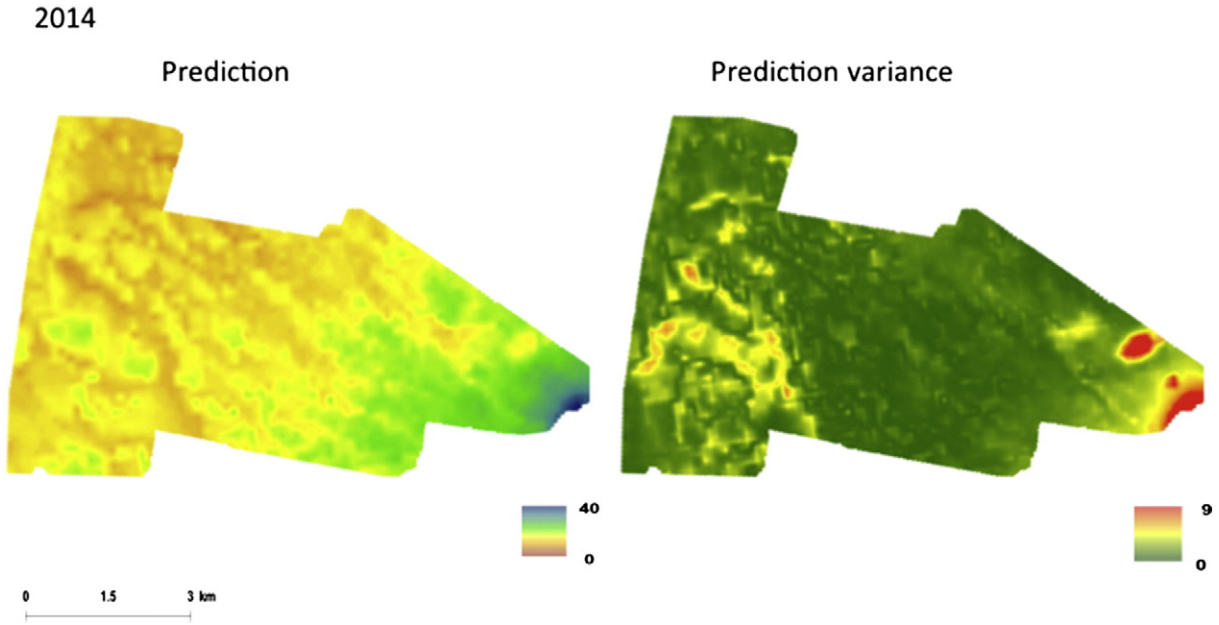

Fig. 4. Prediction and prediction variance of C stock in topsoil of Nowley farm.

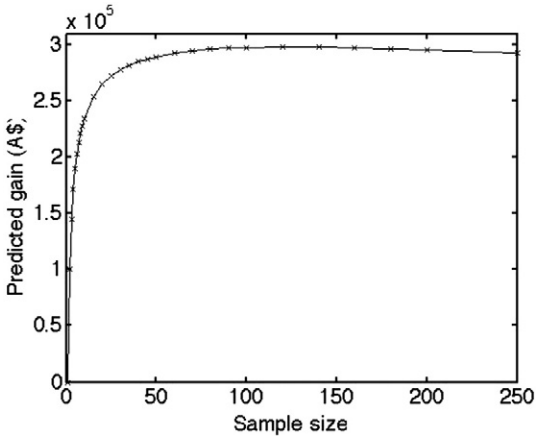

Fig. 6. Predicted gain [A$] as a function of first round sample size, using *Ospats* stratification with 10 strata (see Fig. 5).

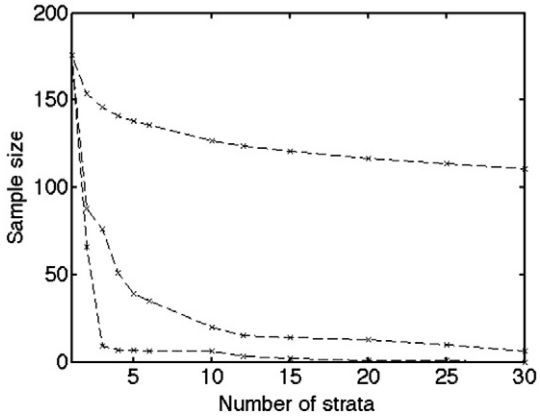

Fig. 7. Optimal total sample size (upper line), maximum sample size per stratum (middle line), and minimum sample size per stratum (lower line) as a function of first round stratum number.

and minimum allocated sample sizes change with increasing stratum number.

To optimize the number of strata, we applied Eq. (25) to a range of stratum numbers. See Fig. 8 for the predicted incremental gain as function of H, relative to $H = 1$ (no stratification). This figure shows that the more strata, the higher gain is predicted, although at an ever slower rate. For instance, using 12 strata instead of 10 renders an increase of A$970. It appears that 12 is the highest number of strata whereby all strata receive at least 3 samples via Neyman allocation. So in this case 12 turns out to be the optimal number of strata under the condition that 3 is the allowed minimum.

8.2. Realization of the first round sampling

Ospats was used to stratify the farm into 10 strata (Fig. 5), and 5 sample points were selected at random from each stratum. The survey was conducted in 2015, with locations determined using a GPS. Topsoil samples were collected at each location using a core with a diameter of 72 mm and height 75 mm. Sub-samples were air-dried and ground, and C concentration was determined using a VarioMax CN Analyser. C stock was then calculated as C concentration times bulk density times core height.

The statistics of the sample data are given in Table 2. The estimated mean Carbon stock for the farm is 15.17 $Mg \cdot ha^{-1}$, with an estimated standard error of 0.62 $Mg \cdot ha^{-1}$. The standard error predicted by *Ospats* is 0.90 $Mg \cdot ha^{-1}$. Ideally, if both the estimate and the prediction were errorless they should have been equal, but both figures have their uncertainty.

The data can also be used to estimate the sampling variance when Simple Random Sampling (SRS) would have been applied with the same sample size. The spatial variance of the area $S^2(C)$ was estimated by:

$$\widehat{S^2}(C) = \widehat{\overline{C^2}} - \left(\widehat{\overline{C}}\right)^2 + \widehat{V}\left(\widehat{\overline{C}}\right) \tag{31}$$

c.f. Equation 7.16 in de Gruijter et al. (2006). Divided by the sample size (50) this yielded a sampling variance for SRS of 0.752. The relative efficiency as compared to SRS equals 1.96, which is equivalent to 98 samples if it was conducted by SRS.

In conclusion, the *Ospats* stratification based on the available digital map of C stock was very efficient.

Table 2
Statistics of C sample data from Nowley farm, based on the *Ospats* stratification with 10 strata and 5 samples per stratum.

Strat.	Relative size	Mean	St. error estimated	St. error predicted	Optimal sample size
1	7.52	11.56	0.83	3.34	11
2	9.01	11.27	1.27	3.08	12
3	12.48	11.70	1.16	2.64	15
4	16.10	13.37	1.44	2.55	18
5	7.63	10.98	1.25	2.99	10
6	15.98	17.06	2.13	2.75	20
7	12.16	14.35	2.01	2.68	15
8	7.89	16.72	1.24	2.93	10
9	7.46	28.12	4.00	2.85	10
10	3.75	25.19	2.54	3.34	6
Farm	100.00	14.82	0.62	0.90	127

8.3. Optimizing the second round sampling

Given the methods of optimal stratification and allocation, respectively *Ospats* and Neyman, the remaining design parameters to be optimized are the number of strata H and the total sample size n. To update the stratification for the second round, one may improve the predictions by more advanced modeling and by using more predictive prior information. In this case we calculated an updated carbon map using a multiple linear regression model (like for the first round), now predicting C content from elevation, gamma radiometric K, terrain wetness index and weathering index. This model was calibrated with the sample data collected in 2014 (80) and 2015 (50). Again, the residuals showed no spatial auto-correlation. See Fig. 9 for the updated maps of

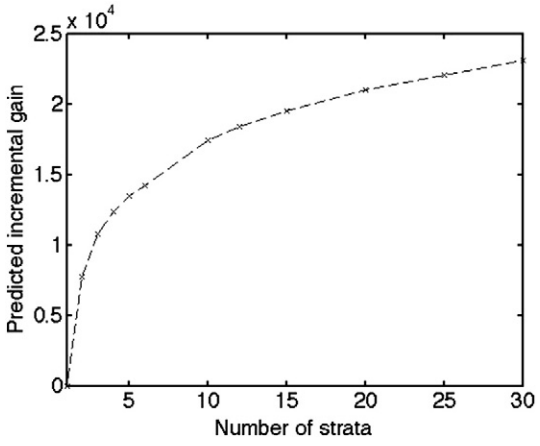

Fig. 8. Predicted incremental gain as a function of first round stratum number.

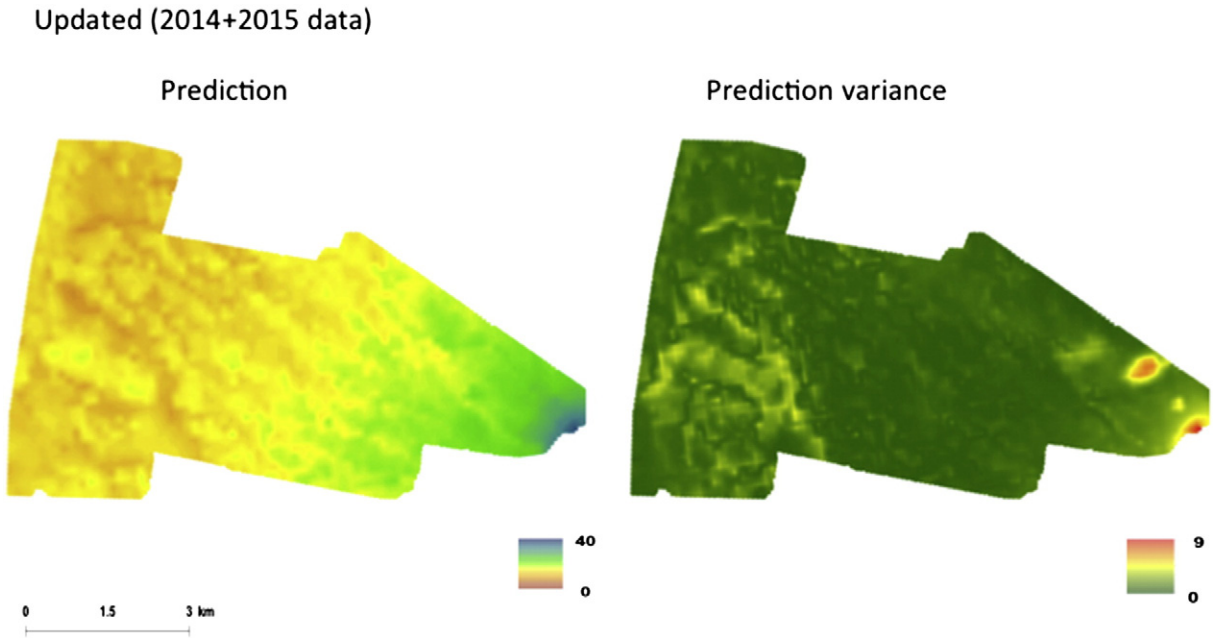

Fig. 9. Updated prediction and prediction variance of C stock in topsoil of Nowley farm.

predictions and prediction variances. The updated *Ospats* stratification with 10 strata is displayed in Fig. 10.

To find the optimal sample size for 10 strata, we used the gain Formula (27), $V_1 = 0.3844$ as the variance estimated from the sample data, and $\overline{O}_2 = 1.0942$ resulting from the updated stratification. The gain as function of the sample size is shown in Fig. 11. It appears that the optimal sample size is only 15, implying that 10 strata is too many under the condition that each stratum receives at least 3 samples. Therefore we determined the optimal sample size and Neyman allocation for a range of lower stratum numbers, see Fig. 12. This led to a maximum of 6 strata and a sample size of 22.

The reason why only 6 instead of 10 strata and 22 samples instead of 50 suffice for the second round, is that updating the carbon map with the first round sample data has enabled an even more efficient stratification than in the first round. This is shown in Fig. 13, presenting $\overline{O}$ as a function of stratum number for both rounds.

9. Discussion

The method devised contains two novel elements. First, a new method (*Ospats*) for optimal stratification (de Gruijter et al., 2015), is used here for soil carbon auditing. It facilitates effective exploitation of all relevant prior information about soil carbon in the project area, as condensed in a carbon map with associated uncertainty. Second, we developed a data value technique to optimize the number of strata as well as the sample size, which is novel in the context of carbon auditing. The optimization criterion of our technique, i.e. the predicted financial gain from a demonstrated amount of sequestration, should lead to decisions on sampling that are more rational than via general statistical criteria.

The information needed to start the optimization process, i.e. optimization for the first sampling round, is a carbon map with associated uncertainty. As carbon maps at reasonably high resolution are becoming available, prior data collection in the field will not be necessary. For instance, soil and landscape grids of Australia have associated uncertainty, and could be down-scaled if necessary.

The method is intended for auditing, not for monitoring or management. For the latter purposes there is generally no need for the restriction not to return to the same sites in subsequent sampling rounds. Efficiency of long-term monitoring may well profit from returning to

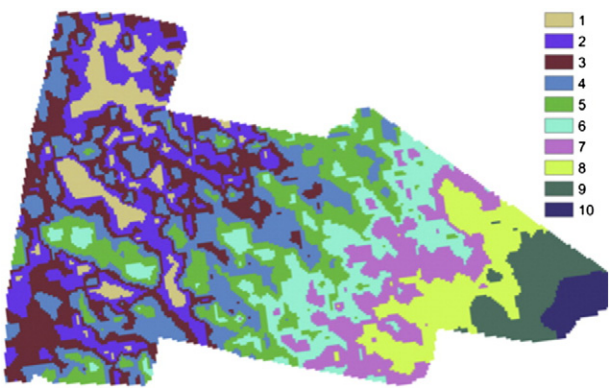

Fig. 10. Updated stratification based on predictions and error variances in Fig. 9.

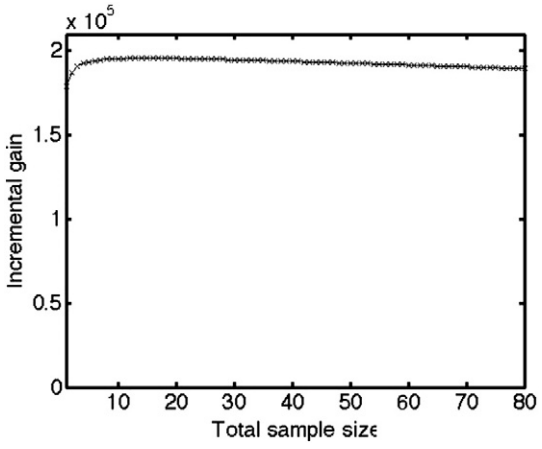

Fig. 11. Predicted gain [A$] as a function of second round sample size, using *Ospats* stratification with 10 strata (see Fig. 10).

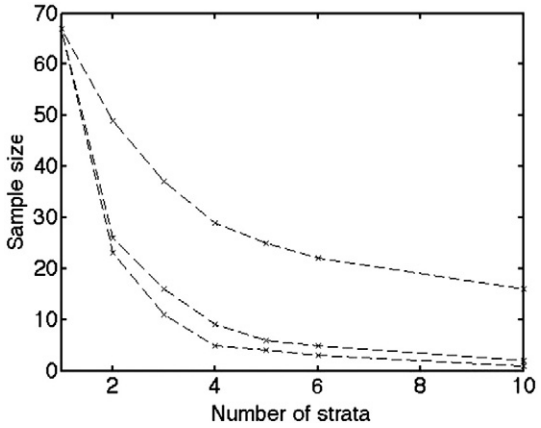

Fig. 12. Total sample size (upper line), maximum sample size per stratum (middle line), and minimum sample size per stratum (lower line), optimized for the second sampling round, as function of stratum number.

(part of) the sites, see Brus and de Gruijter (2013). Also, the intended usage of monitoring results is usually complex, which makes the data value approach unfeasible.

As shown by the case study, updating the map with first round sample data may improve the resulting stratification considerably, and hence reduce sampling costs. However, this updating option does not exist if the sample sites are re-visited, because then the stratification too must stay unchanged.

In the case study only the top 7.5 cm was sampled. This is shallower than usual in soil carbon auditing, but it is enough to demonstrate the method, as this can be applied likewise in projects involving deeper sampling.

The method has the following limitations and underlying assumptions;

1. The data value approach as devised here does only account for the costs that vary with the sample size, i.e. the costs of taking samples and laboratory analysis. Costs of travel to the farm and office work (administration, GIS and computing) are not accounted for. This means that the gain predictions as calculated by the method can only serve to optimize a sampling design, not to decide on starting an audited sequestration project.
2. The gain predictions may be hypothetical because underlying assumptions are that the amount of carbon that will be sequestration by the farm does not reach a physical limit, and that there is no regulatory set bound to it. However, if necessary the method can be easily adapted to account for a known limit.

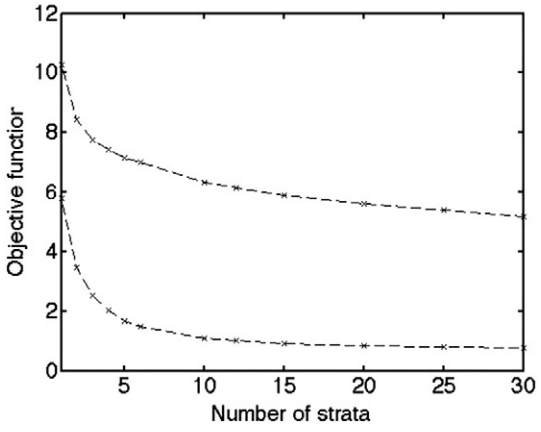

Fig. 13. Objective function $\overline{O}$ of stratifications for first round (upper line) and second round (lower line) as function of stratum number.

3. The optimality of stratifications calculated by *Ospats* is only warranted as far as the uncertainty of the predictions is correctly quantified. At present we do not know how sensitive the stratification quality is for misrepresentation of the uncertainty.
4. Two sources of error are disregarded in this study: error in locating the sampling sites in the field and measurement errors in the laboratory. We expect that the disturbing effects of these error sources on the optimization will be moderate in general.

10. Conclusions

We presented a novel method for soil carbon auditing, which uses prior information in the form of a carbon map with associated uncertainty. The method is based on stratified random sampling and design-based inference about the amount of sequestered carbon. Stratification, total sample size and sample sizes per stratum are mathematically optimized in conjunction. The criterion used is the expected financial gain (excluding fixed costs) for the farmer. This is maximized by a data value technique on the basis of assumptions about the costs of sampling and measurement and the price of sequestered carbon, given a required level of certainty about the amount of sequestered carbon.

An application on an Australia farm has shown that soil carbon changes across farms and regions can be audited effectively using the proposed stratification method and data value technique. The stratification method implies that strata will be created that are typically of unequal size and spatially non-contiguous. The former means that also the optimized sample sizes per stratum are unequal and, as a consequence, sample bulking across strata is unfeasible.

Updating the initial carbon map with sample data from the first round may considerably improve the efficiency of the stratification for the second round. As this stratification differs from the initial one, returning to the same sampling sites is unfeasible for design-based inference. Another reason not to return to the same sites is that it is not recommendable for auditing purposes, in order to avoid possible fraudulent practices and disturbance of sites.

Future research may focus on sensitivity of the auditing method for incorrect quantification of the uncertainty of the initial carbon map. Other research issues are the effects of spatial location error and measurement error on the optimization process, and how these error sources could be accounted for.

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