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Mapping soil carbon stocks across Scotland using a neural network model

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ABSTRACT

A neural network model was trained to predict soil organic matter content, bulk density and soil organic matter density at different soil profile depths across Scotland. These predictions were then used to predict soil organic carbon content. The data used to train the model was developed from the National Soil Inventory of Scotland (NSIS) datasets, along with spatial datasets for topographic and climatic variables, and for geology, soil type and land cover. The trained network was tested and found to explain 79.8% of the variance in organic matter content, 77.9% of the variance in bulk density and 57.3% of the variance in profile depth. Various statistical measures were used to evaluate the predictive ability of the model, showing that it was suitable for predicting the carbon stocks of soils. The neural network model was used to make predictions from the surface to 1 m in 1 cm intervals, at 100 m spatial resolution, across Scotland. This allowed us to make a prediction of the distribution, spatially and at depth, of carbon stocks to 1 m across Scotland and to make estimates of the total carbon stock of Scottish soils (2954 Tg) and the amount stored in different soil types across the country. We found that our estimate of the amount of carbon stored in Scottish soils was in agreement with previous estimates. Mineral and organo-mineral soils are predicted to hold a large amount of carbon in the upper portion, and in terms of carbon stock are almost as important as peat soils. At increased depth, a much smaller proportion of the total Scottish soil carbon stock is held in soils not classified as organic. We provide information about the distribution of carbon stocks with depth and soil type and under different land use/land cover types. Finally, we discuss the relevance of this information in relation to efforts to store carbon within Scottish soils in the medium to long term.

1. Introduction

Mapping of soil carbon stocks across the UK is necessary for a number of reasons, including providing baseline data for monitoring the effects of climate change, carbon accounting, and informing land management decisions. Actual or potential variation in soil organic carbon stocks is now a factor considered in climate change negotiations, implying a need to accurately map the spatial distribution of soil organic carbon. Examples of monitoring frameworks incorporating soil carbon stocks include France (Martin et al., 2011), Ireland (Xu et al., 2011) and China (Wiesmeier et al., 2011; Liu et al., 2012). For each of these examples, the spatial distribution of soil organic carbon (SOC) stocks was modelled as a function of environmental and soil variables.

In addition to providing carbon stock assessment for political, regulatory and conservation purposes, any map of soil carbon that includes information about variation with depth will be useful for providing baseline data and parameterisation for soil profile models. These models could then be used to make more accurate predictions about the effects of land management and climate change over time. Hong et al. (2010) for example, produced maps of various soil water characteristics for South Korea, based on soil carbon profile predictions. Recent work on modelling soil carbon dynamics, such as that of Nieto et al. (2010) using RothC, Aitkenhead et al. (2011) using MOSES, or Oelbermann and Voroney (2011) using Century, is reliant on direct measurements of the distribution of soil carbon in the profile.

Several different approaches have been used for national-scale soil carbon stock mapping, including interpolation between sample points (Bradley et al., 2005), characterisation by map unit (Batjes, 2010); estimation from point data (Chapman et al., 2013) and raster-based soil process modelling (Smith et al., 2007; Smith et al., 2010a,b). In regions where the landscape is heterogeneous, it can be difficult to make accurate predictions of soil carbon stocks without (A) information about the relationships between landscape character and soil carbon content, and (B) high-resolution spatial datasets of the relevant environmental parameters, such as vegetation and topography. Development of models of soil organic carbon for heterogeneous landscapes requires sufficiently detailed field survey data. Examples of such models include the use of pedotransfer functions (Han et al., 2010) and kriging using existing survey point data (Dlugoss et al., 2010; Ungar et al., 2010). The work by Poggio and Gimona (2014) on modelling soil organic carbon stocks in Scotland integrated several approaches, including General Additive Modelling (GAM), and kriging of residuals to account for local variation. This approach is highly flexible, being able to incorporate a wide variety of spatial covariates, and also provides a method for determining levels of uncertainty at each location. The work presented here uses a different

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though still flexible approach (neural networks) and is used to generate maps with a different resolution (100 m instead of 1 km) and also to generate estimates with a finer profile depth resolution (1 cm instead of 5 cm); however, it is not as robust in terms of uncertainty assessment as the method of Poggio and Gimona (2014).

In addition to the measurement of soil organic carbon content at specific points, accurate national-scale assessment of SOC requires an ability to relate soil organic content to proxy data. This allows more detailed assessments to be carried out at reduced cost, or where soil assessments have not been detailed enough (Xu et al., 2011). Several approaches have been taken to modelling SOC content, ranging from statistical regression (Bauer et al., 2006; Li et al., 2010), through the development of pedotransfer functions that include multiple parameters at each point of interest (e.g. Chapman et al., 2013), to the use of approaches based on artificial intelligence (AI) and using environmental parameters (Sarmadian et al., 2009; Allahyaripour and Fazli, 2011). The use of approaches taken from AI to model environmental characteristics often includes the application of neural networks to develop predictive models from large, noisy and complex datasets. For soils, this kind of approach has been very successful in producing more accurate models of soil character than existing pedotransfer functions (e.g. Allahyaripour and Fazli, 2011; Haghverdi et al., 2012).

Historically, as most SOC stock estimates require information about the proportion of the soil that is organic matter, it has been important to have an accurate estimate of the bulk density (BD) of the soil. Methods of estimating this include relationships between organic matter content and BD (e.g. Prevost, 2004; Perie and Ouimet, 2008; Ruehlmann and Koerschens, 2009). It is important however to be able to predict BD from parameters other than organic matter content alone, as otherwise there will be a tendency to rely twice on the accuracy of the OM content assessment, leading to potential error propagation (Chapman et al., 2013). Heuscher et al. (2005) and Crowe et al. (2006) demonstrated that a number of parameters such as moisture content, texture and depth in the profile could also be used as predictors of bulk density. Texture in particular has been shown as effective in predicting bulk density in mineral soils (Keller and Hakansson, 2010; Brahim et al., 2012). Approaches that incorporate additional environmental parameters such as parent material and vegetation type have also been shown to be effective (Jalabert et al., 2010; Sakin, 2012). Having said this, any pedotransfer function or model predicting bulk density for topsoils must also incorporate some information about organic matter content, as variation in this single soil characteristic has a stronger effect on bulk density than any other.

Values given for LOI are often assumed to indicate the concentration of organic matter within the soil. For mineral soils with low organic matter content, or those soils containing carbonates or with high clay content, this assumption is incorrect (Salehi et al., 2011). At low organic matter content values, it has been shown that a significant fraction of the mass loss during LOI analysis is in fact due to water loss from certain minerals (Hoogsteen et al., 2015), meaning that using LOI to estimate soil organic matter or carbon content will lead to an overestimate if the common assumption is made that a simple ratio can be used to derive carbon content from LOI.

The estimation of soil organic carbon has historically been achieved by dividing the soil organic matter content by a value of 1.724 (the van Bemmelen factor). The use of this factor over the last 180 years is described in a useful, informative and entertaining review by Pribyl (2010), who demonstrates that a value closer to 2 is more accurate, although it is also argued that using a single conversion factor is not generally appropriate. There is evidence that the conversion factor should be (A) related to depth, with larger values nearer the surface where more labile organic matter contains a lower proportion of carbon, and (B) related to organic carbon content itself, with more organic soils containing a higher proportion of recaltricent organic matter with a relatively high proportion of carbon (and therefore having a lower conversion factor).

Depth within the profile is often shown to be an important predictor of bulk density (e.g. Suuster et al., 2011). The variation of bulk density, and therefore carbon content, with depth can be modelled effectively using parameterised functions of depth (e.g. Minasny et al., 2006). The effects of overburden pressure on bulk density at depth through compaction vary between soil types (Stutter et al., 2009), and between soils under different land cover types (Bachmann and Hartge, 2006). In order to successfully predict the variation of bulk density with depth across a country such as Scotland, which has a very complex landscape with a number of different soil types, any predictive model of bulk density variation with depth should either include a number of different factors, or be calibrated for site conditions (e.g. Hollis et al., 2012). Either way, specific information about each site is required. The model we demonstrate here includes topography, geology, soil and vegetation information to predict bulk density, soil organic matter content and soil carbon density with depth, in a single unified approach.

Here we demonstrate an approach to mapping soil organic matter, bulk density and soil organic carbon (SOC) content across Scotland to develop a pedotransfer-like model that is applied at a relatively fine spatial scale (100 m). This reduces two of the largest contributing factors to soil organic carbon estimate uncertainty, namely variation with soil density and variation at small scales. The modelling approach relies on neural networks, the use of which for modelling soil characteristics has been shown to be successful (Baker and Ellison, 2008; Borgesen et al., 2008).

2. Methods

2.1. Soil data

The data used in this work are contained within the Scottish Soils Database (SSD), one of the most detailed and systematic collections of national soil data in Europe. Formation of the SSD was initiated at the Macaulay Institute in the late 1970s, with several studies and surveys resulting in a completed database in 1987 (Brown et al., 1987). This database contained soil profile descriptions and chemical and physical analyses for several thousand sample points. One of the most significant components of the SSD is information from the National Soils Inventory of Scotland (NSIS) dataset, which is derived from an objective sampling of Scottish soils. Soil and site conditions of 721 locations throughout Scotland were sampled on a 10 km grid across the entire country, aligned with the National Grid of Great Britain (Lilly et al., 2010). Samples were taken at multiple depths from soil pits and analysed to determine their physical and chemical properties.

2.2. Soil data preparation

Not all of the data points in the Scottish Soils Database contain full records of every parameter. For this work, we selected those points that had the following information:

- Dry bulk density average
- Soil organic carbon (SOC) (only a subset of the data used had this information)
- LOI (loss on ignition) at 900 °C (values at 450 °C were also available and would have been preferred as the lower temperature gives a clearer measurement of organic matter content, but there were not as many measurements available at this temperature)
- Sample depth (i.e. the depth from the surface at which the sample was taken, this was taken as the mean value of the depths given for the top and bottom of the sampling depth).

As we are interested in the quantities of organic carbon stored in the soil but do not have direct information about organic carbon content for each of the samples used, it was necessary therefore to derive OC (organic carbon) content values from LOI using a neural network-based pedotransfer function. This pedotransfer function predicted C content from depth and LOI, data for which was extracted from the Scottish Soils Database. In order to predict OC content within a given volume of soil, it was also necessary to predict bulk density values. Multiplying together organic carbon content and bulk density gave a value for organic carbon density, which we have termed here OCD.

Each sample location in the soil survey data did not produce only a single data point; instead, each location provided several data points from samples at different depths. This not only provided information from multiple depths from each profile visited, but also a method of approximating the profile depth. Working on the assumption that the profile would have been dug either until some artificial limit was reached (in practice, this was 70–80 cm) or until it became difficult to penetrate the soil further (at which point, arguably, the bottom of the profile has been reached), we took the deepest sample depth for each profile to be the depth of that profile. Therefore, each data point could also be given an estimate (or at least a lower limit estimate) of the depth of the profile from which it came, allowing us to include profile depth as an output in the model. This approach to taking the depth of the deepest sample as the profile depth is obviously less reliable for deeper soils than for shallow ones, as the sampling depth limit may be arbitrarily chosen; however, discussions with field surveyors who actually carried out the work indicates that if the soil was penetrable to at least 70–80 cm, then it was reliably dug to that depth and usually further.

The estimation of profile depth is important as it allows us to determine a cut-off point below which any carbon content estimate is not included in the total for that profile. The assumption made about profile depth is acknowledged to be generally but not universally true, as there were some instances where the profile was not dug any deeper due to flooding of the pit or some other safety issue. However, for the majority of these it would also be true that the profile had been explored beyond the 'carbon bearing depth' of the profile, which is the literal definition of what is meant here by the term 'profile depth'. For organic soils deeper than 1 m, the profile was generally dug at least to this depth.

2.3. Spatial datasets

The following spatial datasets were used for the mapping work, both in generating training data for the model and for mapping soil organic carbon once the model was trained:

- DEM (Digital Elevation Map) — OS Land-Form PROFILE dataset 1:10,000 scale (Ordnance Survey, 2003).
- LCM2007 — Land Cover Map 2007 with minimum mappable unit at 0.5 ha (Centre for Ecology and Hydrology, 2007).
- LCS88 — Land Cover of Scotland (1988) at 1:25,000 scale (Macaulay Land Use Research Institute, 1993).
- Soil map units — major soil subgroup (and soil parent material) from the 1:250,000 Soil Survey of Scotland subsampled to 100 m resolution from the original data (Macaulay Institute for Soil Research, 1984).
- Mean monthly temperature — taken from 1460 Meteorological Office Stations from 1941 to 1970 interpolated to a 100 m resolution across Scotland (Matthews et al., 1994, MacDonald et al., 1994).
- Mean monthly rainfall — taken from the same sources as the temperature data.

From the DEM, a total of 7 further topographic spatial datasets were generated. These included slope, overall curvature (second derivative of the DEM, or slope of the slope), profile curvature (curvature in the direction of maximum slope) and plan curvature (perpendicular to the direction of maximum slope), aspect, aspect from North and aspect from East. These last two are the minimum angle between the actual aspect and North and East, respectively, and provide values for aspect that do not have a large discontinuity between values slightly east and slightly west of North. As such, for the cost of increasing the number of input parameters by one, we remove any nonlinearity in this input parameter. There are a number of other parameters that can be derived from elevation data and for future work, we would anticipate developing these.

For the LCM2007 and LCS88 datasets, a reduced categorisation was generated with only 10 classes, which allowed a separate map to be generated for each of the two land cover maps. The broad categorisation of land cover that was used was selected to allow both LCM2007 and LCS88 maps to be translated easily and consistently, and included the following categories: arable, improved grassland, rough grassland, heath, peat, bare ground, water, montane, coniferous forest and deciduous forest. The number of categories within the two original datasets is large (in particular for the LCS88, which has 127 individual classes and over 1200 including 'mosaic' classes), making it difficult to represent the reclassification that was carried out.

Using the map of soil mapping units, we produced nine new maps, each providing values for the percentage of presence of the relevant class within the mapping units. The nine soil classes used were: alluvial, alpine, bare, brown earth, gley, peat, podzol, ranker and regosol. Also from the soil map information, we produced a map of parent material that contained at each point one of 19 broad parent material types. As for the land cover datasets, the number of different soil types within the soils map is too high to demonstrate the reclassification in tabular form. However, this information can be obtained from the authors upon request.

The above spatial datasets were resampled to a 100 m resolution common grid. This was in preparation for later mapping work, but also to enable us to determine the relevant parameter values from each soil sampling point. The resolution of 100 m was selected as it reflects many landscape-scale features of relevance (e.g. agricultural fields) and was appropriate in relation to the minimum mapping unit size of the vector maps used (land cover and soil maps). Where a spatial dataset had a coarser spatial resolution than 100 m (e.g. temperature and rainfall monthly means), it was interpolated linearly between the existing points. Where a dataset had finer resolution than 100 m (e.g. the land cover maps), the nearest neighbour approach was used.

For each of the sampling points taken from the soil database, a set of parameters was generated corresponding to the location on each of the spatial datasets listed above. This gave a total of 81 input parameters for modelling soil BD and LOI values (1 for depth, 8 for topography, 20 for land cover, 9 for soil type, 12 for temperature (one for each month), 12 for rainfall and 19 for parent material). The resulting dataset, with 81 input parameters and 3 output parameters (BD, LOI and profile depth), contained 1134 data points. As each data point was derived from a sample acquired at a specific depth (taken as the middle of the sample depth range, which was a few centimetres), this gave depth-specific data. For estimating parameters using the trained network, the depth for which the estimation was made (1–100 cm) was included as an input.

2.4. Neural network model

A neural network model approach was selected for several reasons. Firstly, it has been shown to be successful in estimating soil organic matter content using environmental variables (Aitkenhead et al., 2015). Secondly, neural networks are known to provide good modelling capabilities for complex, noisy environmental datasets where the relationships between input and output parameters are not well understood. And while it is possible to make a neural network model over-fit the data, this is also an issue with other modelling approaches and can be avoided with careful design and training of the model. While NNs are often derided as 'black box' models it is no more difficult to extract the information they develop on the modelled system than with other approaches (although that was not our intention here). Finally, the authors are familiar with the design and operation of neural network models and so selected this approach for reasons of ease of use.

In order to train the predictive model effectively, the dataset of 1134 sample data points obtained from the 721 profiles was split into two datasets, using a random selection of 850 (training) and 284 (testing) points. This enabled us to develop a model and validate its performance appropriately. Examination of the training and testing datasets showed that there was no significant difference in the mean or variance for any of the input or output parameters, between the two datasets. Our objective was to develop a neural network model that could take information about the environmental characteristics (topography, land cover, soil type, climate, parent material) and a selected depth within the profile, and make predictions of BD and LOI at that depth and of the total depth of the profile to the C horizon.

One consideration was that the above approach may not have been as rigorous as using k-fold cross validation, which is considered one of the 'best practise' approaches for model training and validation. This approach involves splitting the available data into k equally-sized subsets, and training k models using all but one of the subsets, with each model having a different subset left aside for validation. We tested the k-fold cross validation approach using values of k equal to 2, 5 and 10, and found that while the performance of the models developed gave results no different to the approach identified above, the use of k-fold cross validation increased the processing time greatly. For this reason, we adopted the approach described above.

The backpropagation neural network (Bishop, 1995; Aitkenhead and Cooper, 2007) was used. The network architecture was of the form X:H:H:Y, where X was the number of input nodes, H was the number of hidden nodes in each of two hidden layers, and Y was the number of output nodes. The number of input nodes X equalled the number of input parameters which exist in the training dataset (81, see Section 2.3), and the number of output nodes Y equalled the number of output parameters (3, see Section 2.3). The number of hidden nodes H equalled twice the maximum of X and Y, in accordance with Kolmogorov's theorem for neural network modelling that states that the number of nodes in the hidden layers should be twice the maximum in the input or output layers in order to guarantee the perfect fit of any continuous function (Bishop, 1995).

Training of the neural network was carried out using the backpropagation gradient descent algorithm, one of the most commonly used neural network training approaches (Bishop, 1995). Repeated exposure to randomly-selected members of the training dataset with a learning rate of 0.05 and a momentum rate of 1 was found to give best results with the test dataset at between 20,000 and 25,000 training iterations, through trial and error. A training regime of 25,000 steps was therefore adopted. All input parameters were normalised to lie within the range [0, 1], while the output parameters were normalised to lie within the range [0.25, 0.75]. This was done to allow for output estimates that lay outside the ranges encountered.

Statistical evaluation of the trained neural network was carried out for each output parameter, including R^2 of the linear regression between actual and predicted values, mean error (ME), mean absolute error (MAE) and root mean squared error (RMSE).

2.5. Organic carbon distribution with depth

A pedotransfer function for proportional organic carbon content using LOI and depth was developed using a secondary neural network model trained with data from the Scottish Soils Database. Fewer data values were available for training and testing this model, which was one of the main reasons for not developing a model that estimated organic carbon directly. This NN had the same training algorithm, but only two input nodes (one each for LOI and depth), and one output node (organic matter to carbon content conversion factor, ranging between 1 and 5). In each of the two hidden layers, four nodes were used. The dataset used for training this network contained LOI and organic C data from the soils database (depth was directly input from the recorded sample depth), and was split into 75% for training and 25% for testing. Input parameters were adjusted to fit the range [0, 1], while the output parameter was normalised to fit into the range [0.25, 0.75]. Using a single model for all OC proportion values in this way ignores all other factors that could be of influence. The distribution between organic matter content in the data is biased slightly towards the mineral soils, but testing of the model showed that the model estimates were not biased towards the conversion factors found in mineral soils (see Section 3.2).

Estimates of organic carbon proportion were derived by applying the secondary neural network to the bulk density and LOI maps generated by the primary neural network. These estimated were used to produce an estimate of organic carbon density (g cm^{-3}) at every 1 cm depth within the profile. While this increased the processing time required over mapping every 5 or 10 cm depth down the profile, it did allow us to produce organic matter content estimates for very shallow soils in addition to deeper soils. Using an estimate of profile depth (see below) as the cut-off for summing the organic carbon mass per unit area down the profile, we were then able to make an estimate of the total carbon content of the soil.

A map of the bulk density, LOI and organic carbon density was produced for every 1 cm depth to a depth of 1 m for Scotland, at a spatial resolution of 100 m. This was achieved using the trained neural network models and the existing spatial datasets described above to provide input parameters. The result was a series of 300 maps (three for each centimetre down to one metre depth), each between 250 and 300 MB in size, which took approximately seven months to generate using a standard PC with an Intel 4-core 3.16 GHz processor.

2.6. Profile depth estimation

Estimates of LOI and BD (and organic carbon density) were made by the neural network models for every 1 cm depth from the surface (1 cm) to 1 m. If the assumption was made that all soils were at least 1 m deep over the parent material, then simply summing the predictions of organic carbon density for the 100 layers would suffice. However, this assumption cannot be used as many soils are shallower than 1 m. Therefore, an estimate of profile depth was required as a cut-off for inclusion of the contribution of the profile at each point to the total soil carbon. The method for estimating profile depth is given in Section 2.2.

To reiterate, for each 1 cm-thick layer an estimate was made of LOI, BD and profile depth. If the current depth of the layer was greater than the profile depth estimate made for that layer, then the layer was not included. Profile depth estimates were given for every 1 cm layer in order to provide an indication of how much the estimates varied for one profile — in practice, the variation in estimates between the upper centimetre and the bottom of the profile was very small — less than a centimetre in more than 99% of cases.

2.7. Map evaluations

The series of maps representing organic carbon content at successive 1 cm depths was used, with the profile depth cut-off, to produce a map of organic carbon distribution across Scotland and to summarise the total amount of organic carbon by depth. We also used this map to summarise soil organic carbon by vegetation type and by soil type. As the soil map contains information about the percentage of each type within a soil unit, not what soil type is present at each point, we summarised by soil type by multiplying the proportional presence of each soil type by the carbon stocking density, to produce a map of 'contribution to carbon stocking density' for each soil type. The total carbon represented in each of these maps was then divided by the sum of all proportional values for soil presence, to give values for the proportional contribution of each soil type to carbon stocking rates in Scotland.

3. Results

3.1. Neural network model

Testing accuracy for each output parameter was measured using R^2 values for linear regression, ME or bias, MAE and RMSE. Table 1 gives these values for each of the output parameters for the trained neural network model, along with minimum, mean and maximum measured values for each.

The neural network model predicted BD and LOI values well, with LOI being predicted with low mean error and the highest R^2 value. There was a slight positive bias (mean error) in prediction of BD, which would lead to an overly high estimate of organic carbon stock if the bias were consistent across all soils. However, the bias was much lower (0.026 g cm^{-3}) when taken across only the low bulk density soils (BD < 0.5 g cm^{-3}), meaning that the proportional error was still relatively low. Profile depth (PD) was poorly predicted, with a large negative bias that was largely due to underestimation of profile depth for the deeper soils (>100 cm).

3.2. Organic carbon content

The neural network-based pedotransfer function for organic carbon content had a regression R^2 value of 0.540. Examination of the prediction errors for different ranges of LOI showed that in relation to the use of a simple ratio (the van Bemmelen factor) to relate LOI (assumed here to be the same as OM content) to organic carbon content, the pedotransfer approach used here did not greatly reduce the mean absolute error between the actual and predicted organic carbon content for high organic matter content soils. For soils with an LOI of greater than 50%, the MAE value using a ratio of 1.724 was 0.0399, while the MAE for the same soils using the pedotransfer function was 0.0385. However, for soils with an LOI of less than 50%, the pedotransfer function did improve the MAE, with values of 0.2138 for the use of a simple proportion and 0.0955 for the pedotransfer function. We found that the conversion factor predicted ranged between 1.368 and 5, with a mean of 2.410. For samples with an organic matter content of less than 20%, the mean conversion factor value was 2.725 and the values ranged from 1.482 to 5.000 (the maximum permissible by the pedotransfer function). For samples with organic matter content greater than 20%, the mean conversion factor value was 1.837, with a range between 1.368 and 2.752.

In addition to a decrease in mean absolute error, the use of the pedotransfer function greatly reduced the bias in prediction of organic carbon proportion of LOI/OM content, from a bias of 0.1869 using a simple conversion factor of 1.724 to a bias of 0.0148 using the pedotransfer function. Again, this reduction in bias was seen most strongly for soils with low organic matter content.

3.3. Profile depth

The neural network profile depth estimation tended to underestimate profile depth, as shown in Table 1. In addition to this, we were already working with the assumption that the lowest sampling point was where the profile bottom was reached, an assumption that is likely also to underestimate the actual profile depth. Using the neural network model and adjusting the predictions of profile depth based on the bias seen in Table 1, we have produced a map of predicted soil depth (Fig. 1), with a cut-off at 100 cm. Comparing this with a map of predicted bulk density for the top 1 cm of the soil profile (Fig. 2), it is possible to see how these two important soil properties are predicted to vary spatially across the country.

Table 1
Accuracy assessment of neural network model for predicting bulk density (BD), loss on ignition (LOI) and profile depth (PD).

	BD (g cm^{-3})	LOI (%)	PD (cm)
R^2	0.779	0.798	0.573
Min	0.046	0.870	0.000
Mean	0.572	41.519	54.19
Max	1.795	98.766	160
ME	0.051	1.902	−23.54
MAE	0.173	11.924	17.20
RMSE	0.223	17.078	22.27

3.4. Map evaluations

Using the estimate of profile depth to the C horizon as a cut-off for including carbon in the stock estimate, we produced an estimate of the total organic carbon stock per hectare and from this generated a map of total organic carbon for Scotland (Fig. 3). This map shows that Scotland's organic carbon is distributed heterogeneously across the country, with large areas of large stocks in Lewis and Harris (the northern part of the large islands in the north-west), and in the far north. However, there are also significant stores of organic carbon in the south of the country, with the east coast agricultural areas generally showing the least carbon stock levels.

Using the map shown in Fig. 3, we produced an estimate of the total organic carbon stock in Scotland's soils to a depth of 100 cm. The total value obtained was 2954 Tg. To obtain an estimate of uncertainty in this estimate, we determined the mean absolute error in prediction at different ranges of predicted soil organic carbon (range sizes of 0.01 g cm^{-3}, from 0 to 0.2 g cm^{-3}). Applying the appropriate error estimate to each 1 cm layer in each 100 m grid cell, we have estimated the uncertainty in the total stock value to be 703 Tg, giving minimum and maximum values of 2251 and 3657 Tg, respectively. In order to determine the distribution of this total stock amongst different landscapes, we summarised the total organic carbon stock by broad vegetation type (Table 2), and by broad soil type (Table 3). For both these tables, we showed carbon stocks as a total and per hectare of the relevant classes. Table 2 shows that peatland vegetation, as expected, has the greatest carbon stock density while heath has the greatest carbon stock overall. Bare ground was also found to have a certain carbon stock, which is initially surprising until considering the fact that urban areas are considered within the bare ground class. A large proportion of urban areas comprises gardens, parks and other vegetated areas, so it is reasonable to expect that soil carbon stocks will exist under this class. The values in Table 2 are greater than estimates in Chapman et al. (2013), with greater variation between the two estimates for Arable (111.5 t/ha), Improved grassland (138.1 t/ha) and Rough or semi-natural grassland (185.2 t/ha) than for Woodland (267.5 t/ha), Moorland/Heath (290.8 t/ha) and Bog (528.3 t/ha). The average value across Scotland given by Chapman et al. (2013) was 265.8 t/ha whereas ours was 378.7 t/ha.

Table 3 also shows that peat soil types have both the greatest carbon stocking per hectare and the greatest carbon stock of any soil type. We have used the Scottish Soil Classification system here (Macaulay Institute for Soil Research, 1984), and the (very) approximate translation between this and the WRB soil classification is as follows:

- Alluvial (Fluvisols)
- Alpine (can be alpine podzols or gleys)
- Bare ground (Bare ground)
- Brown earth (Cambisols/Umbrisols)
- Gley (Gleysols/Stagnosols)
- Peat (Histosols)
- Podzol (Podzols)
- Ranker (Leptosols)
- Regosol (Regosols).

Small areas of some other WRB soil types do exist in Scotland (Lilly et al., 2012). We have distinguished alpine subgroup soils here as they generally have low organic horizon thickness. Rankers, regosols and

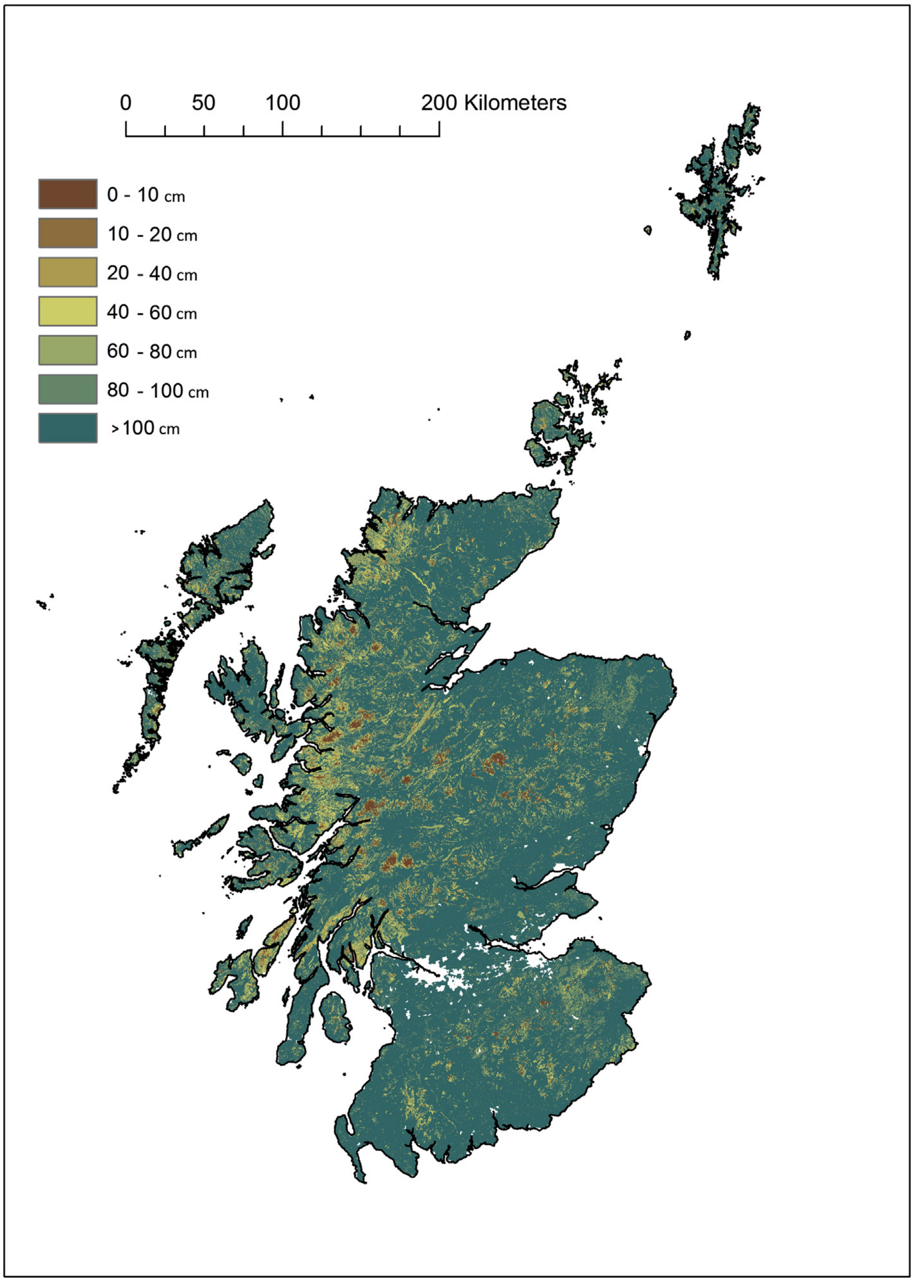

Fig. 1. Map of predicted soil profile depth to the C horizon.

bare ground are also shown to have carbon stock densities greater than expected (although these soils can contain a lot of organic carbon in the top few centimetres, the organic layer is usually too thin to contribute much to soil carbon stocks). Although these result in small contributions to the total, do require explanation. Areas of bare ground or thin, weakly-developed soils are often in soil map units with deeper, organic-rich soils such as peats. Due to the fact that the soil map used to produce Table 3 contained information about percentage of soil type within mapping units that were larger than 1 ha, the spatial distribution of these soil mosaics is not given. This results in a misappropriation of carbon within certain soil classes due to a lack of knowledge about which soils lie where within a mapping unit.

Using the map of predicted profile depth and the individual layers of predicted organic carbon density, we were able to calculate the total organic carbon stock at each centimetre depth. Fig. 4 shows this information, along with carbon stock with depth for soils classed as peat under the Scottish system of soil classification (>60% organic matter content for all depths within the top 50 cm) and non-organic, or mineral/organo-mineral. From this graph we can see that as expected, the total stocking density decreases with depth with a gradient that becomes shallower with depth. We also see that taken all together, mineral and organo-mineral soils contain greater total organic carbon stock than organic soils at all depths, although there is a greater decrease in stocking density with depth for mineral/organo-mineral than for organic soils. This shows that according to the model, organic carbon in mineral soils is more strongly accumulated in the upper horizons, while in organic soils the organic carbon density remains more consistent with depth. An analysis of the predictions showed that the carbon values did not change with depth in ways that were unrealistic (e.g. sudden increases/decreases over a single centimetre, rapid increase with depth).

To highlight the relationship between stocking rates at different depths between organic and mineral/organo-mineral soils, Fig. 5 shows the ratio between organic carbon stocking density (per hectare) for these two types of soil. This shows that at the surface, the ratio is

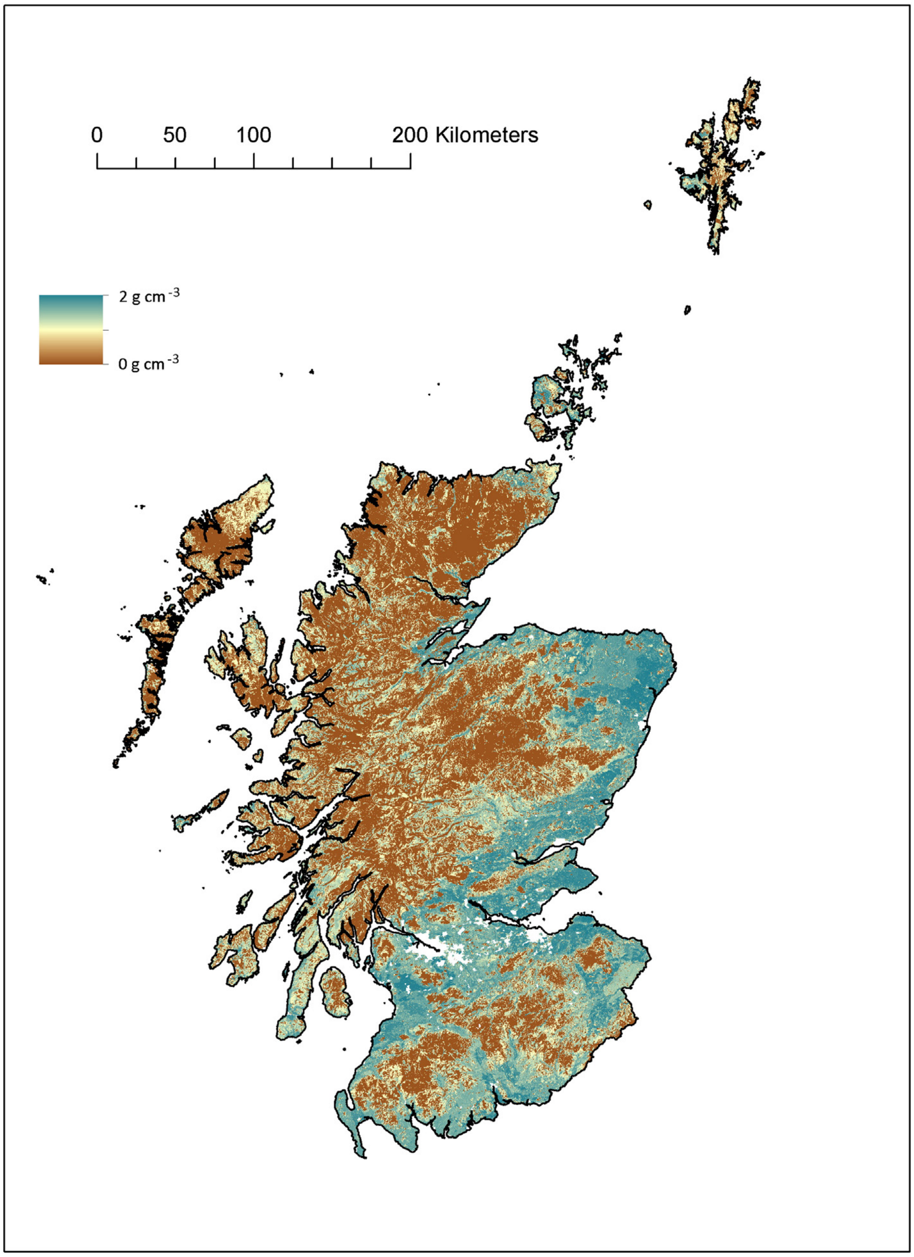

Fig. 2. Map of predicted soil bulk density in the top 1 cm.

close to 1 with organic soils having slightly more organic carbon per hectare than non-organic soils. As the depth increases so does the ratio, indicating that the relative importance of organic soils for carbon storage increases with depth.

4. Discussion

We have demonstrated an approach to mapping soil organic carbon contents that predicts bulk density and loss on ignition values, allowing an estimation of organic carbon density at different depths down to 100 cm. The estimation to a 1 cm vertical resolution is higher than the resolution at which the sample measurements were made, so this could be taken as giving a false sense of precision. However, we have not attempted to estimate the rate of change with depth to this resolution (which would have been inappropriate) but have instead used this information to provide total-profile estimates.

Table 3 shows that peats are predicted to contribute only 27.6% of the total soil carbon stock in the top 1 m with a value of 813.9×10^6 kg, whereas Chapman et al. (2009) gave an estimate of 56% within the top 2 m and a total value of 1610×10^6 kg. While the percentages initially seem very different, the fact that peats contain much more organic carbon than other soils at depth allows us to approximate, using a doubling of the total peat organic carbon depth from 1 m to 2 m, that (A) the two estimates for total peat organic carbon stock are not as different as at first sight, and (B) the percentage of total carbon stock due to peats at 1 m should be less than the percentage at 2 m, as other soils will contain little or no organic carbon below 1 m depth. In actual fact, as peat bulk density is likely to increase with depth due to overburden pressure (in addition to a probable increase in the proportion that is carbon), while not all peats will extend to 2 m depth, the estimate that we can make for total stock at 2 m is approximately double the value of 813.9×10^6 kg.

The method Poggio and Gimona (2014) used for estimating Scotland's soil carbon stock produced a higher level of uncertainty than the approach described here, and modelled values that were generally higher than those measured. However their approach gave a more robust estimate of uncertainty than ours and is amenable to improvement given

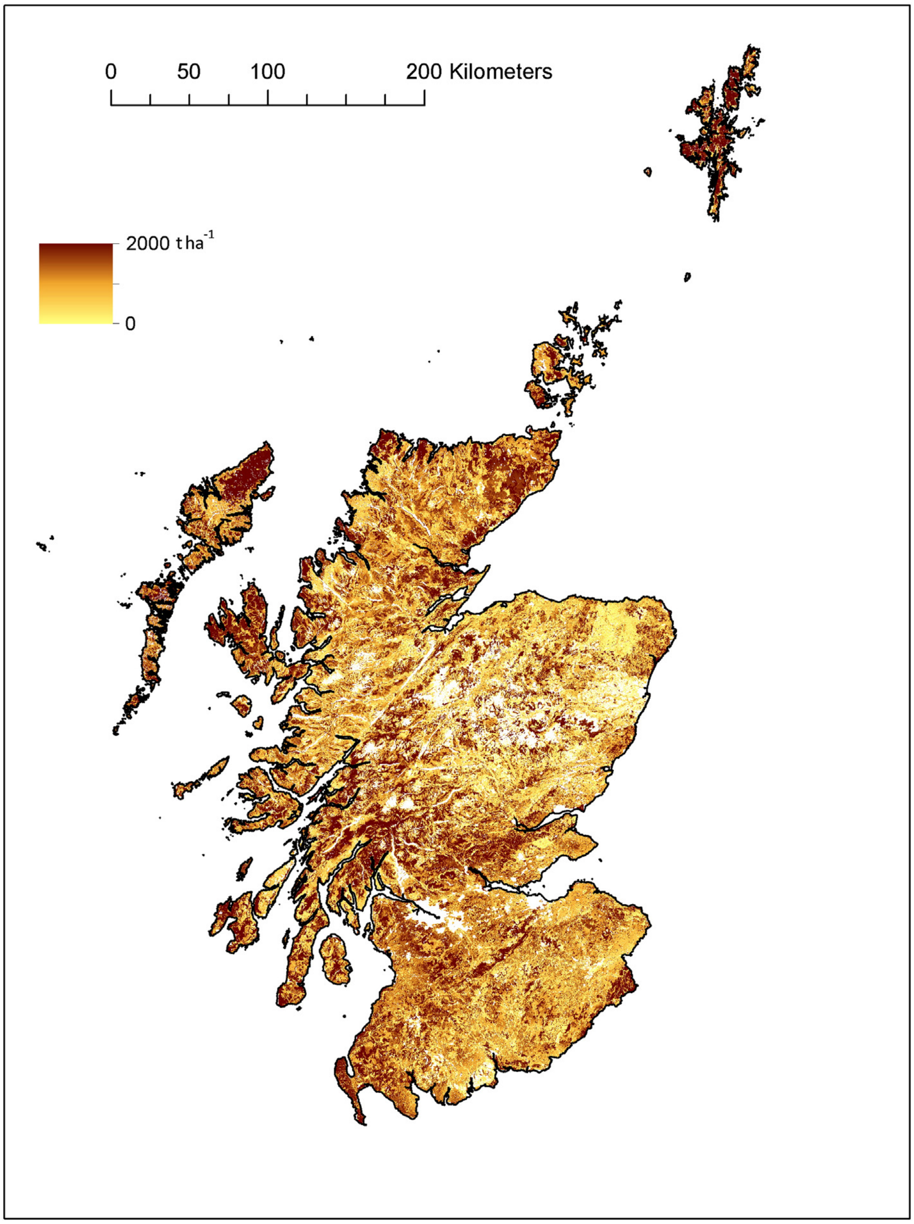

Fig. 3. Map of predicted soil organic carbon stock, in units of 10^3 kg/ha (t/ha).

additional spatial covariate data to that used. Both approaches suffer from the use of large numbers of covariates that are correlated with one another and the need to deal with this issue, and both are computationally intensive. Model simplification and accuracy improvement are needed for both.

To estimate organic carbon density, a pedotransfer function was used that took the estimates of bulk density, loss on ignition and depth, and used these as inputs to a second model. This model was shown to improve estimation of organic carbon content over the use of a simple ratio, although there is still some error introduced at this point. Linking the organic carbon estimation to predictions of profile depth enabled us to estimate the carbon stocking rate per hectare across Scotland. Estimation of profile depth was less accurate than that of bulk density or loss on ignition and we consider this to have been the source of the greatest amount of uncertainty in the overall carbon stock estimate. Improvement of our ability to estimate profile depth, particularly in organic soils where significant amounts of carbon can be stored at depth, is considered a priority area for improvement. Examination of

Table 2
Organic carbon (OC) stock by vegetation class, as a total and per hectare.

Vegetation	Total OC (kg)	OC (kg/ha)	Vegetation	Total OC (kg)	OC (kg/ha)
Arable	152.3×10^9	245.1×10^3	Bare ground	69.9×10^9	225.7×10^3
Imp. grass	474.5×10^9	450.9×10^3	Water	0	0
Rough grass	225.5×10^9	473.0×10^3	Montane	119.5×10^9	400.3×10^3
Heath	1043.5×10^9	443.9×10^3	Coniferous	315.8×10^9	345.9×10^3
Peat	475.3×10^9	631.2×10^3	Deciduous	77.8×10^9	376.8×10^3

Table 3
Organic carbon (OC) stock by soil class, as a total and per hectare.

Soil type	Total OC (kg)	OC (kg/ha)	Soil type	Total OC (kg)	OC (kg/ha)
Alluvial	40.8×10^9	246.2×10^3	Peat	813.9×10^9	468.6×10^3
Alpine	145.7×10^9	380.9×10^3	Podzol	536.6×10^9	295.5×10^3
Bare ground	50.5×10^9	302.0×10^3	Ranker	82.6×10^9	326.3×10^3
Brown earth	590.3×10^9	369.6×10^3	Regosol	19.0×10^9	435.0×10^3
Gley	645.4×10^9	404.3×10^3			

Fig. 1 shows that shallower soils are predicted in areas of steep slopes and/or high elevation, with deeper soil more dominant in low-level areas and on shallow slopes. The underestimation of profile depth for deeper soils would not introduce much error in carbon stock estimation for mineral and organo-mineral soils as the amount of carbon at depth in these soils is low; however, for organic soils that are often deeper than 1 m, an underestimate of depth would greatly reduce the estimate of carbon storage. Even though we are only making predictions of organic carbon storage within Scottish soils to 1 m depth, this would still result in the depth of many organic soils being incorrectly estimated at less than 1 m, with a lower portion down to 1 m depth being left out of our calculations. The improvement seen in our model for predicting the proportion of LOI that is organic carbon is greatest when predicting organic carbon stocking densities for mineral soils where values are already low, and so may not have a very large impact on the total carbon stock estimate for Scotland.

We also found that the approach used for mapping soils across Scotland may lead to under- and over-estimates of the stocks for specific soil classes. The mapping of soil 'map units' usually containing a mix of more than one soil type in estimated proportions, does not allow us to identify the exact soil type at a specific location and therefore to relate this to an estimated carbon stock density. The effect of this will be to allocate a proportion of the soil carbon from soils with large stocks estimates to soil types that are associated with lower stocks, and to do the opposite with soils, such as peats, which are associated with greater stocks. The overall effect of this will be to smooth out the estimates of soil carbon by soil types, with peats being lesser and bare ground/arable soils being greater than the reality. This is in fact what was seen in the results, resulting in some disagreement with the estimates by others, particularly Chapman et al. (2013).

Distribution of organic carbon with depth shows that mineral soils contain more organic carbon overall than organic soils, particularly near the surface. By unit area and on average, organic soils contain slightly more organic carbon at the surface than mineral soils, but with depth their relative importance for carbon storage increases. The implication of this, particularly when considered next to the fact that some mineral soils contain almost as much organic carbon as peats at the surface, is that mineral topsoils may be more important than is often considered for carbon storage. This is an important factor to consider when managing soils for carbon storage. Organic soils are an obvious storage medium for carbon and already contain a significant store; however, denser soils with lower organic matter content can not only provide an important carbon store but can also have their ecosystem service provision enhanced through increased organic carbon content. Many mineral soils in Scotland are used for agriculture, and the organic matter component of these soils is important for soil fertility, water holding capacity and erosion control in addition to provide carbon storage. There is an argument to be made therefore that targeted management of all soil types should be achieved in order to maintain or increase their carbon storage capabilities.

An important topic that has not been tackled in this work is the form that mineral topsoil organic carbon takes — it is possible that this carbon is turned over rapidly, with the labile fraction being lost at the same rate as it is being input to the system, and as such is not appropriate as a potential long-term 'store' of carbon. Increasing the organic carbon stocks of mineral soils may be more difficult due to their more intensive use and the demand for functions other than carbon storage. Management strategies that work the soil for cost-effective productivity are usually, if not always, the same strategies that lead to loss of organic matter through erosion and increased organic matter turnover.

Possible improvements to the approaches used in this work include the optimisation of the neural network models through parameterisation of the learning rate and network architecture, and the use of multiple neural networks to obtain consensus values that are often more accurate than the use of single models. We also feel that using additional terrain parameters may improve model accuracy. A priority is the development of an improved model for the prediction of profile depth, particularly in organic soils, in order to make more accurate assessments of the storage of organic carbon deep within the soil profile. In order to accomplish this, it is necessary to develop a set of field observations for peat depths that is sufficiently large and diverse to allow a model applicable to the whole of Scotland to be developed. Currently, there is insufficient data available to do this although numerous small surveys have been carried out over the last 60 years. Integration of this legacy data may allow us

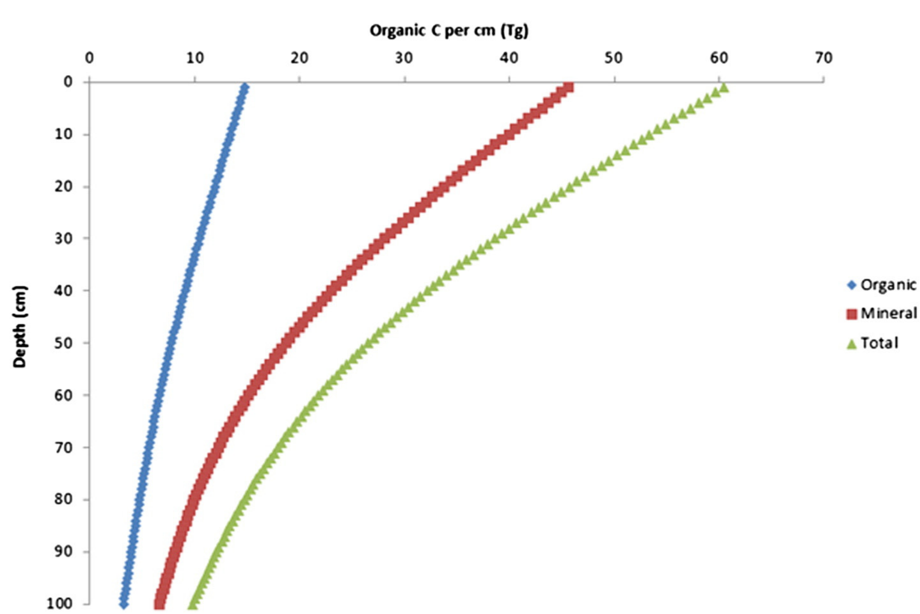

Fig. 4. Distribution of predicted organic soil, mineral soil and total soil organic carbon with depth.

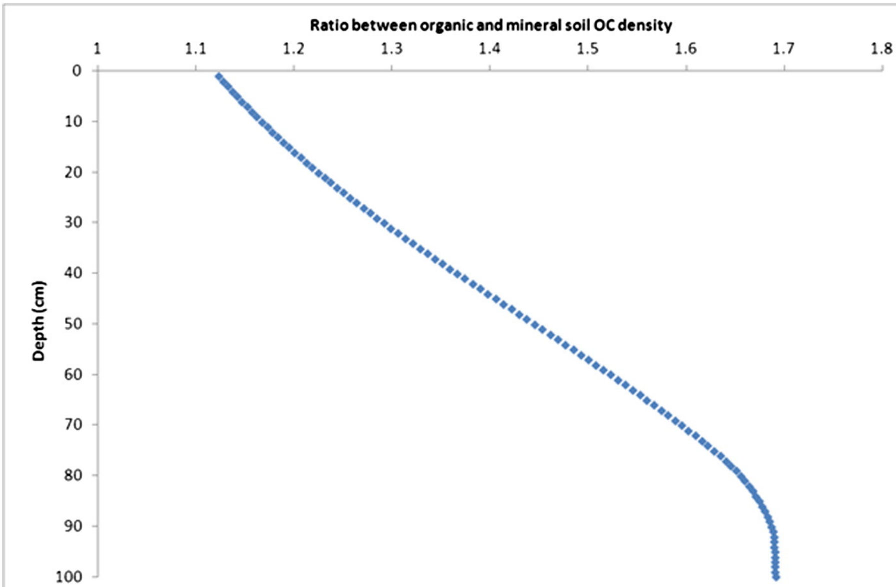

Fig. 5. Variation with depth of ratio between organic carbon density of organic and non-organic soils.

to develop a partial dataset, although very little peat depth survey work has been done on blanket bogs and upland bogs and some field work is therefore still required.

In addition, it is necessary to better consider the role of inorganic carbon on soil carbon assessments where calcareous soils are present (Rawlins et al., 2011), or where charcoal accumulation takes place due to biochar additions (or naturally occurring carbon deposits such as surface seams of coal or glacial drift containing coal fragments).

The adoption of standard protocols was important in the National Soil Inventory of Scotland (Lilly et al., 2010), a body of work that has been carried out over several years and the importance of which for developing this work cannot be overstated. Multiple methods exist for developing national or regional soil carbon inventories, although certain commonalities exist for those that rely on field data and are designed to be 'future proof'. Van Wesemael et al. (2011) discuss important features of soil inventories, including archiving of samples for comparison with future assessments and the recording of land use/land cover and other environmental information that may be important in relating soil characteristics to formation factors. VandenBygaart and Angers (2006) identified important parameters and modes of measurement that improve the effectiveness of SOC inventories for multiple uses and research purposes.

5. Conclusions

For Scotland, estimates of total soil carbon stocks to 1 m depth vary, with values including 2187 Tg (Bradley et al., 2005), 2055 Tg (Chapman et al., 2013, Chapman, pers. comm.), and ~3000 Tg (Campbell et al., 2012). The value we have obtained, 2954 Tg, is higher than that given by Bradley et al. (2005) and Chapman et al. (2013), but is comparable with the value given by Campbell et al. (2012). One important characteristic of our predicted distribution of carbon is that it shows a large amount of soil organic carbon in soils of relatively high bulk density and low organic matter content, particularly in the south and south-west of Scotland. While the majority of the soil organic carbon is contained within peats in the top metre (and more will exist in peats below this depth), there is more soil carbon predicted in these mineral soils than previously expected. In relation to soil carbon stock management this is an important finding as it indicates a need to consider how best to manage these soils in order to retain their carbon.

An important part of estimating total soil carbon stocks is the quantification of uncertainty levels, which are not always provided. Goidts et al. (2009) showed that several factors can influence variations in soil organic carbon (SOC) estimates, including laboratory errors and high spatial variability of soil organic carbon content in relation to sampling density. While we have assumed that the laboratory measurements that were used to develop the model were accurate, we have not accounted for variation within the 100 m scale. In some areas, large variation at this scale is less likely (e.g. homogeneous arable land, forestry or grassland). However, there are some parts of Scotland where topography varies greatly over short distances, resulting in small-scale variation. This work could potentially be repeated using topographic data at a resolution of 10 m, which is available over the whole of Scotland, although the computational costs would be greatly increased. It would also be necessary if redoing some aspect of this work to resample the climate data that was used, possibly using a more sophisticated approach than the linear interpolation that was used.

The value we obtained for total soil organic carbon stock to 1 m depth was consistent with other estimates in the literature. In addition, we were able to produce estimates of distribution of this organic carbon between different vegetation classes, and between different soil classes. We found that peatland vegetation had the greatest stocks followed by heath, with grassland also contributing significantly. Peat soils, as expected, are predicted to contain the greatest stocks of organic carbon although gley soils are also predicted to contain a high density. Certain classes of mineral and organo-mineral soil, while having lower proportional organic matter content than 'organic' peat soils, nevertheless have much greater bulk density values and therefore contain almost as much organic carbon per unit volume as peats.

The use of a neural network-based pedotransfer function for prediction of organic carbon density at depth has enabled us to produce a three-dimensional map of Scotland's soil carbon stocks. The input parameters used to develop this map include topography, climate, vegetation and geology, which are commonly mapped in most other countries. The methodology applied here is therefore applicable for other regions of the world, and could potentially be used to provide maps of soil organic carbon where little information exists about this important environmental characteristic. It is different from approaches used in some Digital Soil Mapping (DSM) work (for example the consortium GlobalSoilMap.net, which usually use interpolation approaches, but which use comparable underlying data). However, a lot of DSM work in the literature has also used multivariate modelling (e.g. neural network, Bayesian) approaches.

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