



**SOC estimation by  
robust external-drift  
kriging**

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This discussion paper is/has been under review for the journal Geoscientific Model Development (GMD). Please refer to the corresponding final paper in GMD if available.

# Estimating soil organic carbon stocks of Swiss forest soils by robust external-drift kriging

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Received: 11 November 2013 – Accepted: 9 December 2013 – Published: 23 December 2013

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Published by Copernicus Publications on behalf of the European Geosciences Union.

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## Abstract

Accurate estimates of soil organic carbon (SOC) stocks are required to quantify carbon sources and sinks caused by land use change at national scale. This study presents a novel robust kriging method to precisely estimate regional and national mean SOC stocks, along with truthful standard errors. We used this new approach to estimate mean forest SOC stock for Switzerland and for its five main ecoregions.

Using data of 1033 forest soil profiles, we modelled stocks of two compartments (0–30, 0–100 cm depth) of mineral soils. Lognormal regression models that accounted for correlation between SOC stocks and environmental covariates and residual (spatial) auto-correlation were fitted by a newly developed robust restricted maximum likelihood method, which is insensitive to outliers in the data.

Precipitation, near-infrared reflectance, topographic and aggregated information of a soil and a geotechnical map were retained in the models. Both models showed weak but significant residual autocorrelation. The predictive power of the fitted models, evaluated by comparing predictions with independent data of 175 soil profiles, was moderate (robust  $R^2 = 0.34$  for SOC stock in 0–30 cm and  $R^2 = 0.40$  in 0–100 cm). Prediction standard errors (SE), validated by comparing point prediction intervals with data, proved to be conservative.

Using the fitted models we mapped forest SOC stock by robust external-drift point kriging at high resolution across Switzerland. Predicted mean stocks in 0–30 cm and 0–100 cm depth were equal to  $7.99 \text{ kg m}^{-2}$  (SE  $0.15 \text{ kg m}^{-2}$ ) and  $12.58 \text{ kg m}^{-2}$  (SE  $0.24 \text{ kg m}^{-2}$ ), respectively. Hence, topsoils store about 64% of SOC stocks down to 100 cm depth. Previous studies underestimated SOC stocks of topsoil slightly and those of subsoils strongly. The comparison further revealed that our estimates have substantially smaller SE than previous estimates.

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## 1 Introduction

Greenhouse gas (GHG) reporting for the sector “LULUCF – Land Use, Land-Use Change and Forestry” of the United Nations Framework Convention on Climate Change and the Kyoto Protocol requires national estimates of soil organic carbon (SOC) stock. Stock estimates are needed as baseline and for quantifying carbon (C) sources and sinks caused by land use change. Switzerland, as an example, accounts in a Tier-2 approach (IPCC, 2003) for stock changes due to conversion between settlements, wetlands, forest-, crop-, grass- and other land (FOEN, 2012a). Respective estimates are reported for the five ecoregions Jura, Central Plateau, Pre-Alps, Alps and Southern Alps (Brassel and Lischke, 2001) and for the whole country.

Mean SOC stocks were estimated by various approaches in previous studies: the simplest is to use the arithmetic mean of the available SOC stock data as a national estimate (Weiss et al., 2000). “Class-matching” (CM) estimates mean stocks for bioclimatic (Chiti et al., 2012), land use or soil map strata (Xu et al., 2011; Krogh et al., 2003) or intersections thereof (Arrouays et al., 2001; Lettens et al., 2004, 2005a; Meersmans et al., 2009) and combines them for a national estimate by formulae for stratified random sampling (STR). Hence, CM capitalizes on benefits of spatial stratification, but Perruchoud et al. (2000) demonstrated that respective gains may be small.

Perruchoud et al. (2000) and other authors (e.g. Leifeld et al., 2005; Meersmans et al., 2008, 2011, 2012a) used therefore linear models (LM) to relate SOC to covariates characterizing soil formation by climate, vegetation, topography, geology and land management. More recently, Grimm et al. (2008); Martin et al. (2011) and Wiesmeier et al. (2011) used non-linear machine learning (ML) methods to the same end. Such statistical modelling of SOC needs covariates that are available contiguously in space because mean stocks are estimated by averaging LM or ML point predictions for the nodes of a fine-meshed grid over a region of interest, which is equivalent to a discrete approximation of the geostatistical block kriging approach (e.g. Gotway and Young, 2002). This restriction generally limits the predictive power of fitted models seriously,

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because accurate spatial information on important, soil-related, SOC controlling covariates (pH, clay content, reactive aluminium and iron, mineral surface charge density, soil temperature and moisture; Schmidt et al., 2011) is commonly unavailable.

If linear and ML models fit SOC data only poorly then spatially structured variation in data becomes likely apparent as residual spatial autocorrelation. Beside ordinary kriging (Mishra et al., 2009), regression kriging (RK, Hengl et al., 2004), a variant of external-drift kriging (EDK), was used by Mishra et al. (2010, 2012) and Kumar et al. (2012) to map SOC stock at regional scale. Mishra et al. (2010, 2012) demonstrated that RK indeed improves on LM and CM by exploiting autocorrelation when computing SOC predictions. Considering autocorrelation is also essential for unbiased significance testing of hypotheses on relations between SOC and environmental covariates. Many studies that built statistical SOC models based on significance testing (e.g. Leifeld et al., 2005; Meersmans et al., 2008, 2012a; Wiesmeier et al., 2013) neglected autocorrelation. The studies by Perruchoud et al. (2000) and Wiesmeier et al. (2012) are here notable exceptions.

Besides precision, also honest modelling of estimation errors of national SOC stocks matters for GHG inventories, e.g., to test the statistical significance of estimated stock changes (Lettens et al., 2005a, b; Meersmans et al., 2009, 2011). Quantification of uncertainties of spatial mean stock estimates (and changes) is straightforward for CM, where STR formulae can be employed. However, care is needed when mean stock estimates are obtained by averaging LM, EDK or ML point predictions: the point prediction errors for the nodes of the prediction grid are then mutually correlated. This is true even if there is no residual autocorrelation because predictions are computed from a common model. Thus, ignoring the correlation of fitted regression coefficients of LM as in Meersmans et al. (2008, 2011, 2012b, personal communication, 2013) and in Martin et al. (2011, personal communication, 2013) likely biases the standard errors (SE) of estimated mean stocks. If there is residual autocorrelation then the correlation of prediction errors at adjacent nodes of the prediction grid is stronger. Neglecting it biases SE even more.

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The truthfulness of reported SE is best checked with independent validation data, along with the actual precision of mean stock estimates. We are currently not aware of any study that validated modelled SE of stock estimates, and only few studies (Mishra et al., 2009, 2010, 2012; Wiesmeier et al., 2011; Kumar et al., 2012) tested the precision of the estimates with independent data. Grimm et al. (2008); Martin et al. (2011) and Meersmans et al. (2012b) used cross-validation to the same purpose, which is clearly better than merely reporting notoriously over-optimistic goodness-of-fit  $R^2$  values, as done in most studies.

The choice of transformations for SOC data is a further issue that requires some care. Statistical inference for CM, LM and EDK relies on the assumption of normally distributed errors with constant variance. Frequently, this assumption is violated by SOC data as empirical distributions are often positively skewed and their dispersion increases with the mean (e.g. Mishra et al., 2009, 2010; Chiti et al., 2012; Kumar et al., 2012; Wiesmeier et al., 2012, 2013). SOC data should then be log-transformed for statistical analyses as in Mishra et al. (2010); Kumar et al. (2012) and Wiesmeier et al. (2012). Neglecting data transformations (Meersmans et al., 2009; Chiti et al., 2012) will likely affect stock estimates only mildly but will invalidate reported SE. Another error is to fit LM to untransformed SOC stocks, but at the same time to assume that the prediction errors have constant relative dispersion (Meersmans et al., 2011).

Last but not least, outliers are a common nuisance in SOC data sets (Meersmans et al., 2008; Mishra et al., 2009; Martin et al., 2011; Chiti et al., 2012; Wiesmeier et al., 2012, 2013). In most instances, they are genuine observations that do not follow the “majority pattern” of a data set. A common but suboptimal recipe is to exclude such observations (Chiti et al., 2012) from the analyses. Outlier deletion biases statistical inference if not properly taken into account (Maronna et al., 2006, chap. 1). A better approach is therefore to use robust methods that are insensitive to outliers. Excepting Martin et al. (2011) and Wiesmeier et al. (2011), no robust procedures were used so far to estimate mean SOC stocks.

This review shows that there is scope to improve on previously used statistical methodology for estimating SOC stocks at the regional and national scales. When estimating SOC stocks stored in the mineral soil of Swiss forests, our objectives were therefore,

- i. to employ a statistically sound, robust lognormal EDK approach that accounts for dependence of SOC stock on environmental covariates and autocorrelation;
- ii. to fit such models for mapping SOC stocks of two compartments (0–30 cm, 0–100 cm depth) of the mineral soil with 100 m spatial resolution across Switzerland;
- iii. to rigorously validate both precision of predictions and truthfulness of modelled SE with independent validation data, and
- iv. to compute reliable estimates and associated SE of mean stocks for whole Switzerland and its ecoregions – stratified further by altitude into the groups  $\leq 600$  m, 600–1200 m,  $> 1200$  m a.s.l. – by robust lognormal block EDK.

The present study is confined to mineral soils under forest. Comprehensive, harmonized and georeferenced SOC data is for the time being available only for this land use. Data on SOC stock stored in organic layers of Swiss forest soils is at present too scarce to allow for a similar analyses, and comprehensive legacy data on SOC stocks of Swiss crop- and grasslands will become available in the future only, as this data is currently digitized and geo-referenced. Nonetheless, mineral forest soil stocks are important for GHG reporting because forest cover 45.5 % of the vegetated area of Switzerland (Hotz et al., 2005). Furthermore, the currently available stock estimates for topsoils suggest that forest soils store 1.5 times more organic carbon (OC) cropland and still 1.2 times more SOC than grassland soils (FOEN, 2012a). These figures underpin the importance of forest SOC stock, which, in our view, justifies a separate analysis of the respective data.

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## 2 Materials and methods

### 2.1 Study area

As our study focused on forest soils, we had to delimit the forest area of Switzerland (Fig. 2). We used the same criteria as Giamboni (2008): six categories rendered by VECTOR25 (Swisstopo, 2011b) as forest plus former forest areas, devastated in 1990 and 1999 by two hurricanes (Bundesamt für Umwelt BAFU, 2010) and currently not classified as forest by VECTOR25. Areas shared with the National Mire Inventory (FOEN, 2012b) were excluded. This removed some but not all organic soils because the inventory does not cover all bogs and fens under forest, in particular, if these had been drained in the past.

According to this definition, forests cover 11 800 km<sup>2</sup> (29 % of total area of Switzerland). Forests extend over altitudes from 190 m to 2390 m a.s.l. (Swisstopo, 2011a). Climatic conditions therefore vary notably within this area: mean annual precipitation ranges from 600 mm to 2900 mm and mean annual temperature from -1 to 13 °C (MeteoSwiss, 2011). Two thirds of the forested area is dominated by coniferous trees, deciduous forests prevail only at lower altitudes in the regions Jura, Central Plateau, Pre-Alps and Southern Alps (Swiss Federal Statistical Office, 2000b). Considerable variation is also found in geologic parent material for soil formation: predominantly limestones in the Jura and in parts of the Pre-Alps, fluvioglacial sediments of several quaternary glaciations and of the Tertiary on the Central Plateau and igneous and metamorphic rocks in the Alps and Southern Alps. This large variation of pedogenetic factors is reflected in the development of very diverse soils (Walthert et al., 2004) with variable conditions for mineralization and accumulation of SOC.

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## 2.2 Data

### 2.2.1 Soil data

#### Soil profiles

We used data of 1033 forest soil profiles (Fig. 2), studied by the Swiss Federal Institute for Forest, Snow and Landscape Research (WSL) in various surveys over the past 30 yr (mostly 1990–2000). Use of legacy soil data is typical for many SOC inventories (e.g. Krogh et al., 2003; Lettens et al., 2004, 2005b; Kumar et al., 2012). Two WSL surveys chose 269 sites on square grids with 1 km and 8 km spacing, respectively. The remaining sites were selected purposively by field surveyors to best represent soils typical for given vegetation types. The position of the soil profiles was recorded in the field on topographic maps (scale 1 : 25 000), hence the error in the coordinates is about  $\pm 25$  m.

We assigned 175 out of the 1033 soil profiles to the validation set, which was used to check the predictive power of the fitted statistical models, and the remaining 858 soil profiles formed the calibration set, used to build and fit these models. All except three sites of the validation set with organic soils lay on the 1 km (38 sites) and 8 km grid (134 sites), respectively. This selection resulted in a fairly even and spatially representative distribution of the validation sites across Switzerland (Fig. 2). When splitting the data, we strived for a balanced representation of soil map units and vegetation types between calibration and validation set.

The thickness of all soil horizons was recorded in the field on the faces of soil pits and subsequent soil sampling and laboratory analyses were all done by pedogenetic horizons.

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## Stone content

The volumetric content of stones (particles with size > 2 mm) was estimated visually on the face of soil profiles, which is a common procedure (Baritz et al., 2010). These estimates are bound to some error that is very difficult to quantify because surveys were done by different staff. However, neglecting stone content as in many other studies would lead to overestimation of SOC stocks as stone content is large for many Swiss forest soils.

## Soil density

The density of the soil fraction with particle size  $\leq 2$  mm was measured for 440 out of ca. 5000 mineral soil horizons with soil samples of fixed volume (Walthert et al., 2004, p. 702) collected from the soil profiles. In addition, a field estimate (penetration resistance of blade) of soil density was available for all soil horizons (ordinal variable with 5 levels, Walthert et al., 2004, p. 695).

We computed the median of the measured densities for each level of this variable and assigned these medians to all soil samples without density measurements. The accuracy of this pedotransfer function (PTF) was evaluated by tenfold cross-validation (by re-estimating and re-assigning the median densities, computed from 9 cross-validation subsets, to the 10th subset). The median of the cross-validation errors was equal to  $0.002 \text{ g cm}^{-3}$  and the median absolute deviation (MAD, see below) was equal to  $0.256 \text{ g cm}^{-3}$ . For comparison, we used also the PTF by Adams (1973) and Honeysett and Ratkowsky (1989), which performed best for forest soils in the evaluations of De Vos et al. (2005) and Baritz et al. (2010). Bias and MAD of the cross-validation errors ranged between 0.33–0.34 and 0.50–0.52  $\text{g cm}^{-3}$  without re-calibration and if the coefficients of the PTF were re-estimated with our own data these measures were 0.06 and  $0.30 \text{ g cm}^{-3}$ . Hence, our PTF had better predictive power.

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## SOC content

SOC content was measured for all mineral soil samples by an elemental C/N-analyser (combustion at 1000 °C, Walthert et al., 2010). When pH of a soil sample was larger than 6.0 then carbonates were removed by fumigation with hydrochloric acid prior to measuring C. Below this pH carbonates were assumed to be absent, and the SOC content of the sample was assumed to be equal to its total C content (Walthert et al., 2010).

## SOC stock

The SOC stock  $S_i$  stored in horizon  $i$  per unit area [ $\text{kg m}^{-2}$ ] was calculated from the total volume  $V_i$  of the horizon per unit area [ $\text{m}^3 \text{m}^{-2}$ ], its volumetric stone content  $G_i$  [ $\text{m}^3 \text{m}^{-3}$ ], soil density  $\rho_i$  [ $\text{kg m}^{-3}$ ] and its SOC content  $C_i$  [ $\text{kg kg}^{-1}$ ] by

$$S_i = V_i(1 - G_i)\rho_i C_i, \quad (1)$$

and the stock  $S$  in a given depth compartment was summed by

$$S = \sum_{i=1}^h w_i S_i, \quad (2)$$

where  $h$  is the number of horizons fully or partly included in the compartment and  $w_i$  is the fraction of the thickness of horizon  $i$  within the compartment.

## 2.2.2 Covariates for statistical modelling

### Parent material and soil

Detailed information on soils and parent material is not available for whole Switzerland. Therefore, an overview soil map discriminating 25 units (map scale 1 : 200 000,

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Swiss Federal Statistical Office, 2000a) was used as a coarse representation of geologic and pedogenetic conditions. Being mainly designed for agricultural usage, certain map units did not well reflect contrasting conditions of forest soil development. To lessen this drawbacks five additional units were created by intersecting the soil map with selected polygons of the Geological Map of Switzerland (map scale 1 : 500 000, Swisstopo, 2005) and the maps of the Last Glacial Maximum (map scale 1 : 500 000, Swisstopo, 2009) and of the Biogeographic Regions of Switzerland (see Table S2 in Supplement, Gonseth et al., 2001). Besides, we used the geotechnical map (map scale 1 : 200 000, BFS, 2001) to extrapolate soil information (for details on sampling see Appendix 2, Walthert et al., 2004) available only at the 1033 soil profile sites to whole Switzerland. Median values of soil properties measured at those sites that lay within a given geotechnical map unit were assigned to the respective unit. Then we checked whether these newly generated covariates correlated with SOC stocks. This was true for cation exchange capacity, iron and calcium stocks and mass of soil particles < 2 mm that we consequently retained for the statistical analyses.

## Climate

Three climate data sets were available to us with spatial information on mean annual/monthly temperature and precipitation, cloud cover, sunshine duration, radiation, degree-days, continentality index (Gams, 1935), temperature variation, ratio of actual to potential evapotranspiration and site-water-balance (Grier and Running, 1977). Two data sets contained spatial information (resolution 25 m and 2 km, respectively) on climatic means for period 1961–1990 (Zimmermann and Kienast, 1999; MeteoSwiss, 2011) and the third for 1975–2010 (spatial resolution 250 m). Since it was not a priori clear, which data set would be best, we used them all as covariates in the statistical analyses.

## Vegetation

The percentage of coniferous trees was derived from spectral imagery (Swiss Federal Statistical Office, 2000a) and species composition data of the National Forest Inventory (NFI, Brassel and Lischke, 2001, both covariates rasterized with 25 m resolution).

5 The SPOT5 mosaic of Switzerland (Mathys and Kellenberger, 2009) with spectral reflectance in green, red and near-infrared bands, band ratios, IHS colour space transformations and the Normalized Differenced Vegetation Index (NDVI, Krieglner et al., 1969) were available. Moreover, canopy height (difference of digital surface to digital elevation model of 2 m resolution, Swisstopo, 2011a) was included in the set of covariates.

## 10 Topography

Two digital elevation models (DEM, resolution 2 and 25 m, Swisstopo, 2011a) allowed to compute a broad range of terrain attributes covering multiple scales: elevation, slope angle, aspect, north- and eastness, planar, profile and combined curvatures and smoothed versions of these attributes. Furthermore, topographic position indices were  
15 calculated based on Zimmermann (2000) and Jenness (2006) with radii ranging from 6 m to 2 km. Flow accumulation area and topographic wetness indices, computed by single and multi-flow algorithms (Tarboton, 1997), were available, too.

## Accounting for errors in locations of soil profiles

We mentioned above that coordinates of soil profiles had been recorded with a likely  
20 error of about  $\pm 25$  m, which exceeds the resolution of the highly resolved DEM clearly. Therefore, the values of all covariates were averaged for circular neighbourhoods, centred on the recorded profile locations and having radii equal to 13 m, 19 m or 26 m. Depending on the type of data, different summary statistics were computed: arithmetic means for real numbers, medians for integers and the most frequent category for nominal or ordinal variables. However, values of covariates aggregated with the different  
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radii were highly correlated, Therefore, we used for statistical analyses only summaries computed with a radius of 26 m.

## 2.3 Statistical analyses

### 2.3.1 Model

5 Given past experiences (Mishra et al., 2010; Kumar et al., 2012; Wiesmeier et al., 2012) and exploratory analyses (Fig. 3), we decided to use a lognormal model for the SOC stock  $S(\mathbf{s})$  at location  $\mathbf{s}$ :

$$Y(\mathbf{s}) = \log(S(\mathbf{s})) = \mathbf{x}(\mathbf{s})^T \boldsymbol{\beta} + Z(\mathbf{s}) + \varepsilon(\mathbf{s}), \quad (3)$$

10 where  $\mathbf{x}(\mathbf{s})^T \boldsymbol{\beta}$  is the external drift that accounts for dependence of  $S$  on environmental covariates  $\mathbf{x}$ , (with  $\boldsymbol{\beta}$  the regression coefficients),  $^T$  denotes transpose and  $Z(\mathbf{s})$  is a stationary autocorrelated Gaussian random field with zero mean and isotropic exponential variogram with sill  $\sigma^2$  and range  $\alpha$

$$\gamma(h) = \sigma^2 (1 - \exp(-h/\alpha)). \quad (4)$$

15  $\varepsilon(\mathbf{s})$  is a zero mean, spatially uncorrelated variable with nugget variance  $\tau^2$ . In our robust geostatistical approach  $\varepsilon(\mathbf{s})$  need not be Gaussian, allowing thereby for outliers in the data. The coefficients  $\boldsymbol{\beta}$ , the variogram parameters  $\boldsymbol{\theta}^T = (\tau^2, \sigma^2, \alpha)$  and the values  $\mathbf{Z}^T = (Z(\mathbf{s}_1), Z(\mathbf{s}_2), \dots, Z(\mathbf{s}_n))$  at the  $n$  soil profile locations  $\mathbf{s}_i$  are unknown and must be estimated from the data.

### 2.3.2 Model building

20 We used only the calibration set for model building, which involved the following steps:

1. Positively skewed covariates (e.g. some terrain attributes) were transformed by square root or natural logarithm.

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2. Strongly correlated and therefore redundant covariates were eliminated based on correlation-biplots (Gabriel, 1981).
3. The least absolute shrinkage and selection operator (LASSO, Hastie et al., 2009, Sect. 3.4) – an algorithm that likely excludes non-relevant covariates – was used with various sets of covariates, partly enriched by first-order interactions between pairs of covariates, to find an external drift that minimized the mean squared error (MSE) in tenfold cross-validation.
4. The parameters of the geostatistical model (Eq. 3) were then estimated by a novel robust restricted maximum method (REML, Künsch et al., 2011, 2013) for the external drift selected by LASSO.
5. Using still the external drift of the optimal LASSO fit, an optimal value of the tuning constant  $c$  that controls the robustness of REML was chosen by tenfold cross-validation. We used the continuous ranked probability score (CRPS, see below and Gneiting et al., 2007) as main criterion for choosing the tuning constant (and for selecting covariates in step 6). We further tested whether other variogram functions (spherical, Whittle-Matérn, etc., e.g. Diggle and Ribeiro, 2007) improved the fit but this was not the case.
6. Non-relevant covariates were then removed step by step by tenfold cross-validating the robust REML fit (and added back along with interaction terms at later stages if cross-validation results justified this).
7. The levels of categorical covariates (in particular of the soil map) were merged based on partial residual plots (e.g. Faraway, 2005) and cross-validation CRPS to obtain a final parsimonious geostatistical model.

The improvement of the cross-validation MSE from step 3 to 6 is shown in Fig. S1 of the Supplement.

### 2.3.3 Mapping SOC forest soil stocks across Switzerland

After having tested the final model with the validation set (see below), we fitted it once more to the merged calibration and validation data to get better parameter estimates and to use all data for mapping. SOC stocks were then predicted by robust lognormal kriging (Cressie, 2006; Künsch et al., 2013) for the nodes of a 100 m grid by

$$\tilde{S}(\mathbf{s}) = \exp(\tilde{Y}(\mathbf{s}) + 1/2\{\hat{\tau}^2 + \hat{\sigma}^2 - \text{Var}[\tilde{Y}(\mathbf{s})]\}), \quad (5)$$

with

$$\tilde{Y}(\mathbf{s}) = \mathbf{x}(\mathbf{s})^T \hat{\boldsymbol{\beta}}_{\hat{\theta}} + \boldsymbol{\gamma}_{\hat{\theta}}(\mathbf{s})^T \boldsymbol{\Gamma}_{\hat{\theta}}^{-1} \hat{\mathbf{Z}}_{\hat{\theta}}, \quad (6)$$

where  $\hat{\cdot}$  denotes robust REML estimates,  $\boldsymbol{\gamma}_{\hat{\theta}}(\mathbf{s})$  is the vector with the estimated covariances between  $\mathbf{Z}$  and  $Z(\mathbf{s})$ ,  $\boldsymbol{\Gamma}_{\hat{\theta}}$  is the estimated covariance matrix of  $\mathbf{Z}$  and

$$\text{Var}[\tilde{Y}(\mathbf{s})] = \left( \boldsymbol{\gamma}_{\hat{\theta}}(\mathbf{s})^T \boldsymbol{\Gamma}_{\hat{\theta}}^{-1}, \mathbf{x}(\mathbf{s})^T \right) \cdot \text{Cov} \left[ \begin{pmatrix} \hat{\mathbf{Z}}_{\hat{\theta}} \\ \hat{\boldsymbol{\beta}}_{\hat{\theta}} \end{pmatrix}, \begin{pmatrix} \hat{\mathbf{Z}}_{\hat{\theta}}^T \\ \hat{\boldsymbol{\beta}}_{\hat{\theta}}^T \end{pmatrix} \right] \begin{pmatrix} \boldsymbol{\Gamma}_{\hat{\theta}}^{-1} \boldsymbol{\gamma}_{\hat{\theta}}(\mathbf{s}) \\ \mathbf{x}(\mathbf{s}) \end{pmatrix}. \quad (7)$$

Künsch et al. (2011) give in their Eq. (19) an approximation for the covariance matrix of  $(\hat{\mathbf{Z}}_{\hat{\theta}}^T, \hat{\boldsymbol{\beta}}_{\hat{\theta}}^T)$ . Approximate, lognormal kriging variances were obtained from

$$\text{Var}[S(\mathbf{s}) - \tilde{S}(\mathbf{s})] = \exp \left( 2 \mathbf{x}(\mathbf{s})^T \hat{\boldsymbol{\beta}}_{\hat{\theta}} + \hat{\tau}^2 + \hat{\sigma}^2 \right) \cdot \left\{ \exp(\hat{\tau}^2 + \hat{\sigma}^2) - 2 \exp(\text{Cov}[\tilde{Y}(\mathbf{s}), Y(\mathbf{s})] + \exp(\text{Var}[\tilde{Y}(\mathbf{s})]) \right\}, \quad (8)$$

where

$$\text{Cov}[\tilde{Y}(\mathbf{s}), Y(\mathbf{s})] = b \left( \boldsymbol{\gamma}_{\hat{\theta}}(\mathbf{s})^T \boldsymbol{\Gamma}_{\hat{\theta}}^{-1}, \mathbf{x}(\mathbf{s})^T \right) \cdot \mathbf{M}^{-1} \begin{pmatrix} \boldsymbol{\gamma}_{\hat{\theta}}(\mathbf{s}) \\ \mathbf{x}^T \boldsymbol{\gamma}_{\hat{\theta}}(\mathbf{s}) \end{pmatrix} \quad (9)$$

and  $b$ ,  $\mathbf{X}$ ,  $\mathbf{M}$  as in Künsch et al. (2011). Since outliers receive small weight when computing  $\hat{\boldsymbol{\beta}}_{\hat{\theta}}$  and  $\hat{\mathbf{Z}}_{\hat{\theta}}$  by the robust REML algorithm, the prediction of SOC stock by Eqs. (5) and (6) is also insensitive to outlying observations.

### 2.3.4 Predicting regional and national mean SOC stocks

The mean SOC stocks in the five ecoregions (and for whole Switzerland), stratified by altitude, were computed from the robust lognormal point kriging predictions at the nodes of the 100 m grid by

$$\tilde{S}(B_k) = 1/N_k \sum_{s_j \in B_k} \tilde{S}(s_j), \quad (10)$$

where the notation  $\sum_{s_j \in B_k}$  means summation over the  $N_k$  nodes of the grid falling into region  $B_k$ . Equation (10) is a discrete approximation to the lognormal block kriging predictor (e.g. Cressie, 2006, Eq. 14). The block kriging variance, i.e., the variance of the prediction error,  $S(B_k) - \tilde{S}(B_k)$ , for region  $B_k$  can similarly be approximated by the covariance (Eq. S2 in Supplement)

$$\text{Var}[S(B_k) - \tilde{S}(B_k)] = \frac{1}{N_k^2} \sum_{s_j \in B_k} \sum_{s_l \in B_k} \text{Cov}[S(s_j) - \tilde{S}(s_j), S(s_l) - \tilde{S}(s_l)]. \quad (11)$$

However,  $N_k$  is usually too large (in our case:  $10^4 - 10^5$ ) to evaluate the double sum of Eq. (11) in acceptable computing time. We used therefore a Monte-Carlo approximation for Eq. (11), where the covariances were repeatedly computed and averaged for randomly selected subsets of nodes in  $B_k$ . Full details can be found in the respective appendix of the Supplement. Of course, this approximation can also be used if there is no residual autocorrelation, and it is straightforward to derive analogous expression for untransformed data. For sufficiently large regions, one can safely assume – due to the central limit theorem – that the prediction errors  $S(B_k) - \tilde{S}(B_k)$  are normally distributed, in spite of the fact that point prediction errors follow lognormal laws.

### 2.3.5 Evaluating predictive performance of statistical models

The predictive power of the fitted geostatistical models was tested by comparing predicted (Eq. 6) with calculated SOC stocks (Eq. 2). The same criteria were used in model

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building by cross-validation (see above). Marginal bias and overall precision were assessed by

$$\text{BIAS} = -\frac{1}{n} \sum_{i=1}^n \frac{S(\mathbf{s}_i) - \tilde{S}(\mathbf{s}_i)}{S(\mathbf{s}_i)}, \quad (12)$$

$$\text{robBIAS} = -\text{median}_{1 \leq i \leq n} \left( \frac{S(\mathbf{s}_i) - \tilde{S}(\mathbf{s}_i)}{S(\mathbf{s}_i)} \right), \quad (13)$$

$$\text{RMSE} = \left( \frac{1}{n} \sum_{i=1}^n \left( \frac{S(\mathbf{s}_i) - \tilde{S}(\mathbf{s}_i)}{S(\mathbf{s}_i)} \right)^2 \right)^{1/2}, \quad (14)$$

$$\text{robRMSE} = \text{MAD}_{1 \leq i \leq n} \left( \frac{S(\mathbf{s}_i) - \tilde{S}(\mathbf{s}_i)}{S(\mathbf{s}_i)} \right), \quad (15)$$

where MAD stands for median absolute deviation. We computed summaries of the relative prediction errors because the lognormal model implies constant relative dispersion, i.e., constant coefficient of variation. We standardized the prediction errors by  $S$  instead of  $\tilde{S}$  to have a common standardization when comparing different models.

We also computed a standard and robust  $R^2$  by

$$R^2 = \frac{\text{Cov}[S(\mathbf{s}_i), \tilde{S}(\mathbf{s}_i)]^2}{\sqrt{\text{Var}[S(\mathbf{s}_i)]\text{Var}[\tilde{S}(\mathbf{s}_i)]}}, \quad (16)$$

$$\text{rob}R^2 = 1 - \left( \frac{\sum_{i=1}^n |S(\mathbf{s}_i) - \tilde{S}(\mathbf{s}_i)|}{\sum_{i=1}^n |S(\mathbf{s}_i) - \text{median}_{1 \leq i \leq n}(S(\mathbf{s}_i))|} \right)^2. \quad (17)$$

Although the latter is tailored for robust L1 regression (Croux and Dehon, 2003), we found it useful for our approach.

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In addition, we compute the strictly proper scoring criterion CRPS (Gneiting et al., 2007), which is equal to the integral over the Brier score (BS):

$$\text{CRPS} = \int_{-\infty}^{\infty} \text{BS}(u) \, du \approx \sum_{i=1}^n \text{BS}(S_{(i)}) \cdot (S_{(i+1)} - S_{(i-1)})/2, \quad (18)$$

where  $S_{(i)}$  is the  $i$ th largest calculated stock,  $S_{(0)} = S_{(1)}$ ,  $S_{(n+1)} = S_{(n)}$  and

$$\text{BS}(u) = \frac{1}{n} \sum_{i=1}^n \{\tilde{F}_i(u) - I(S(\mathbf{s}_i) \leq u)\}, \quad (19)$$

with  $\tilde{F}_i(u)$  the (estimated) lognormal predictive distribution of the  $i$ th datum and  $I(A)$  an indicator equal to one if  $A$  is true and zero otherwise. CRPS measures the *sharpness* of predictive distributions (smaller values signal sharper  $\tilde{F}_i$ ), hence depends both on prediction precision and quality how prediction uncertainty is modelled. Modelling of prediction uncertainty was further tested by counting how many observation fall into two-sided 95 %-prediction intervals and by checking the empirical distribution of the probability integral transform (PIT, Gneiting et al., 2007)

$$\text{PIT}_i = \tilde{F}_i(S(\mathbf{s}_i)), \quad (20)$$

which should be uniformly distributed.

All statistical computations were done in  $\mathbb{R}$  (R Core Team, 2013), using several add-on packages, in particular `georob` (Papritz, 2013) for robustly fitting geostatistical models and for robust kriging. Processing and mapping of spatial data was done in ArcGIS 10.0 (ESRI, 2010).

## 3 Results

### 3.1 Calculated SOC stocks

SOC stock stored in the top 30 cm of the mineral soil at the 1 033 sites varied considerably from 0.8 to 36.1 kg m<sup>-2</sup> (median 6.3 kg m<sup>-2</sup>), and to 100 cm depth stocks ranged from 1.0 to 96.4 kg m<sup>-2</sup> (median 9.2 kg m<sup>-2</sup>). Stocks in both depths were strongly correlated (Spearman correlation 0.91). On average, calculated stocks were slightly larger for the validation set (Table S1 of Supplement). Except for the Central Plateau and the Southern Alps, mean stocks down to 1 m depth increased with altitude (Fig. 3). For most strata, the frequency distribution of stocks was positively skewed and dispersion increased with the mean, calling for log-transformation for the statistical analyses.

### 3.2 Models for SOC stocks in 0–30 cm and 0–100 cm depth

Not surprisingly, given the strong correlation of stocks in the two depths, the structure of the external drifts did not differ much. Both drifts were parsimonious, with 10 and 12 fitted coefficients, respectively, and included covariates characterizing soils, vegetation, climate and topography (see Table 1 as well as Tables S3 and S4 of Supplement).

Tenfold cross-validation resulted for both depths in similar  $\text{rob}R^2$  (0.31). However, based on CRPS, the fit was better for topsoil stocks (0.238 vs. 0.252). Residuals of both models were spatially autocorrelated, but spatial dependence was rather weak with nugget/total-sill ratios and effective ranges of 0.37 and 600 m for 0–30 cm and 0.41 and 660 m for 0–100 cm depth (see Table S5 of Supplement).

The optimal tuning constant was equal to  $c = 2$  for both models, and robustly estimated parameters fitted the data better than customary Gaussian REML estimates (cross-validation CRPS of 0.239 for non robust model fit for 0–30 cm and of 0.253 for 0–100 cm depth).

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### 3.3 Validation of SOC stock predictions with independent data

Figure 4 shows calculated SOC stocks in 0–30 and 0–100 cm of the mineral soil, plotted against respective predictions for the independent validation set. The solid lines of the loess smoothers are close to the 1 : 1-lines, indicating absence of conditional bias.

This is confirmed by the BIAS and robBIAS statistics (Table 2). Irrespective how the statistics were computed, relative marginal bias was less than 15 %. However, variation of the data around the 1 : 1-line was quite large, which was reflected in large root mean squared relative errors. robRMSEs were about 40 % and non-robust RMSE 49 % for topsoils and 56 % for stocks down to 100 cm. As seen from the (non-)robust  $R^2$ , the models explained about 35 % of the variation of calculated SOC stock in 0–30 cm and 40–48 % of stocks in 0–100 cm. The kriging variances overestimated the prediction errors somewhat: only 3.4 % of the validation observations (both models) were outside of 95%-prediction intervals (Fig. S5 in Supplement). Overestimation of prediction uncertainty was also indicated by convex-shaped PIT histograms (Fig. S6 in Supplement), which had more probability mass in the centre than in the tails.

### 3.4 Prediction of SOC stocks for Swiss forest soils

For computing the predictions, the parameters of the final models (Table 1) were estimated with data of 1022 sites (combined calibration and validation sets, excluding 11 sites with missing covariate information). Robust lognormal kriging predictions of stocks stored to 100 cm depth are mapped in Fig. 5 for the nodes of the 100 m grid. The map with the predicted topsoil SOC was very similar and is therefore not shown. Block kriging predictions of the mean stocks for the five ecoregions and for the entire Swiss forest area are shown in Fig. 6.

Largest SOC stocks were predicted for higher altitudes and for the Southern Alps in general. Predicted stocks were smallest for the Central Plateau and for lower altitudes of the Pre-Alps, where stocks down to a depth of 100 cm remained below  $10 \text{ kg m}^{-2}$ . For whole Switzerland, predicted mean SOC stocks in 0–30 cm were equal

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to  $7.99 \text{ kg m}^{-2}$  (SE  $0.15 \text{ kg m}^{-2}$ , 95 %-prediction interval [7.69, 8.29]  $\text{kg m}^{-2}$ ). Down to 100 cm a SOC stock of  $12.58 \text{ kg m}^{-2}$  SOC was predicted (SE  $0.24 \text{ kg m}^{-2}$ ) resulting in a 95 %-prediction interval of [12.11,13.05]  $\text{kg m}^{-2}$ . Thus, about  $4.5 \text{ kg m}^{-2}$  SOC are stored in subsoils (30–100 cm) of Swiss forests.

Our estimates do not include carbon stored in forest floor horizons. Spatially explicit estimation was not possible for this compartment because we largely lacked C and soil density measurements. Based on the available data, Nussbaum et al. (2012) estimated that about  $1.7 \text{ kg m}^{-2}$  (SE  $0.08 \text{ kg m}^{-2}$ ) of C are stored in forest floors of Swiss forests.

## 4 Discussion

### 4.1 Model building and covariate selection

The model building procedure effectively reduced the 360 potential covariates and their first-order interactions to a small and meaningful set. Precipitation was a covariate of both models (with positive coefficients, Figs. S2 and S3 in Supplement). Perruchoud et al. (2000); Martin et al. (2011); Meersmans et al. (2012b); Kumar et al. (2012); Chiti et al. (2012) and Wiesmeier et al. (2013) previously reported that wet climate favours SOC accumulation. Near-infrared reflectance of the forest canopy was also selected for both models: smaller reflectance of conifers for wavelength of 750 to 1300 nm (Cipar et al., 2004) and negative regression coefficients imply larger SOC stocks under conifers than deciduous trees. Additionally, information on parent material was important for SOC prediction: aggregated units of the overview soil map were meaningful covariates despite representing the heterogeneous pedogenetic conditions typical for Switzerland only coarsely (see Figs. S2 and S3 in Supplement).

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## 4.2 Residual spatial autocorrelation

Spatial autocorrelation of residuals remained weak in both models, suggesting that spatial patterns in calculated SOC stocks were reasonably well modelled by the external drifts. Due to short-ranged spatial dependence, only 5% of the nodes of the prediction grid were within a distance equal to the effective variogram ranges of the soil profile sites. Although kriging predictions differ only within these zones from predictions obtained by the regression models, consideration of autocorrelation was important for accurate modelling of prediction uncertainty.

## 4.3 Robust parameter estimation

Moderate robustification of the parameter estimation procedure (tuning constant  $c = 2$ ) increased the predictive power of the fitted models in cross-validation slightly compared to customary REML and kriging. A further advantage of robust estimation is clear labelling of data that are fitted only poorly by the models. Scrutinizing environmental conditions for those observations revealed that these were: (i) sites on calcareous bedrock in inner Alpine valleys where recurring drought hinders OC mineralization, resulting in thick forest floor and SOC rich A horizons (Walthert et al., 2004), and (ii) sites in the Southern Alps with acid podsollic soils that show pronounced humus translocation down the profile. Moreover, these sites are influenced by forest fires (leading to accumulation of black carbon) and stabilize SOC effectively by large content of aluminium and iron weathered from silicate rich bedrock (Blaser et al., 1997). Using robust procedures ensured that SOC data resulting from sites subject to such special conditions did not confound statistical analyses.

## 4.4 Predictive performance of fitted models

Random dispersion of the prediction errors remained large as our robRMSEs of 39% and 42% demonstrated. This was also reflected in rather modest  $R^2$  of 0.35 and 0.48

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(Table 2). Further validation data from Swiss soil monitoring networks were predicted with somewhat larger errors (Nussbaum et al., 2012, Table 4). Other studies found (cross-)validation  $R^2$  (all non-robust) of similar magnitude: Martin et al. (2011) obtained by cross-validation  $R^2 = 0.36$  for predicting topsoil SOC stocks of forests in France. Mishra et al. (2009) found  $R^2 = 0.46$  for stocks in 0–50 cm and  $R^2 = 0.56$  for 0–100 cm, and Kumar et al. (2012) reported  $R^2 = 0.36$  for stocks down to 100 cm depth. The latter two studies validated with independent data predictions of OC stocks in soils under various land-uses in the US states Indiana and Pennsylvania.

On the one hand, incompleteness and partly insufficient quality of covariates is likely responsible for the modest predictive power of the fitted models. In particular, spatial information on soil or vegetation parameters controlling SOC turnover was completely lacking in our set of potential covariates. Also, data on forest management and land use history (e.g. stand age), found to be relevant by Schroeder et al. (2009) and Schulp et al. (2013), was missing.

On the other hand, causes for the moderate precision of our predictions lie in the missing soil density measurements (Schrumpf et al., 2011). For most horizons soil density was derived from a PTF, which proved to be unbiased, but nevertheless added additional variation to the data.

### 4.5 Spatial structure of SOC stock predictions

So far, no maps of SOC stocks have been published for Swiss forests that could be used for verification of Fig. 5. Nevertheless, several patterns in our SOC stock map matched our expectations: small SOC stock was predicted for acid soils at lower altitude on the Central Plateau. Very small total SOC stock was estimated for areas in the Eastern Pre-Alps and Alps where Permian Verrucano sand stones form the bedrock. On these sites, SOC accumulates in the forest floor. The map shows large stocks up to  $40 \text{ kg m}^{-2}$  in parts of the Eastern Pre-Alps where large annual precipitation and water-logged soils prevail, and also in the Jura region, where large stocks are likely related to organic matter stabilisation by calcium (Walthert et al., 2004). Very large SOC stock

was predicted for the Southern Alps, where a combination of forest fires and Al-rich soil on metamorphic parent material led to an accumulation of organic matter, even in deeper soil horizons. Excepting the special conditions in the Southern Alps, predictions of the mean stocks by ecoregions and altitudinal class (Fig. 6) reflected the increase of SOC stock with altitude described by Hagedorn et al. (2010).

#### 4.6 Comparison with SOC stock estimates of previous studies

Perruchoud et al. (2000) estimated for whole Switzerland a mean SOC stock of  $7.59 \text{ kg m}^{-2}$  (SE  $0.30 \text{ kg m}^{-2}$ ) for the top 30 cm of the mineral soil and  $9.82 \text{ kg m}^{-2}$  (SE  $0.53 \text{ kg m}^{-2}$ ) for mineral soils down to bedrock, which are both significantly smaller than our current estimates ( $p$  values of one-sided  $z$  tests: 0.004 and  $< 10^{-12}$ , respectively). The estimate of  $11.86 \text{ kg m}^{-2}$  (SE  $0.54 \text{ kg m}^{-2}$ ) by Bolliger et al. (2008) for total SOC stock (forest floor plus mineral soil down to bedrock) of Swiss forests is also smaller than our estimate for 0–100 cm. Our standard errors (0–30 cm:  $0.15 \text{ kg m}^{-2}$ ; 0–100 cm:  $0.24 \text{ kg m}^{-2}$ ) are smaller (by a factor of about two) than those of Perruchoud et al. (2000) and Bolliger et al. (2008). Since we validated uncertainty modelling for point predictions and used a coherent framework to quantify the uncertainty of our regional and national mean estimates, one can trust that these figures accurately represent the uncertainty of our estimates.

Perruchoud et al. (2000) estimated that about 77 % of SOC stock of Swiss forests is stored in the mineral topsoil (0–30 cm), whereas we predicted a proportion of only 64 %, which matches the proportion of 64.3 %, computed directly from the observed SOC data ( $n = 1033$ ) very well.

### 5 Summary and conclusion

Greenhouse gas reporting requires estimates of regional or national mean SOC stocks that are computed from observations with quasi-point support. The geostatistical block

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kriging approach is method of choice for such change-of-support problems as it guarantees that estimates are unbiased and precise and prediction standard errors correctly account for the spatial averaging. Rather surprisingly, our study seems to be the first to employ such an approach in the context of GHG reporting.

5 Based on spatially referenced data about 1 033 soil profiles, we built parsimonious, pedologically interpretable, geostatistical models for SOC stocks in two depth compartments (0–30 cm, 0–100 cm) of mineral soils of Swiss forests. The models relate calculated stocks to environmental covariates that characterize the pedogenetic conditions at the profile sites and account for residual spatial auto-correlation. The fitted models  
10 were rigorously validated by comparing predictions with independent data. Using the models, we mapped forest SOC stock across Switzerland by robust external-drift kriging at high spatial resolution and aggregated the kriging results coherently to come-up with reliable block kriging estimates (and standard errors) of national mean SOC stocks in Swiss forests.

15 A comparison with earlier studies on SOC in Swiss forest revealed that previous estimates of SOC stock down to 1 m depth were distinctly smaller than our estimate. Moreover, our (independently validated) standard errors were only half as large as the previously reported SE. As we used a substantially larger database and sound geostatistical methods we trust our estimate more and conclude that SOC stocks of  
20 Swiss forests have been considerably underestimated in the past.

**Supplementary material related to this article is available online at**  
**[http://www.geosci-model-dev-discuss.net/6/7077/2013/  
gmdd-6-7077-2013-supplement.pdf](http://www.geosci-model-dev-discuss.net/6/7077/2013/gmdd-6-7077-2013-supplement.pdf)**

25 *Acknowledgements.* We thank the Swiss Federal Office for the Environment (FOEN) for funding this work. A special thank goes to the WSL for collecting and analysing innumerable soil samples and to the WSL GIS group for providing the infrastructure for spatial data processing.

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**Table 1.** Covariates of external drift selected by model building procedure for soil organic carbon (SOC) stocks in 0–30 cm and 0–100 cm depth.

	SOC stock 0–30 cm	SOC stock 0–100 cm
soil	categorical covariate with 5 aggregated soil map units	categorical covariate with 9 aggregated soil map units
	mass of soil particles < 2 mm assigned to geotechnical map units	
climate	mean annual precipitation (square root)	mean March precipitation (square root)
vegetation	near-infrared band (SPOT5 mosaic)	near-infrared band (SPOT5 mosaic)
topography	topographic position index with radius 500 m (Jeness, 2006) for soil map units rich and poor in clay	slope (resolution 2 m)

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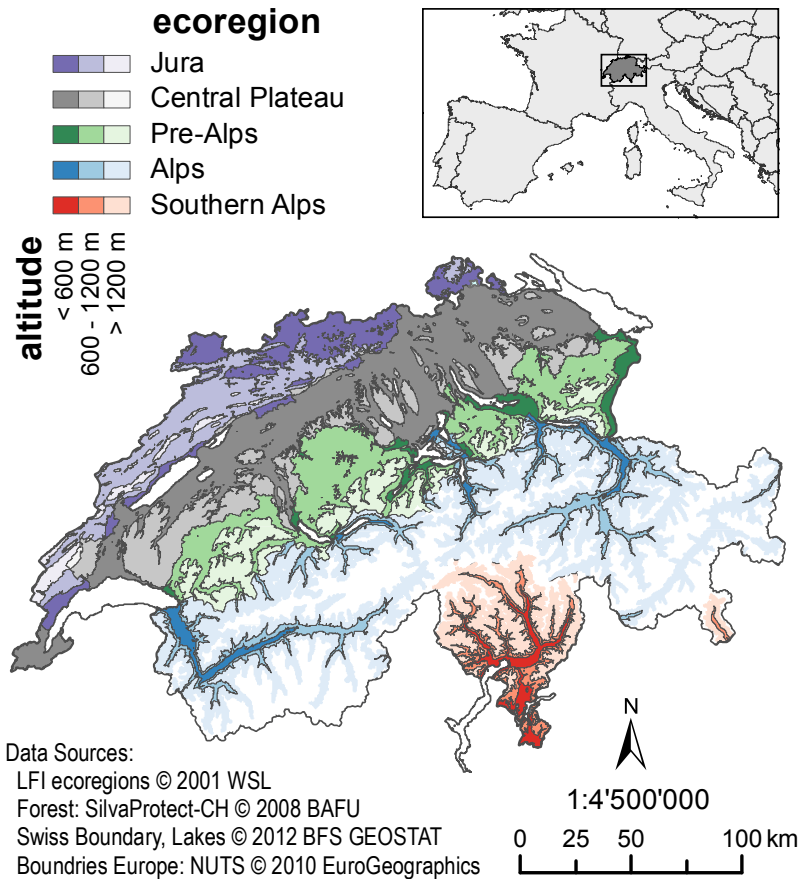
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**Table 2.** Statistics of relative soil organic carbon (SOC) stock prediction errors computed for the validation set in two depth compartments 0–30 cm and 0–100 cm.

	BIAS	RMSE	$R^2$	robBIAS	robRMSE	rob $R^2$	CRPS
0–30 cm	0.135	0.488	0.346	0.070	0.388	0.337	0.221
0–100 cm	0.152	0.556	0.477	0.066	0.420	0.403	0.247



**Fig. 1.** Ecoregions of Switzerland, stratified by altitudinal class.

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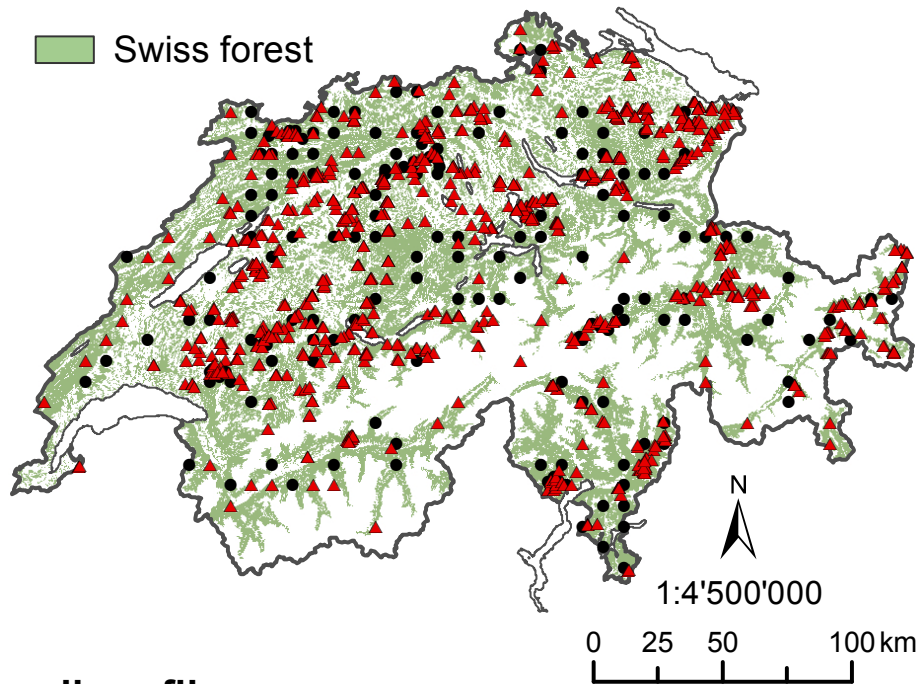
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## soil profiles

- ▲ calibration set (858 sites)
- validation set (175 sites)

Data Sources:  
 Soil profile points © 2011 WSL  
 Forest: SilvaProtect-CH © 2008 BAFU  
 Boundary, Lakes © 2012 BFS GEOSTAT

**Fig. 2.** Locations of the 1 033 soil profiles and Swiss forest area (subdivided into calibration and validation sets).

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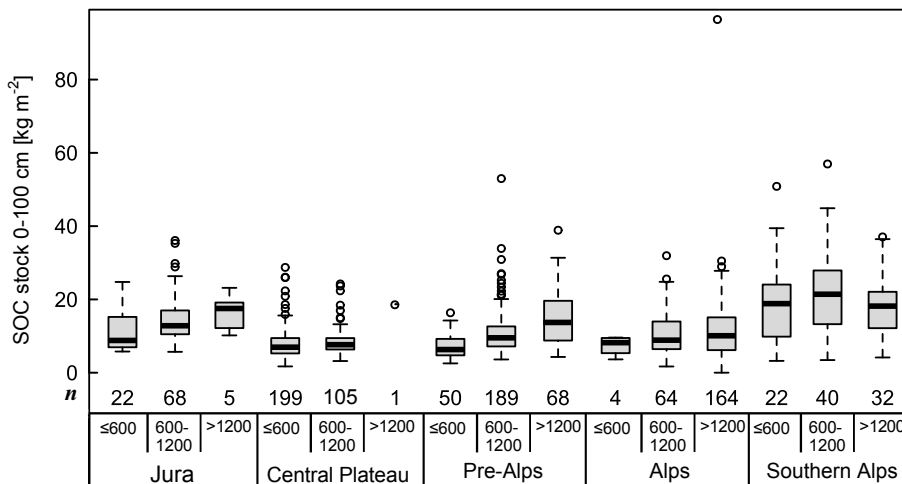
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**Fig. 3.** Boxplots of soil organic carbon (SOC) stocks in 0–100 cm depth by ecoregion and altitudinal class (*n*: number of sites).

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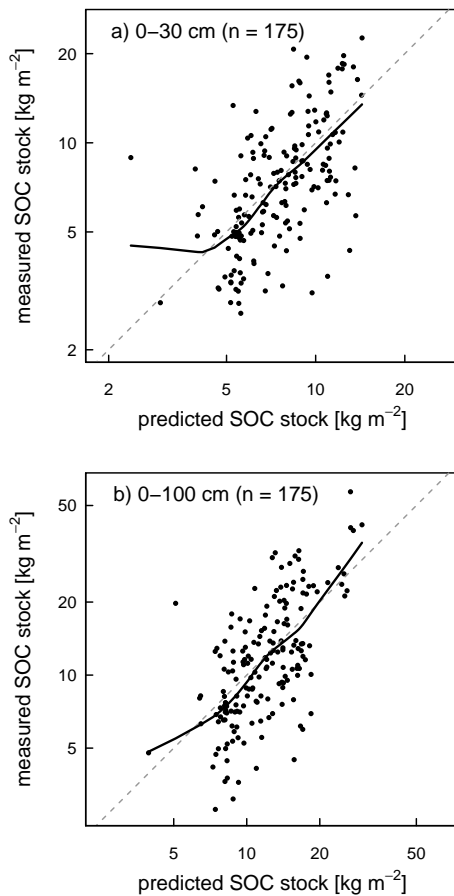
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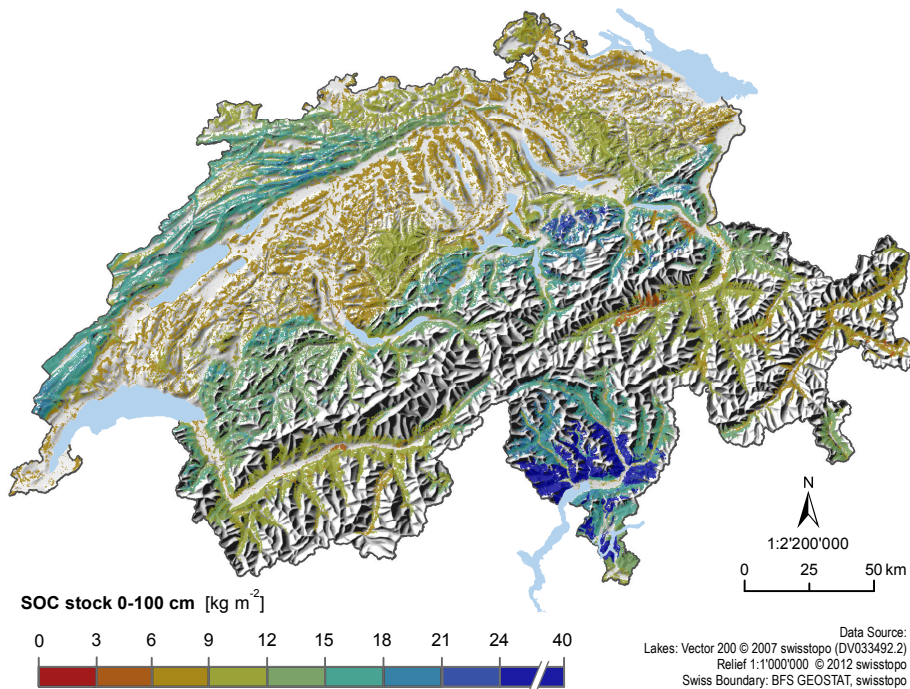
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**Fig. 4.** Scatter plots of measured against predicted soil organic carbon (SOC) stocks in 0–30 cm **(a)** and 0–100 cm **(b)** of the mineral soil, computed with the calibration data for the sites of the validation set (solid line: loess scatter plot smoothers,  $n$ : number of sites).



**Fig. 5.** Robust lognormal kriging prediction of the soil organic carbon (SOC) stock in 0–100 cm of the mineral soil of Swiss forests (computed with best-fit model with covariates according to Table 1 and tuning constant  $c = 2$ , smoothed with focal mean with a radius of 1 pixel = 100 m).

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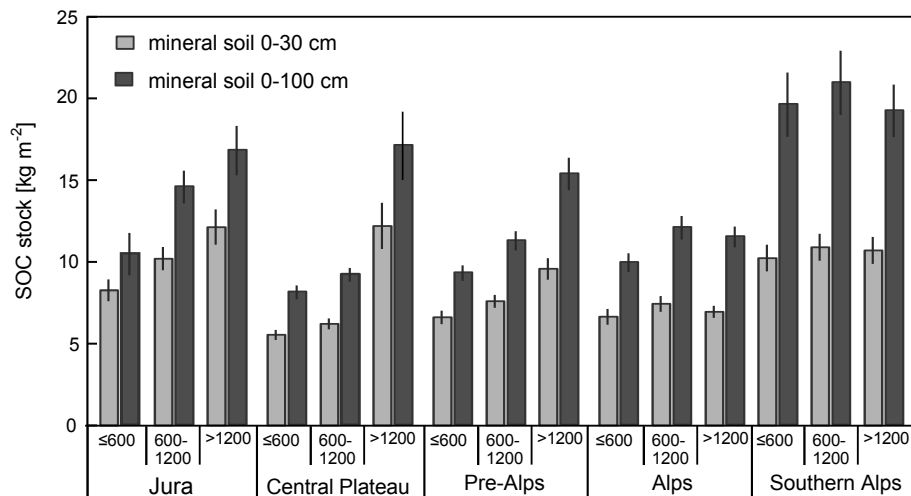
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**Fig. 6.** Block kriging predictions of the soil organic carbon (SOC) stocks in 0–30 cm and 0–100 cm soil depth in the five ecoregions stratified by altitude asl [m] into three classes (vertical lines: prediction intervals).

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