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Research Article

Deriving regional pedotransfer functions to estimate soil bulk density in Austria

Ableitung regionaler Pedotransferfunktionen um Bodenlagerungsdichten in Österreich zu schätzen

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Summary

Soil bulk density is a required variable for quantifying stocks of elements in soils and is therefore instrumental for the evaluation of land-use related climate change mitigation measures. Our motivation was to derive a set of pedotransfer functions for soil bulk densities usable to accommodate different levels of data availabilities. We derived sets of linear equations for bulk density that are appropriate for different forms of land-use. After introducing uncertainty factors for measured parameters, we ran the linear models repeatedly in a Monte Carlo simulation in order to test the impact of inaccuracy. The reliability of the models was evaluated by a cross-validation. The single best predictor of soil bulk density is the content of soil organic carbon, yielding estimates with an adjusted R^2 of approximately 0.5. A slight improvement of the estimate is possible when additionally, soil texture and soil depth are known. Residual analysis advocated the derivation of land-use specific models. Using transformed variables and assessing land-use specific pedotransfer functions, the determination coefficient (adjusted R^2) of the multiple linear models ranged from 0.43 in cropland up to 0.65 for grassland soils. Compared to pedotransfer function, from the literature, the performance of the linear modes were similar but more accurate. Taking into account the likely inaccuracies when measuring soil organic carbon, the soil bulk density can be estimated with an accuracy of +/- 9 to 25% depending on land-use. We recommend measuring soil bulk density by standardized sampling of undisturbed soil cores, followed by post-processing of the samples in the lab by internationally harmonized protocols. Our pedotransfer functions are accurately and transparently presented, and derived from well-documented and high-quality soil data sets. We therefore consider them particularly useful in Austria, where the measured values for soil bulk densities are not available.

Keywords: Land-use, regional calibration, multiple regression, Monte Carlo, cross validation

Zusammenfassung

Die Bodenlagerungsdichte ist eine notwendige Variable bei der Berechnung von dem im Boden gespeicherten Bodenkohlenstoff und ist deshalb auch ein wichtiges Instrument bei der Evaluierung von landnutzungsbasierten Minderungsmaßnahmen gegen den Klimawandel. Unsere Motivation war, ein Set von Pedotransferfunktionen für die Bodenlagerungsdichte zu entwickeln, die für unterschiedlichen Datensätze nutzbar sein könnten. Wir entwickelten ein Set linearer Funktionen für landnutzungsabhängige Bodenlagerungsdichten basierend auf Daten aus Österreich, der Schweiz und Südtirol in Italien. Nach dem Einfügen von Unsicherheitsfaktoren für gemessene Bodenparameter wurde die Ungenauigkeit der Gleichungen mittels einer Monte Carlo Simulation ermittelt. Die Glaubwürdigkeit der Modelle wurde anhand von Kreuzvalidierung bestimmt. Der Gehalt von organischem Bodenkohlenstoff ist mit R^2 = 0.5 die Bestimmungsvariable, die am besten die Bodenlagerungsdichte voraussagt. Wenn Bodentextur und Aufnahmetiefe bekannt sind, ist eine geringe Verbesserung des Bestimmtheitsmaßes möglich. Die Residuen-Analyse empfiehlt landnutzungsspezifische Modelle. Mit transformierten Variablen reicht das Bestimmtheitsmaß (R^2) der landnutzungsspezifischen Pedotransferfunktionen von 0.43 in Ackerböden bis zum 0.65 für Grünlandböden. Die Ergebnisse sind ähnlich aber mehr präzise im Vergleich mit Modellen aus der Literatur. Unter Berücksichtigung der Unsicherheit von gemessenen Bodenkohlestoffwerten, kann die Bodenlagerungsdichte abhängig von der Landnutzung mit einer Genauigkeit von +/- 9% bis 25% geschätzt werden. Wir schlagen vor, dass die Bodenlagerungsdichte an standardisierter volumsgerechter Proben, die mittels Stechzylindern geworben wurden und im Labor nach internationalem Standard gemessen wird. Wenn gemessene Werte für Bodenlagerungsdicht nicht vorhanden sind, bieten diese Pedotransferfunktionen eine Alternative besonders, weil sie einerseits den Geltungsbereich und anderseits die Schwankungsbreiten und Unsicherheiten transparent angeben.

Schlagwörter: Landnutzung; regionale Kalibrierung, Multiple Regression; Monte Carlo; Kreuzvalidierung

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1. Introduction

When assessing the carbon pool in terrestrial ecosystems, soils play a dominant role. The seminal papers of Dixon et al. (1994), Batjes (1996) and Pan et al. (2011) provide widely cited estimates of the soil carbon pool in different types of ecosystems. The soil carbon pool is estimated from the content of organic carbon (mg OC g^{-1}) and the soil mass. The content of soil carbon is measured with high accuracy in the lab and the volume of the fine soil is calculated by reducing the total soil volume (1 m × 1 m × depth of a soil horizon) by the volume of coarse material (Cools and De Vos, 2016). The carbon-by-mass is finally converted to carbon-by-volume (stock) by multiplication with soil bulk density (g cm^{-3}). An efficient and commonly used method of soil sampling is to open a soil pit and collect material from the individual horizons. Methods for the precise measurement of coarse material and soil bulk density are available (Walter et al., 2016). However, despite the importance of soil bulk densities for the calculation of nutrient or carbon stocks, this parameter is often let out of soil surveys, mostly because it is laborious and time-consuming (Kätterer et al., 2006; Sequeira et al., 2014).

In the database BORIS (https://www.umweltbundesamt.at/boris), we have a huge collection of regional and local soil data from previous soil surveys. BORIS is the most comprehensive and quality controlled collection of physical and chemical soil properties including site and land-use information in Austria. Even so, few measured soil bulk densities have been recorded. In order to estimate changes in soil organic pools over time, we need to use this limited historical data there is, and estimate soil bulk density where such measured values are missing.

Pedotransfer functions for the estimation of soil bulk density have been developed for several land-use categories and geographical zones. Several pedotransfer functions use the content of organic carbon as a single predictor (Adams, 1973; Leifeld et al., 2005; Manrique and Jones, 1991; Rawls, 1983; Saini, 1966; Schrumpf et al., 2011). More complex models also include soil type, soil depth, soil texture, and land-use (Callesen et al., 2003; Chen et al., 2018; De Vos et al., 2005; Hollis et al., 2012; Keller and Håkansson, 2010; Manrique and Jones, 1991; Nussbaum et al., 2016; Ruehlmann and Körschens, 2009; Wiesmeier et al., 2012).

The published equations illustrate two general patterns, both correlating with the content of soil organic carbon and management, regularly managed cropland soils have a higher bulk density than forest and grassland soils because of more frequent management measures with heavy machinery (Schrumpf et al., 2011), and topsoils have a lower bulk density than deeper soil horizons, because the load of heavy machinery compact subsoils more intensively. Whereby there is an exception for intensive grassed pastures where trampling has a higher impact on the upper layers (Bohner et al., 2017). However, the published equations for the estimation of soil bulk density are not generally applicable and can be recommended only for regions that are represented by the dataset (De Vos et al., 2005). In particular, pastures and meadows in mountainous regions may have soil characteristics that are different from grasslands in lowlands due to the influence of climate on soil development and plant growth, and also because of less intensive land management.

Nanko et al. (2014) categorize the approach of established pedotransfer functions as either physical or empirical. One of the most cited empirical models is one based on a huge database all across the United States including Hawaii and Puerto Rico from Manrique and Jones (1991) and has been implemented for various regions (De Vos et al., 2005; Hollis et al., 2012). Weiss et al. (2000) applied in the first Austrian inventory of forests a well validated model of Rawls et al. (1983) adopted by Moore (1998). This is a physical model, which predicts the soil bulk density by the content of soil organic matter (SOM) and the weight of mineral fraction (Nanko et al., 2014). But more often, default values depending on soil texture have been applied for the estimation of missing soil bulk densities (Haslmayr et al., 2018). Unfortunately, the goodness and the uncertainties of these approaches, as applied in Austria, have not been validated or published.

Our motivation was the compilation and evaluation of a dataset that allows the estimation of soil bulk density in Austrian mountainous soils. Whereas data on forest and cropland soils are abundant, we encountered a scarcity of data for mountain grasslands, and therefore, acquired additional data from Switzerland and Southern Tyrol in Italy. We tested two often used pedotransfer functions with different approaches on our dataset and derived in step-by-step analysis a set of regional pedotransfer functions for the estimation of soil bulk density of mountainous soils. The data analysis assumed different levels of data availability and included a span of uncertainties of measured parameter. The intention was to provide functions of different complexity including a range of uncertainty suiting the needs of the respective users.

2. Methods

2.1. Soil data

Data for cropland and forest soils were available from the BORIS database. Soil data for grassland soils in the BORIS data insufficiently represented mountain grassland. In order to better represent mountain grassland soils, we acquired additional data from Switzerland and Southern Tyrol in Italy. We included data where soil depth was recorded and which contained measured value for soil bulk density, of the concentration of soil organic carbon, and soil texture (sand, silt, clay). If necessary, we used the factor 1.724 to convert the content of measured soil organic matter to soil organic carbon. Content of soil organic carbon and soil bulk densities are not significantly different between the datasets. As shown in Table 1, the studied dataset held information from 1,732 samples, of which, 567 are from cropland, 348 from forest and 817 from grassland soils. All the data were sampled from sites above 400 m asl and cover soil types and parent material as heterogeneous as the Alpine landscape itself. The dominant soils are Cambisols, Fluvisols and Chernozems and to a lesser extent Leptosols, Gleysols, Regosols, Podzols and Stagnosols according to the WRB systematic (http://www.fao.org/3/i3794en/I3794en.pdf).

2.2. Analysis and calculations

2.2.1. Dataset and pedotransfer functions from literature

The statistically significant differences between land-use categories in the compiled dataset were calculated with an ANOVA and a post Student-Newman-Keuls test for all the soil parameters. Outliers were not removed because they had no statistical influence on the calculated models.

We tested for the different datasets ("all data"; "cropland"; "forest"; "grassland") the empirical pedotransfer function of Manrique and Jones, (1991) developed on a huge dataset

$$BD = 1.66 - 318 * \%\,SOC^{0.5}$$

as well as a technical equation already used in Austria by Weiss et al. (2000) based on Rawl et al. (1983) and adopted from Moore, (1998) as followed

$$BD = \frac{100}{\left\{\left(\frac{\%\,SOM}{0.244}\right) + \left[\frac{(100 - \%\,SOM)}{1.4}\right]\right\}}$$

whereby SOM was derived from % soil organic carbon by a factor of 1.724.

2.2.2. Building models

General linear models were calculated to derive functions for soil bulk density with different sets of independent variables for the whole dataset and for the datasets of each land-use category. Independent variables were the content of organic carbon, location of the soil sample in the soil profile ("that is to say, its depth") and soil texture (sand, silt, clay). We derived functions of different complexity and used transformed data if necessary. In the simplest model, the only independent variable was soil organic carbon. More complex models included soil texture and soil depth. For the multiple regression, a stepwise variable selection algorithm was used, employing the AIC to determine which parameter significantly improved the model.

Table 1. List of datasets from Austria (AT), Switzerland (CH) and Italy (IT) naming sources, number of samples, land-use and mean, lowest (min) and highest (max) elevation of the sites sampled

Tabelle 1. listet die Datensammlungen aus Österreich (AT), Schweiz (CH) und Italien (IT) mit Quellen, Anzahl Bodenprobe, Landnutzung und mittlere (mean), minimale (min) und maximimale (max) Höhenlage der Probenstellen.

Country	Made available by	number of samples	Land-use	elevation (m asl)			
				mean	min		max
AT	our own dataset	15	Grassland	909	672	-	1554
AT	Upper Austria (BORIS)	567	cropland	540	400	-	1140
AT	Upper Austria (BORIS)	656	Grassland	1047	410	-	2460
AT	BAW (internal dataset)	348	Forest	1024	400	-	2050
AT	A. Bohner (other studies)	18	Grassland	663	420	-	1830
CH	J. Leifeld	116	Grassland	760	430	-	1220
IT	EURAC	12	Grassland	1607	986	-	2043

BORIS = official soil data base (https://www.umweltbundesamt.at/boris); BAW = Bundesanstalt für Wasserwirtschaft, Petzenkirchen; EURAC = Institute of Alpine Environment, Bolzano

In order to justify the derivation of individual general linear models for each type of land-use, we performed an ANOVA of the model residuals complemented by the post hoc Duncan- and Scheffe-tests.

2.2.3 Evaluation and validation

The quality of the obtained linear models as well as the use of the two pedotransfer functions from the literature was judged by the adjusted R^2 and the accuracy of the predicted soil bulk densities by the root mean squared errors (RMSE). Additionally, we tested in a Monte Carlo simulation the impacts of uncertainties from the measured parameters on the prediction of the estimated soil bulk density.

Based on expert judgement, we defined that depth is having an error term of zero and the measured value of the soil organic carbon and texture all have an error term of 10% respectively (Gottschalk et al., 2007). Accordingly, the measured parameters "soil organic carbon", "sand", "silt" and "clay" were modified in a Monte Carlo analysis by including a normally distributed error. This was done by multiplying the original value with a random value from an N (1, 0.1) distribution. This means that the mean is 1 (which means no change) and the standard deviation is 10% of the original value. Each parameter was modified in this way and the estimation of soil bulk density was run n = 5,000 times. The mean percentage of uncertainty (PU) of the estimated soil bulk density was quantified as the mean of the 5,000 resulting standard deviations of the relative residuals:

$$PU = \frac{1}{n}\sum_{i=1}^{n} SD(diff_i)$$

with SD being the standard deviation and diffi being the vector of the k relative differences between the modelled and measured values in the ith iteration of the Monte Carlo simulation:

$$diff = \left(\frac{BDmo_1 - BDme_1}{BDme_1}, \cdots, \frac{BDmo_k - BDme_k}{BDme_k}\right)$$

with BDmo and BDme being the modelled and the measured bulk density, respectively.

Best fit equations have a higher R^2, and lower RMSE and PU. Medians of diff were used for each separate data set ("all data"; "cropland"; "forest"; "grassland") to determine any over- or underestimation of the predicted soil bulk densities.

In order to test the models for overfitting, a cross-validation was carried out. Hereby all datasets from all sites ("all data", "cropland", "forest" and "grassland") were randomly split into four disjoint parts. Each of these parts was alternately once used as validation dataset with measured soil bulk densities, while the other three were used as training data set estimating bulk densities by the best fit models. The cross-validation was repeated 1,000 times for all the land-use categories, and finally, the R^2 of cross-validation was compared between the different loops and to the R^2 of the model. All the computing was done with R-Studio (version R-3.4.4).

3. Results

3.1. Dataset

In Table 2, the descriptive statistics of the whole data sets and divided into the different land-use categories are shown. Except for clay content, the means of all the soil parameters differed significantly between the three land-use categories ($p < 0.05$). Soil organic content in the dataset ranged from 1–295 mg g^{-1} in the order grassland > forest > cropland. Figure 1 A shows a wide scatter of measured soil bulk densities for different forms of land-use. Cropland soils are clustered at higher densities, forest soils have generally lower values, and grassland soils are widely variable, presumably depending on type (pasture or meadow) and intensity of grassland management.

3.2. Linear models

The single best predictor of soil bulk density of the whole dataset (n = 1732) is the content of soil organic carbon with an adjusted R^2 of 0.50 ($p < 0.001$). Including horizon depth and soil texture as additional independent variables increases R^2 only marginally to 0.52 ($p < 0.001$). The relation between soil organic carbon and bulk density, as shown in Figure 1 A), is curvilinear. In order to justify the use of linear models for the prediction of bulk density, we transformed soil carbon to the square root of soil carbon ($SOC^{0.5}$; Figure 1 B). The adjusted R^2 of $SOC^{0.5}$ to bulk density increased to 0.55 ($p < 0.001$).

Figure 2 A) presents the standardized residuals versus fitted values for all data. The three land-use categories are clustered. Values for cropland (stars) are in the upper right part of the graph, forest (triangle) in the right lower part of

Table 2. Mean, minimum (min) and maximum (max) values of soil depth, organic carbon (SOC), sand, silt, clay and bulk density according to the datasets: all data, cropland, forest and grassland (n = number of samples)
Tabelle 2. Mittlere (mean), minimale (min) und maximale (max) Werte der Bodenprobeentnahme, organischem Bodenkohlenstoff (SOC), Sand-, Schuff-, Tongehalten und der Bodenlagerungsdichten (BD) von ‚allen Daten', Ackerböden, Wald- und Grünlandböden (n = Anzahl Proben)

parameter	all data (n = 1732)				cropland (n = 567)				forest (n = 348)				grassland (n = 817)			
	mean	min		max	mean	min		max	mean	min		Max	mean	min		max
Depth [cm]	20	1	-	70	26	10	-	50	27	8	-	60	12	1	-	70
SOC [mg g^{-1}]	39	1	-	295	19	4	-	120	32	10	-	185	55	1	-	295
Sand [mg g^{-1}]	280	0	-	910	217	0	-	721	35	21	-	717	289	18	-	910
Silt [mg g^{-1}]	538	2	-	934	587	172	-	934	446	172	-	703	544	20	-	882
Clay [mg g^{-1}]	184	1	-	701	197	35	-	467	207	36	-	701	167	10	-	560
BD [g cm^{-3}]	1.2	0.3	-	2.2	1.4	0.5	-	1.7	1	0.4	-	2.2	1.1	0.3	-	1.7

the graph, whereas grassland (squares) are widely distributed. Figure 2 B), C) and D) show the performance of the individual land-use categories. The AONVA analysis of the results for the individual land-use categories shows biased predictions for the single categories. Cropland and grassland biases are slightly positive at 0.08 and 0.03 respectively, and the bias of forest soils is -0.20. The Duncan and Scheffe tests both confirmed the differences between the three land-use categories (data not shown), and thereby, the appropriateness of own models for each land-use category.

3.3. Best fit models

The coefficients of the linear models for the estimation of soil bulk density are listed in Table 3. The best fit is achieved for grassland soils (R^2 = 0.65; RMSE 0.190), the

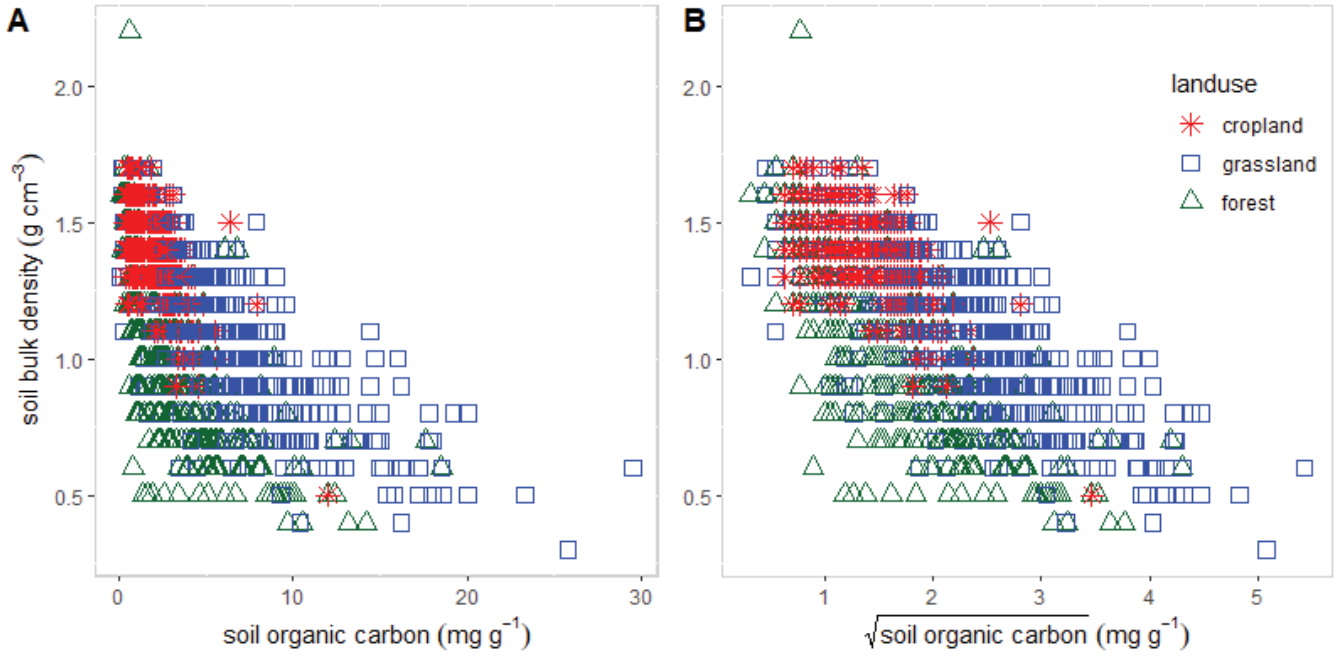

Figure 1. Measured soil bulk densities from cropland (star), forest (triangle) and grassland (squares) soils versus A) soil organic content and B) squared root of soil organic carbon
Abbildung 1. gemessene Bodenlagerungsdichten von Acker- (Sterne), Wald- (Triangel) und Grünlandböden (Quadrate) versus A) gemessenen organischen Bodenkohlenstoff und B) Wurzel des organischen Bodenkohlenstoffs

Table 3. Coefficients of the linear model equations (EQ) and the evaluation of the models by R squared (R^2), root mean squared error (RMSE) and percentage of uncertainty (PU) together with the validation by the mean squared R (mR^2) of the cross validation (CV)
Tabelle 3. Die Koeffizienten der linearen Gleichungen (EQ) und die Evaluierung der Modelle anhand des Bestimmtheitsmaß (R^2), Wurzel der Mittlere quadratische Abweichung (RMSE) und dem Prozent der Unsicherheit (PU) gemeinsam mit dem Ergebnis der Validierung durch mittleres Bestimmtheitsmaß (mR^2) aus der Kreuzvalidierung (CV)

EQ	landuse	Intercept	Depth [cm]	$SOC^{-0.5}$ $[mg\ g^{-1}]^{0.5}$	Silt [%]	Clay [%]	R^2	RMSE	PU [%]	CV mR^2
1	all data	1.650	-0.0022***	-0.3157***	0.0028*		0.58	0.190	21	0.57
2	cropland	1.873	-0.0021***	-0.3042***			0.43	0,105	9	0.41
3	forest	1.523		-0.3199***			0.58	0.205	25	0.56
4	grassland	1.698		-0.2737***	0.0009**	-0.0020**	0.65	0.171	17	0.65
5	all data	1.682		-0.2738***			0.55	0.197	24	
6	cropland	1.720		-0.2306***			0.41	0.107	9	
7	grassland	1.693		-0.2635***			0.65	0.157	18	

*; ** and *** means a significance where p < 0.05; 0.01 and 0.001 respectively

weakest fit for cropland soils (R^2 = 0.43; RMSE = 0.105). The most complex models, that is, with the highest number of predictors, give the best adjusted R^2 and RMSE, although the difference in R^2 to the simpler models is modest. The uncertainty of the model equations slightly increases when only the content of soil carbon as prediction variable is considered but the differences are minor.
If land-use is not specified (dataset "all data"), the parameters of soil depth and content of silt strengthen the estimates of soil bulk densities in EQ 1. The variable "depth" has a significant impact in cropland soils (EQ 2), but is not relevant for forest and grassland soils. In forest soils, only the content of soil carbon has a significant impact in the model (EQ 3) whereas the content of silt and clay increases the quality of estimates in grassland soils (EQ 4). In situations where only the content of soil carbon is known, the strength of the equations for all data (EQ 5), cropland (EQ 6) and grassland (EQ 7) decreases, although the reduction is marginal.

3.4. Evaluation and validation

Monte Carlo simulations showed that a 10% inaccuracy of the measured variables leads to PU of 21% of the estimated soil bulk density for all the data. In the stratified datasets, the PU of the estimated soil bulk densities using all the prediction variables was lower for cropland (9%) and grassland (17%) and higher for forest (25%) as compared to the whole dataset. With the content of soil organic carbon as the only prediction variable, the PU increases only slightly. The cross-validation showed only a minor variation of R^2 between the separate loops and thereby no overfitting was found. Overall, the mean R^2 of the cross validation was slightly lower compared to R^2 of the model equations (Table 3).
In Figure 3, the histograms show that the estimated soil bulk densities for A) the whole dataset and B) cropland are slightly underestimated with median predictor error of -0.020, and -0.005 respectively, whereas for C) forest and D) grassland, the calculated soil bulk densities are overestimated with median predictor error of 0.014 and 0.028.
The equations are not reliable for extrapolation. To avoid very low, or even negative estimated soil bulk density values, for instance, by using data with prediction variables outside the range of the calibration data sets, we introduced a minimum value with the "max" term in the equations above the minimum value of the predicted soil bulk densities was set to the lowest value occurring in the respective dataset described in Table 2. Figure 4 A–D) illustrate the performance of measured versus modelled soil bulk densities in the validation data set using the best fit equations from Table 3:

A) $BD_{all\ data} = \max(0.3, 1.650 - 0.0022 \cdot \text{cm soil layer depth} - 0.3157 \cdot SOC^{0.5} + 0.0028 \cdot \%silt)$
B) $BD_{cropland} = \max(0.5, 1.873 - 0.0021 \cdot \text{cm soil layer depth} - 0.304 \cdot SOC^{0.5})$
C) $BD_{forest} = \max(0.4, 1.523 - 0.3199 \cdot SOC^{0.5})$
D) $BD_{grassland} = \max(0.3, 1.698 - 2.2737 \cdot SOC^{0.5} + 0.0009 \cdot \%silt + 0.002 \cdot \%clay)$

The R^2 of the prediction ranges from R^2 = 0.43 in cropland to R^2 = 0.64 in grassland soils, the RMSE are between 0.105 in cropland and 0.205 in forest. In Figure 4, we

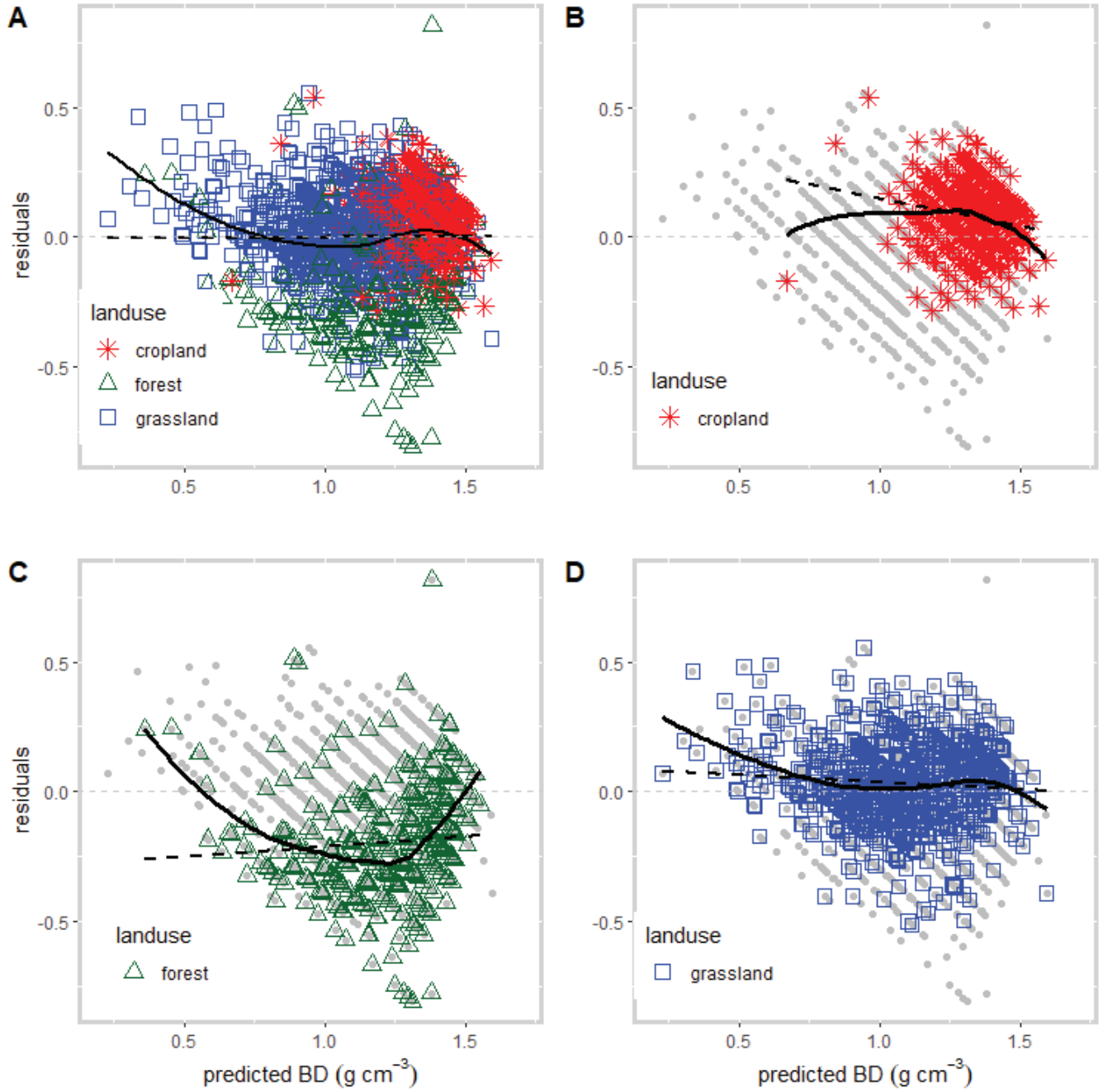

Figure 2. Residuals versus predicted soil bulk densities (BD) with regression line (dashed) and lowest smoothing line (solid) of A) all data, B) cropland, C) forest and D) grassland sites.
Abbildung 2. Die Residuen versus modellierten Bodenlagerungsdichten (BD) mit der lineare Regressionsline (gestrichelt) und LOWESS-Spline-Linie (durchgezogen) von A) ‚alle Daten', B) Ackerböden, C) Wald- und D) Grünlandböden.

see in B) C) D), that low measured soil bulk density values in all the land-use categories are rather overestimated, whereas high values are rather underestimated by the equation EQ 2, EQ 3 and EQ 4 respectively.

R^2 of the Manrique and Jones model and the model used by Weiss et al. (2000) are similar to the results of the regional pedotransfer functions (EQ 1–EQ4) derived in this study, though the accuracy is less good as RMSE for all the datasets are higher and ranges from 0.190–0.248. Results from "all data", "cropland" and "grassland" show that the Manrique and Jones model strongly underestimates the predicted soil bulk density, whereas the predicted values for "forest" are to a high degree overestimated. By the model used by Weiss et al. (2000; Figure 4; I–L), the results show

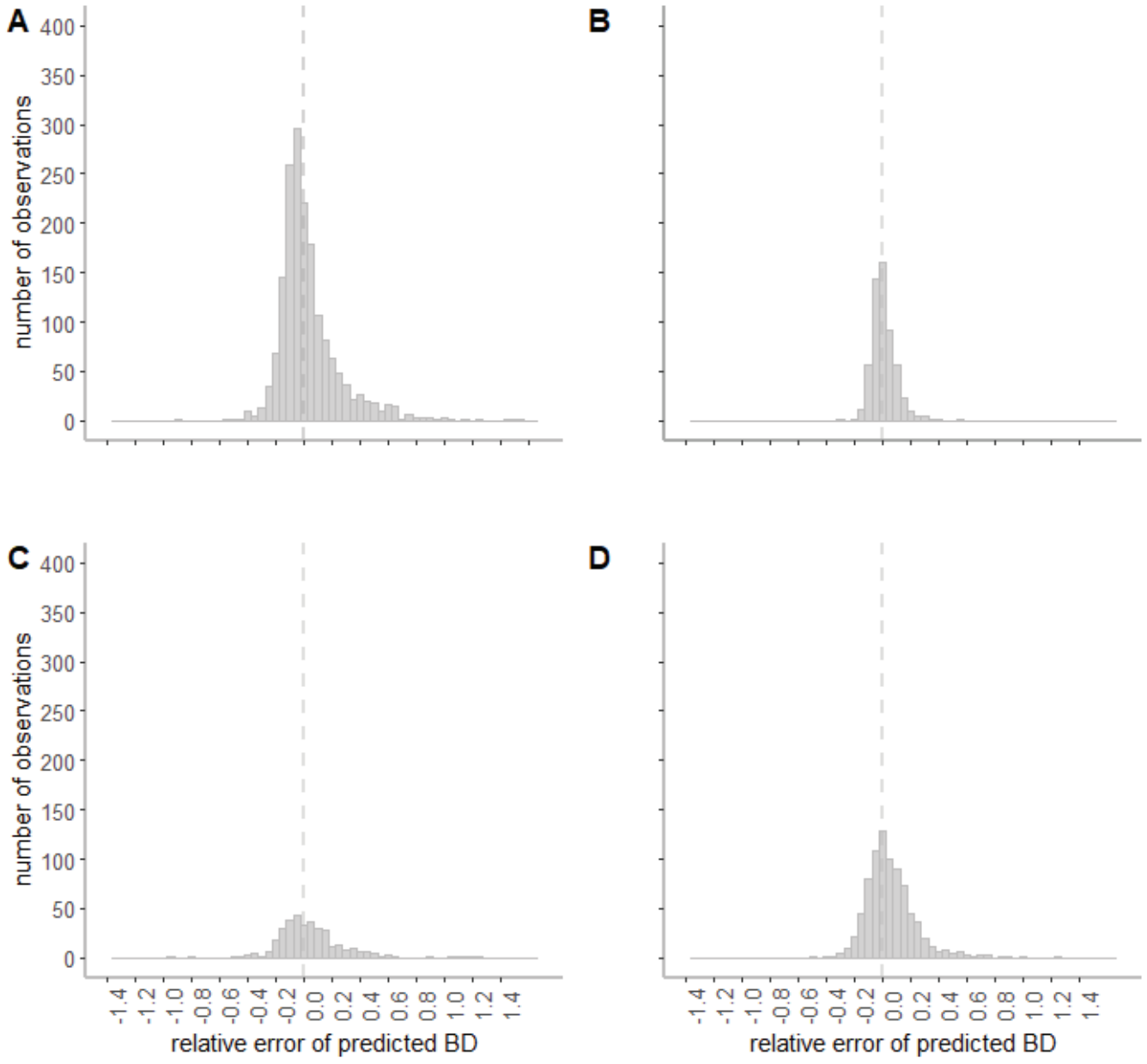

Figure 3. Histograms showing the bias (relative error) of predicted soil bulk density (BD) of A) all data, B) cropland C) forest and D) grassland respectively
Abbildung 3. Histogramm mit der Verzerrung (relative Fehler) der geschätzten Bodenlagerungsdichten (BD) bei A) ‚alle Daten', B) Ackerböden, C) Wald- und D) Grünlandböden

a similar trend, though the model is not able to predict higher soil bulk densities in either of the datasets.

4. Discussion

Estimations of the stock size of elements in soil horizons require the concentration of the respective element, the mass of fine earth, the depth of the respective horizon, and the soil bulk density. High quality data of the measured element concentrations are available from specialized labs. A considerable source of error is introduced by uncertain estimates of the rock content, as discussed in Poeplau et al. (2017). Here, we focus on soil bulk density.

The optimal solution is measuring soil bulk density from all the sampled soil horizons by the collection of undisturbed soil cores that are later processed in the laboratory. Due to operational constraints, this measurement is often omitted and consequently alternatives are sought. In Austria, like in the recent calculations for the Austrian Soil Carbon Map

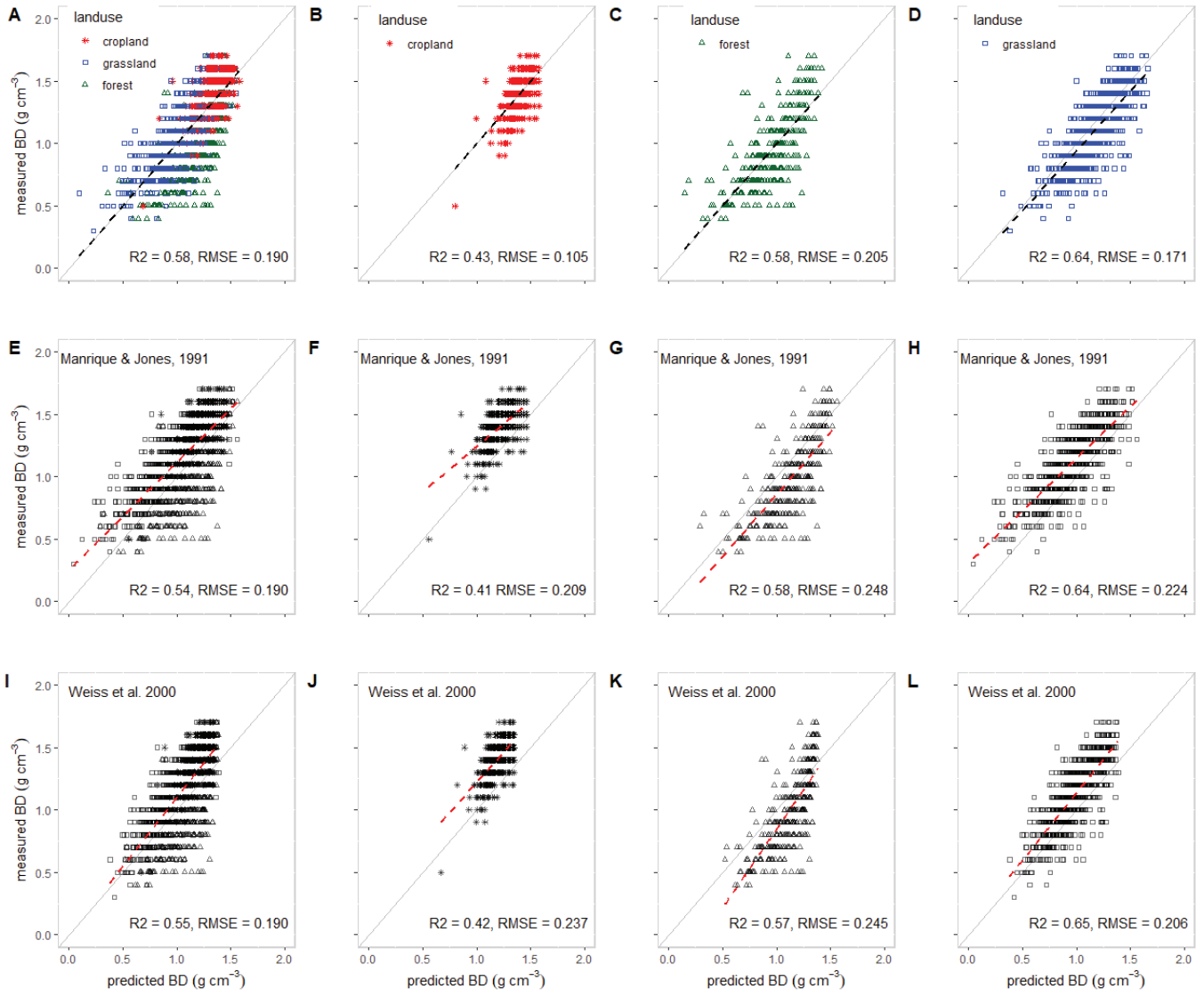

Figure 4. Performance of measured versus predicted soil bulk density (BD) including regression line (dashed) for "all data", "cropland", "forest" and "grassland" datasets applying A – D the best of regional equations from this study, E – H the model of Manrique and Jones (1991) and I – L the model used by Weiss et al (2000). R^2 and RMSE describe the goodness of the functions

Abbildung 4. Modellierte versus gemessene Bodenlagerungsdichten mit Regressionsline (gestrichelt) für alle Datensets (‚all data', ‚cropland', ‚forest' und ‚grassland') in A – D anhand der regional kalibrierten Gleichungen dieser Studie, E – H berechnet mit dem Modell von Manruiqe und Jones (1991) und I – L das Modell verwendet von Weiss et al. (2000). R^2 und RMSE geben die Güte der Gleichungen wieder.

(ASOC; Haslmayr et al., 2018), it is common to use default values for missing values of soil bulk densities. These default values are based on soil texture and are derived from different German surveys. They are elaborately described, for example, by Ad-hoc-Arbeitsgruppe Boden (2005). For the first carbon budget of Austrian forests, Weiss et al. (2000) applied an international published equation based on Rawls et al. (1983). For agricultural soils, a set of estimates for soil bulk density correlated with the soil organic content was used by Gerzabek et al. (2005). The nature of these calculations follows the approach of Körschens and Waldschmidt (1995) but are not further described.

As we see in Figure 4, there are minor differences in model performance between the different models, whereby the equations from this study, as well as the model from Manrique and Jones, are more flexible predicting soil bulk densities from a wider range of measured values. In addition, they are more precise (better RMSE) than the physical approach based on the model used by Weiss et al. (2000) as this model has limited prediction potential for higher soil

bulk densities. All the models overestimate the low measured soil bulk densities and underestimate the high measured values. Sequeira et al. (2014) explain this as a typical trend for datasets including a wide set of measured soil bulk densities, since the empirical as well as the physical model intend to minimize the systematic errors focusing on the mean of the prediction variable (here foremost SOC) in the datasets. This also explains the lower RMSE and PU from the cropland equations, as these samples have less variability in the measured soil bulk densities as well as in the predicting variables of soil organic carbon and soil depth.

We suggest to use regional datasets and multiple linear regression in order to derive and calibrate the pedotransfer equation. The dataset used in this study represents a wide range of management systems and site conditions in the eastern Alps above 400 m a.s.l. Using a regional dataset enabled us to reduce bias and strengthen the predictability of the pedotransfer function (De Vos et al., 2005). We see the performance of the predicted soil bulk densities in A–D (Figure 4) following this approach fit closer to the 1:1 relationship line. The presented pedotransfer equations are valid for sites with soil parameters within the range calibration dataset (Table 2) and open for the inclusion of incomplete databases for local, regional and national soil nutrient or organic carbon stock calculations.

The equations we present in Table 3 are given for soils in general and for different forms of land-use. Bias is low in all the datasets. The best support for the pedotransfer equation is given for grassland soils. In the Alps, there is a wide range of intensities in grassland management, ranging from extensively-used pastures and meadows with one or two cuts a year to intensively used cattle pastures and meadows with four or five cuts per year and fertilizer applications. In the compiled data set, all the grasslands categories were represented.

The pedotransfer functions for cropland gave the weakest prediction of soil bulk densities as only 43% of the estimated soil bulk density can be explained by the variable soil depth and content of soil organic carbon. The results are comparable to the findings of (Chen et al., 2018; Kätterer et al., 2006; Suuster et al., 2011). We suppose the impact of management on one hand explain the lower variability of the measured parameters in the cropped top soil, and on the other hand, the compaction by heavy machinery in the sub soils below the plough-pan layer.

Surprisingly, soil texture only has a significant impact on the soil bulk densities derived from grassland soils. Just as interesting were the negligible differences of model goodness (R^2, RMSE) and PU between more complex models and models with only soil organic content as predicting variable (for instance see Table 3: EQ 4 and EQ 7).

Using any of these equations to estimate the stock of soil organic carbon, a delicate situation occurs. The content of organic carbon is used to estimate soil bulk density, and soil bulk density is used to estimate the soil carbon pool. This is the classic example of a circular argument where the premise includes the conclusion. However, it is elusive to estimate soil bulk density without knowing the organic carbon content. The only remedy is to insist that soil carbon pools can only be estimated using data based on the measured soil bulk densities.

The assessment of uncertainty and variance is indispensable for the measured as well as for the estimated soil bulk densities (Schrumpf et al., 2011). The Monte Carlo simulation shows that, due to the structure of the derived linear model, soil bulk density estimates carry an uncertainty of 9 to 25% according to land-use. It is the task of the user of the equations to evaluate this uncertainty. An argument against the equations may be that an uncertainty of up to 25% is not acceptable. An argument in favor of these equations is that the uncertainty is known at all, and that upper and lower limits and the mean value of the target value (e.g., soil carbon stock of an area) based on soil bulk density can be established. This knowledge sets the equations apart from published formulas and expert judgment.

5. Conclusion

By this step-by-step description of deriving pedotransfer functions, we encourage the use of these derived pedotransfer functions as well as the development of further regional models for other missing variables. Regarding the rather poor predictability, we recommend measuring soil bulk density by standardized sampling of undisturbed soil cores and the post-processing of the samples under laboratory conditions by internationally harmonized protocols. When the measured values for soil bulk density are not available, our set of linear equations, based on a broad range of predicted variables of different land-use offers a regionally calibrated and validated alternative.

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