Prediction of bulk density in Croatian forest Pseudogleys based on contents of soil organic matter and clay

Predikcija volumne gustoće šumskih pseudogleja u Hrvatskoj temeljem sadržaja organske tvari tla i gline

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Abstract

Soil bulk density (BD) is often used to assess soil properties related to soil structure and general soil quality, or to convert weight units to volume/area units. Because collecting undisturbed soil samples (cores) and directly measuring BD is laborious and time-consuming, data on BD are often lacking. Pedotransfer functions (PTFs) can be used to predict BD from more readily available (easily measured) properties. However, specific PTFs for specific range of soils should be developed. In this study, soil organic matter (SOM) and clay contents of 90 forest Pseudogleys horizons, distributed across 11 locations in continental Croatia, were used to develop a multiple linear regression equation that predicts BD. The results have shown that the increase in BD due to the unit increase in clay content is lower than the decrease in BD due to the unit decrease in SOM content. PTF performance was relatively high (R²_{adj}=77.5%, RMSE=0.1 g*cm⁻³, MAE=0.08 g*cm⁻³), showing that missing data on soil BD of Croatian Pseudogleys (or other similar soils, formed on similar parent materials) can be estimated reasonably well by using it. However, care should be taken when dealing with arable soils, which have different properties, compared with the natural soils considered herein.

Keywords: continental Croatia, forest soils, multiple linear regression, pedotransfer function (PTF), soil bulk density estimation, Stagnosols

Sažetak

Gustoća tla volumna (Gv) se često koristi za procjenu svojstava tla povezanih sa strukturom tla i općom kvalitetom tla, ili za pretvaranje težinskih jedinica u volumne/površinske. Obzirom da prikupljanje neporušenih uzoraka tla u cilindrima i izravno određivanje Gv zahtijeva puno rada i vremena, podatci o Gv često nedostaju. Pedotransfer funkcije (PTF) se mogu koristiti za predikciju Gv koristeći lakše dostupna (lakše mjerljiva) svojstva tla. Pritom bi se trebale razviti specifične PTF za specifične raspone tala. U ovom istraživanju, sadržaji organske tvari tla (OTT) i gline u 90 horizonata šumskih pseudogleja distribuiranih na 11 lokacija diljem kontinentalne Hrvatske su korišteni za razvoj jednadžbe višestruke linearne regresije za predikciju Gv. Rezultati su pokazali da je porast Gv zbog jediničnog porasta sadržaja gline niži nego smanjenje Gv zbog jediničnog smanjenja sadržaja OTT. Razvijena PTF imala je relativno dobre pokazatelje (R²_{adj}=77.5%, RMSE=0.1 g*cm⁻³, MAE=0.08 g*cm⁻³), pokazujući da se eventualno nepostojeći podatci o Gv hrvatskih pseudogleja (ili sličnih tala, razvijenih na sličnim matičnim supstratima) mogu relativno dobro procijeniti njenom primjenom. Ipak, u slučaju poljoprivrednih tala, potreban je oprez, obzirom da takva tla imaju različita svojstva od prirodnih, koja su razmatrana u ovom radu.

Ključne riječi: kontinentalna Hrvatska, pedotransfer funkcija, procjena volumne gustoće tla, Stagnosoli, šumska tla, višestruka linearna regresija

Introduction

Soil bulk density (BD) is a soil property that indirectly affects plant (most notably, root) growth/yield (Mouazen et al., 2003; Dexter, 2004; Reichert et al., 2009; Keller and Haakanson, 2010). Accordingly, BD can be used as an indicator of soil quality or site productivity (Tamminen and Starr, 1994; Suuster et al., 2011). This is due to direct relationships between BD and various soil properties, such as soil compaction and porosity, soil organic matter (SOM) content, and soil texture (e.g. Tamminen and Starr, 1994).

Values of BD are commonly used for conversions of weight units to volume or area units. This is often the case with studies on soil moisture, as well as with those in which conversion of stocks of soil organic carbon (SOC) and other soil elements (nutrients) from a mass basis (e.g. g*kg⁻¹) to an area basis (e.g. kg*ha⁻¹) at a specified depth is required (Tamminen and Starr, 1994; Brahim et al., 2012; Sequeira et al., 2014). Due to the global climate change and the fact that soil C accumulation may contribute to its mitigation, estimates of soil C stocks have become increasingly demanded (Eswaran et al., 1993; Smith, 2004).

In spite the importance of BD, this parameter remains a major source of uncertainty in many soil-related assessments. The basic problem is that the data on BD are often lacking in soil databases - mainly because collecting undisturbed samples (soil cores) and directly measuring BD is considered to be labor-intensive, time-consuming, and accordingly expensive (De Vos et al., 2005; Brahim et al., 2012; Sequeira et al., 2014). Secondly, if the data on BD is actually available, it is reliable only if the methodological rigor was high (Barros and Fearnside, 2015).

Due to the above, several pedotransfer functions (PTFs) were developed to estimate BD from other (more readily available) soil properties (Tamminen and Starr, 1994; Benites et al., 2007; Suuster et al., 2011; Barros and Fearnside, 2015, etc.). PTFs have been widely used in soil studies to estimate various soil properties that are

JOURNAL Central European Agriculture ISSN 1332-9049 difficult to measure in the field (Minasny and Hartemink, 2011). Basically, PTFs represent predictive functions that use existing (legacy) data, which is usually easily acquired, as predictor variables (e.g., soil particle size distribution (PSD), SOC content, pH) for prediction of a soil property (response variable) that is more expensive and/or more complicated to measure (e.g. BD, particle density, water retention, cation exchange capacity). In predicting BD, soil organic matter and texture were the most common predictors used (Kaur et al., 2002; De Vos et al., 2005; Benites et al., 2007; Hollis et al., 2011; Brahim et al., 2012). Even though various statistical methods are available, multiple linear regression has been the method most used for developing BD PTFs (Sequeira et al., 2014).

Large differences in the performance of published PTFs are usually recorded after they are applied to environments different than those used for their calibration (De Vos et al., 2005). Therefore, although attempts were made at continental/global level to provide equations that would apply to a wide range of soils (e.g. Benites et al., 2007; Hollis et al., 2011), in order to obtain high accuracy and great precision in estimating BD, an equation specific for each range of soils of relevance to a particular research program should be used, rather than to rely on general PTFs (e.g. Barros and Fearnside, 2015).

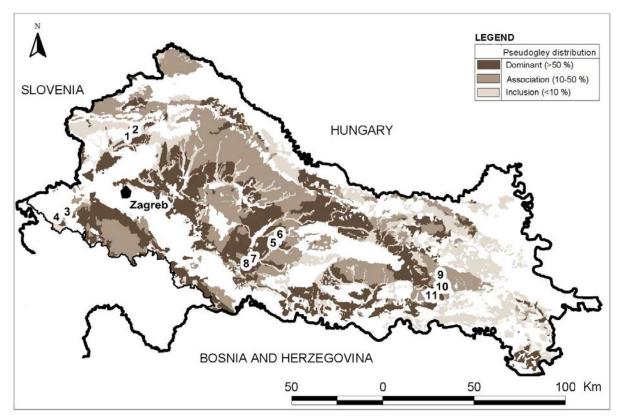
Thus, the objective of this study was to use readily available properties of 33 forest Pseudogley profiles distributed across continental Croatia, in order to develop a region-specific PTF that would allow BD prediction for such (and similar) soils across the wider region. Although Pseudogleys are the most common soils in continental Croatia (Bogunović et al., 1998; Rubinić et al., 2015), such PTF is currently missing.

Materials and methods

Study area, field and laboratory work

The study area (Figure 1) represents the northern part of Croatia, which is found at the southwestern edge of the Pannonian Basin. Climate is moderate continental and largely humid. Albeit several isolated mountains are present, the dominant geomorphic units of the area are the Holocene (alluvial) terraces and the Pleistocene terraces. Pseudogleys have formed on the latter, and their parent materials can generally be labeled as pseudogleyed loess derivates (Rubinić et al., in press). Across such materials, sessile oak and hornbeam forest (*Epimedio-carpinetum betuli*) is the prevailing natural vegetation. Accordingly, to minimize human influence on soil properties, all soils analyzed in this study were found at sites with well-established sessile oak and/or hornbeam forests.

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At each location, three replicate soil profiles were investigated.

Figure 1. Eleven locations with Pseudogley soils studied across the continental Croatia

Total of 11 locations were investigated (Figure 1). At each location, three soil pits were dug. Accordingly, 33 soil profiles were investigated altogether. Soils were described and sampled according to FAO (2006). Disturbed soil samples were taken from each mineral horizon. Undisturbed soil samples, collected in 100 cm³ cores (as triplicates), were taken from only around 70% of all horizons. Namely, the cores could not be taken from the A horizons that were too thin and/or comprised too many roots, nor from some compacted parent materials that were too dry at the time of sampling. In total, 90 soil horizons were used for the development of the PTF. Some properties of soil horizons covered in this study were previously analyzed by Rubinić et al. (2015; 2016), as affected by relief, climate, and profile stratigraphy.

On each location, Pseudogley soils were found. One of the main features of these soils is periodic stagnation of precipitation water on/in their poorly permeable (clayenriched and often massive) subsurface Btg horizon, as well as their low pH (see Rubinić et al., 2015; 2016). Most of these soils correlate with Stagnosols, and some with Stagnic Retisols and Stagnic Luvisols (IUSS Working Group WRB, 2014). Usually, their soil profile can roughly be designated as O-A-Eg-Btg-Cg according to Food and Agriculture Organization (2006).

Prior to performing laboratory analyses, disturbed soil samples were air-dried and sieved through the 2 mm sieve. Soil PSD was determined after Škorić (1982), by pipette-method comprising wet sieving and sedimentation after dispersion with

sodium-pyrophosphate (Na₄P₂O₇, c=0.4 M). SOM content was determined as humus (and not organic carbon) content using the Tjurin method, by acid-dichromate (K₂Cr₂O₇, c=0.4 M) digestion (JDPZ, 1966). Core samples were used to determine BD after drying the soil at 105 °C (HRN ISO 11272:2004). More details on these analyses, including the results of the analyses not covered herein, are found in Rubinić et al. (2015; 2016).

Data handling, descriptive statistics, and PTF development

Statistical analyses were conducted using Statgraphics Centurion VI (StatPoint Inc., USA). After performing descriptive statistics and correlation analysis, the complete data set (n=90) was randomly split into the calibration (training) set (n=60) and the validation (evaluation) set (n=30). The size ratio between the two sets is in accordance with the commonly applied strategies, which use training sets comprising 1/2-2/3 of the complete set (e.g. Dobbin and Simon, 2011).

Subsoil samples (Btg and Cg horizons) comprised around 60% of the complete set, with the rest belonging to the topsoil samples (A and Eg horizons). However, the data were not stratified on the horizon-basis, but were used as a whole to develop a continuous PTF. Namely, stratification of the data set into topsoil and subsoil data has been shown not to improve the overall BD prediction quality, which is why PTFs should be calibrated using samples taken from all horizons, with a higher proportion of subsoil samples (De Vos et al., 2005).

Models have been fit by ordinary least squares method using all combinations of available predictors. Only the predictors that significantly (P<0.01) affect the predicted variable were selected, so that effort and resources can be optimized (e.g. Sequeira et al., 2014) and the risk of overfitting the model, which reduces the prediction accuracy for unseen (new) data, can be reduced (e.g., Aertsen et al., 2010). The best model for estimating BD was selected after comparing the obtained values of commonly-used metrics: root mean squared error (RMSE), coefficient of determination (R^2), adjusted coefficient of determination (R^2_{adj}), and Mallows' Cp statistic (Cp). Including additional variables (predictors) in the model increases R^2 and reduces RMSE, thereby pointing to better performance of the function even when those variables do not significantly contribute to explaining the outcome. Hence, when selecting the model, more robust metrics that penalize inclusion of additional predictors (i.e. adjusted R^2 and, especially, Cp) were primarily considered.

Cp is a measure of model bias, which provides information that enables the selection of a model that has small residual error and as few predictors as possible. The value of Cp should be as close as possible to (or even below) the number of predictors used. Basically, the smaller the Cp, the better the model:

$$Cp = \frac{SS_{RES(p)}}{MS_{RES(FULL)}} + 2p - n$$

where $SS_{RES(p)}$ is the sum of squares for the model with p variables, $MS_{RES(FULL)}$ is the mean squarer error for the full model, *p* is the number of predictors (including the regression intercept), and *n* is the number of observations.

JOURNAL Central European Agriculture 155N 1332-9049 After selecting the best model, its further evaluation followed. Analysis of variance (ANOVA) was performed on the model. To evaluate more aspects of prediction, several validation (goodness-of-fit) indices should be considered simultaneously (e.g. De Vos et al., 2005). Therefore, RMSE, R^2_{adj} , and mean absolute error (MAE) were used to evaluate the reliability/accuracy of the developed PTF. Performance of a PTF increases with the decrease in RMSE and MAE and the increase in R^2_{adj} .

Finally, outliers were searched for and eliminated if found appropriate. For this purpose, studentized residuals (SRs) were used along with visual examinations of residual plots (SRs against individual observations). Observations with studentized residuals greater than 3 and a notable effect on the predictive ability of the PTF were considered as outliers, which were in turn eliminated (in case they obviously resulted from measurement errors, and not natural variability). Because regression analysis assumes homoscedasticity (all residuals to be normally distributed, i.e., randomly scattered around zero), SRs were also plotted against predicted values to assess if there is heteroscedasticity within the data, which would imply the need for data transformation.

After the PTF has been developed on the calibration set, it was tested by regressing the BD values predicted by the developed PTF against the BD values observed in the validation set. In line with Pineiro et al. (2008), the predicted values were plotted on the *x* axis, and the observed ones on the *y* axis. Performance of the PTF was evaluated using the same metrics as during calibration, without removing any possible outliers.

Results and discussion

Descriptive statistics and correlations

As presented in the Table 1, the 90 analyzed soil horizons had averagely 21.1%, 4.8%, and 74.1% of clay, sand, and silt particles, respectively. Thereby, they were generally silt loams. However, due to the notable variations in particle contents across the analyzed samples (Table 1), some were actually silts or silt clay loams. Average content of SOM was 2% (Table 1). Because all samples were taken from forest soils, topsoil horizons usually comprised very high SOM contents (up to 12.5% - Table 1). Consequently, variation in SOM content across the samples was high (Table 1). Accordingly, BD ranged from 0.8 g*cm⁻³ to 1.6 g*cm⁻³, averagely amounting to 1.37 g*cm⁻³.

Measure	Clay content	Sand content	Silt content	SOM ¹ content	BD ² (g*cm ⁻³)	
	(%)	(%)	(%)	(%)	(g chi °)	
	Horizons of the complete set (n=90)					
Average	21.1	4.8	74.1	2	1.37	
SD ³	6.3	1.3	5.6	2.5	0.19	
Minimum	9	1.9	61.9	0.2	0.8	
Maximum	34.8	7.5	86.5	12.5	1.6	
Horizons of the calibration subset (n=60)						
Average	21	4.8	74.2	2.2	1.36	
SD ³	6.8	1.4	6	2.7	0.19	
Minimum	9	1.9	62.1	0.2	0.8	
Maximum	34.3	7.5	86.5	12.5	1.6	
Horizons of the validation subset (n=30)						
Average	21.3	4.7	74	1.9	1.37	
SD ³	5.3	1.2	4.7	2.3	0.21	
Minimum	11	2.1	61.9	0.3	0.8	
Maximum	34.8	6.5	82.6	9.6	1.6	

Table 1. Descriptive statistics	for the selected properties c	of analyzed soil horizons
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¹Soil organic matter, ²Soil bulk density, ³Standard deviation.

SOM content was highly negatively correlated with BD (Table 2). This is in line with previous studies on forest soils (e.g. Tamminen and Starr, 1994). Contents of clay and silt also were highly correlated with BD (positively and negatively, respectively), unlike the content of sand, which was moderately negatively correlated with it (Table 2).

Given the almost perfect correlation between clay and silt themselves (Table 2), the latter was not evaluated as a potential BD predictor, i.e., clay content was selected as the fraction of preference (e.g. Hollis et al., 2011). Later on, contents of clay, sand, and SOM were evaluated as potential predictors while selecting the best model for

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BD estimation (Table 3). Such approach agrees with several other studies that used SOM and texture to develop BD PTFs (Kaur et al., 2002; De Vos et al., 2005; Benites et al., 2007; Brahim et al., 2012). According to some previously developed conceptual models, the main factors determining BD of a soil layer are its SOM content (and its associated density) and its mineral density as determined by its PSD - either the sand or the clay content or both (Hollis et al., 2011).

n=90 ¹	BD	Clay content	Sand content	Silt content	SOM ² content
BD ³		0.7**	-0.32**	-0.71**	-0.79**
Clay content			-0.61**	-0.98**	-0.61**

Table 2. Pearson correlations among the selected soil properties

¹Complete sample size (number of pairs of data values used to compute each coefficient), ²Soil organic matter, ³Soil bulk density, **Significant at P=0.01 level.

Selection and calibration of the regression model (n=60)

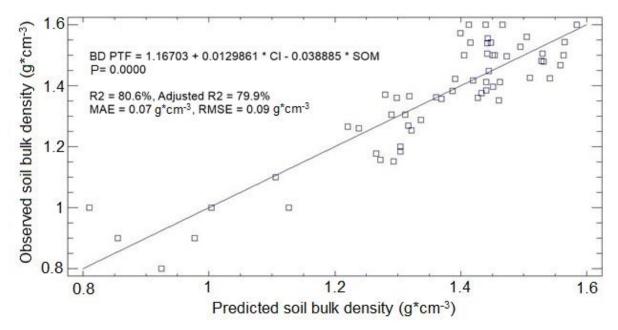
After evaluating the generated regression models, clay and SOM contents were selected as the best predictors (Table 3). This agrees with the results of Husnjak and Rubinić (2016).

Table 3. Values of Mallows' Cp statistic used for the selection of the best model for soil bulk density prediction (n=60)

Predictors ¹	Ср
CI, SOM	3.9
CI, S, SOM	4
SOM	20.3
S, SOM	21.1
CI	33.9
CI, S	34
S	107.6
-	131.5

¹Listed in line with the increasing Cp value. Cl - clay content (%), S - sand content (%), SOM - soil organic matter content (%).

After the selection of the model, an outlier with a studentized residual of 5.9 was detected. It featured BD of 1.6 g*cm⁻³ and SOM content of 5.7% (raw data not shown). Descriptive statistics (Table 1) and the correlation between BD and SOM (Table 2) clearly show that this observation lacks sense, i.e., that it is the product of human error during either field/laboratory analyses or typing. Therefore, it was discarded from the calibration data subset. As a consequence, the performance of the PTF notably increased. One can note that the calibrated PTF explained around 80% of the variability in BD of the analyzed soils, with a mean absolute overestimation of 0.07 g*cm⁻³ (Figure 2). The regression equation clearly shows that the BD of Croatian forest Pseudogleys generally increases with the increase in clay content and the decrease in SOM content (Figure 2). However, as shown by the estimated regression coefficients, the increase in BD due to the unit increase in clay content is lower than the decrease in BD due to the unit decrease in SOM content (Figure 2). In non-cultivated (forest) soils, SOM often has the prevailing effect on BD (e.g. Jalabert et al., 2010).



Evaluation metrics (RMSE - root mean square error, R^2 - coefficient of determination, Adjusted R^2 - adjusted coefficient of determination, MAE - mean absolute error, P - model ANOVA P value) for the pedotransfer function (PTF) calibrated for soil bulk density prediction is shown. BD - soil bulk density (g*cm⁻³), CI - clay content (%), SOM - soil organic matter content (%).

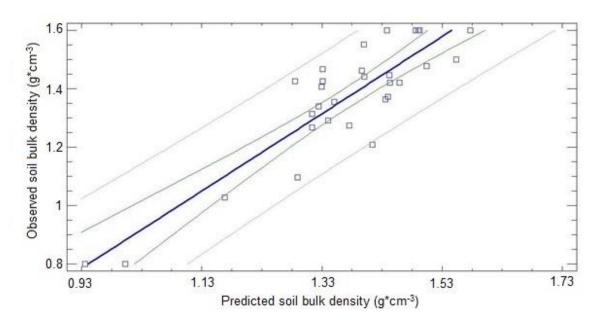
Figure 2. Observed vs. predicted values of soil bulk density for the calibration subset

Given the P-value obtained by ANOVA for the calibrated model (Figure 2), there is a statistically significant relationship at the 99% confidence level between BD and the independent variables in the developed model. Hence, the model itself is highly significant. Plotting the observed BD values vs. the predicted BD values (Figure 2) confirmed the good performance of the developed PTF.

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Validation of the regression model (n=30)

Using the developed PTF to predict BD of the samples in the validation subset showed that the function keeps most of its predictive power outside the data set it was created in (Figures 2 and 3). Most notably, the adjusted R^2 for the validation set (R^2_{adj} =77.5%) was not much lower than the one computed for the calibration set (R^2_{adj} =79.9%). Hence, the variation in BD was explained almost equally well by the chosen predictors even after the PTF was extrapolated out of the calibration subset. However, one should note that the validation data were held out from the same population from which the calibration data originated from. In addition, soils from only 11 different locations were analyzed.



Blue line is the regression line, curved green lines are confidence bounds, and straight gray lines are prediction bounds at 95% confidence level. Evaluation metrics (RMSE - root mean square error, R^2 - coefficient of determination, Adjusted R^2 - adjusted coefficient of determination, MAE - mean absolute error, P - validation model ANOVA P value) for the PTF validation equation of the pedotransfer function for soil bulk density prediction is shown. BDo - observed bulk density (g*cm⁻³), BDp - predicted bulk density (g*cm⁻³).

Figure 3. Observed vs. predicted values of soil bulk density for the validation subset

After validating the PTFs that they have developed using regression to predict BD of forest soils in Brazil, Barros and Fearnside (2015) reported the R² value of 57% for the model comprising 140 observations and using clay content and soil pH as predictors. Regression model created by Bernoux et al. (1998), which used clay, total organic C, soil pH, and sand to describe the variation of BD in the Brazilian Amazon (n=323), achieved the R² value of 56%. Obviously, the R² values reported above for the Brazilian forest soils are notably lower than the one obtained for the forest soils in this study (R²=78.2%). This is probably due to the much larger heterogeneity of soils in the Brazilian studies, than in the soils covered herein. Tamminen and Starr (1994) achieved the R² value of 83% for the BD prediction in 158 samples of Finnish forest

JOURNAL Central European Agriculture 15SN 1332-9049 soils. However, no validation of the derived PTF seems to have been conducted in their study.

Conclusion

A simple continuous PTF for prediction of soil BD in Croatian forest Pseudogleys was selected (n=60), calibrated (n=59), and validated (n=30) using multiple linear regression. It was shown that the increase in BD due to the unit increase in clay content is lower than the decrease in BD due to the unit decrease in SOM content.

When applied to the validation subset, the PTF performed almost equally well $(R^{2}_{adj}=77.5\%, RMSE=0.1 \text{ g}^{*}\text{cm}^{-3}, MAE=0.08 \text{ g}^{*}\text{cm}^{-3})$ as in the calibration subset. Hence, if the data on soil BD of Croatian Pseudogleys (or some other similar soils, formed on similar parent materials) are missing, they can be estimated reasonably well by applying the here-developed PTF. However, care should be taken when predicting BD of arable soils, which may have significantly different properties (lower contents of SOM included), compared with the soils considered herein.

In the future, attempts should be made to develop PTFs for prediction of soil BD (and other relevant soil properties that are not readily available) also for other soils on loess-derived parent materials in continental Croatia. Given the abundance and the relative homogeneity of such parent materials across the region, one PTF could easily prove to be adequate for more than one soil type. To create a highly reliable and robust PTF, a large number of soil profiles (samples), taken from numerous different locations and comprising agricultural soils along with the natural ones, should be considered.

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