Methods of modeling and mapping of the soil bulk density: a case study from Chernivtsi region, Ukraine

Vasyl CHERLINKA, Yuriy DMYTRUK, Liubov CHERLINKA, Mykhailo GUNCHAK, Volodymyr SOBKO

Abstract: *Soil monitoring programs in many countries often do not measure such an indicator as soil bulk density. At the same time, modern problems of assessing the condition of the soil cover require its use in soil management of agricultural landscapes. We see the solution to this problem in geospatial modeling. We have developed a technique for simulating soil bulk density, the algorithm of which consists of five stages: the creation of model maps of agro-industrial soil groups, modeling of a clay content map, construction of a map of humus content, selection of empirical dependences of soil bulk density on humus and clay content with evaluation reliability of these dependencies and their implementation in GRASS GIS and, finally, cartographic modeling of the spatial continuous distribution of soil bulk density. At the same time, parameters for improving the quality of methods modeling and mapping the soil bulk density were established. First of all, this is an increase in the sampling dataset of density, humus, and clay content to improve the reliability of the selected regression formula. It is also an improvement in the quality of spatial modeling of the humus content using geostatistical methods or modeling. To improve the clay content map, it is necessary to increase the resolution of DEM and predictors, to choose more accurate sources of DEM and prediction algorithms. The application of the presented methodology is shown in a part of Chernivtsi region, Ukraine, with the possibility of use on the scale of the entire country.*

Keywords: *soil bulk density, humus, clay, modeling, simulation, morphometric parameters, DEM, predictive algorithms, regression*

Introduction

The soils of Ukraine are very diverse in terms of their genesis and texture, as well as their physico-chemical, physical, and agronomic properties. Large-scale research revealed 634 of their species, and taking into account the granulometric composition, salinity, degree of erosion, and other indicators, the number of soil varieties exceeds 2 thousand (Zinevych 1985), which is due by zonal features of climate and vegetation during their formation (Krupsky and Polupan 1979). Soil bulk density is evaluated as the most generalizing parameter of the physical properties of soils and is used as an indicator of changes in the physical state of the soil. Direct measurement of bulk density, depending on the country, is quite widely used in agricultural research to determine the compaction of soils, primarily of arable land, observed under different tillage systems. In general, this problem is acute both in Ukraine (Medvedev 1997a, Medvedev et al. 2004) and in other countries (Jalabert et al. 2010, Makovníková et al. 2017). The problem of agrophysical degradation of soils, along with other types of it, threatens the sustainable use of soils and the fulfillment of their global functions.

The practical significance of soil bulk density is primarily related to the productivity of agricultural crops, which require a certain ecological optimum of soil conditions and soil indicators: the content of organic matter (humus), macroelements, as well as calcium, magnesium,

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potassium and other ash elements available to plants, acidity, structure soil, the bulk density of the root layer. So, for example, for winter wheat, the optimal density of the arable layer lies in the range of 1.10-1.35 $g \cdot cm^{-3}$, within which the productivity is 80-100%, in the ranges of 1.00-1.09 and 1.36-1.45 $g \cdot cm^{-3}$, productivity decreases to 50% and beyond the mentioned limits, plants begin to struggle for survival due to either excessive aeration or compaction (Cherlinka 2016, 2019, Medvedev 1997a). It is known that plants absorb up to 80-85% of the elements of mineral nutrition from the arable horizon, in which the main mass of roots is located, during the growing season (Nikitin 1987). Therefore, the deviation from the optimum bulk density limits the assimilation of nutrients by plants (Schillaci et al. 2021, Sequeira 2014). It is interesting to note that different crops have a differentiated tolerance to compaction and looseness, which must be taken into account when developing cultivation and cultivation systems. Agricultural production technologies are aimed at ensuring the maximum productivity of agricultural plants by creating optimal soil indicators.

Monitoring of carbon sequestration/emission by soils is no less important in terms of the practical use of the density indicator. It is controlled by determination of carbon stocks in soils (Dent et al. 2022, Stepanchenko et al. 2023). Such calculations are carried out for a certain area using the actual carbon content, the thickness of genetic horizons or soil layers, and soil bulk density (Lal 2009, Schillaci et al. 2021, Tadiello et al. 2022). With the same carbon content in soils, but different bulk density, the carbon reserves will differ significantly. In the monitoring of the neutral level of soil degradation, it was found that the decrease in the actual content of organic carbon is accompanied by a decrease in soil porosity, water-holding capacity, and acceleration of erosion.

Field soil surveys play a major role in planning production volumes and monitoring changes in soil parameters. But in Ukraine, in the five-year cycle, only the main agrochemical parameters (NPK content, humus, and pH) are studied, and other indicators, including soil density are analyzed from time to time or not at all (Balyuk et al. 2010, Balyuk et al. 2012, Yatsuk 2018). The soil texture, for example, is determined almost once, as a rule, when constructing soil maps on a scale of 1:10,000, and the study of soil bulk density is the prerogative of separate scientific studies, although the most common core method for determining bulk density is not too complicated for analytical laboratories. Given the intensive mechanization, we believe that this is a gap in monitoring programs, but the application of existing methods (ISO 11272:2017) is not yet widely implemented in production processes and analytics (Jalabert et al. 2010, Medvedev 1997a, Sequeira 2014, Suuster et al. 2011, Taalab 2013, Yatsuk 2018).

Although many studies show a certain dependence of soil bulk density on its genesis, it is most often fully revealed when analyzing the full soil profile (Chestnykh and Zamolodchikov 2004). However, for soils used in agriculture, especially of the top layer, genetic features are significantly reduced by constant anthropogenic influence. The indicators of the soil texture, content of organic matter, exchangeable cations, that is, some of the indicators of the soil absorbing complex (Cherlinka 2019, Nazarenko et al. 1998, 2000) come first. But this kind of research requires a sufficiently voluminous sample of data to reliably establish relationships of density with other soil indicators and to build appropriate cartographic models.

Research background

Existing practical tillage technologies lead to the physical degradation of soils, first of all to their compaction. Thus, according to Medvedev (1997b), the bulk density of chernozem soils increased by 0.14 $g \cdot cm^{-3}$ from 1970 to 1990, and of dark chestnut soils by 0.27 $g \cdot cm^{-3}$. Compaction led to the deterioration of other agronomically and ecologically important soil properties. The dependence of the soil bulk density on human production activity is manifested not only in how and when the soil is cultivated, but also in the content of humus (Makovníková et al. 2017, Meurer et al. 2020, Taalab 2013) or features of the indicators of the soil absorption complex (Cherlinka 2001, Nazarenko et al. 1998, 2000). In particular, the peptization of the finely dispersed part of the soil or, conversely, its aggregation depends on the composition of exchangeable cations, which is reflected in the value of the soil bulk density (Manrique and Jones 1991, Heuscher et al. 2005). Therefore, there are correlations between the soil bulk density and the above-mentioned indicators, which we consider as resultative and factor characteristics, respectively. Since in some cases the connection can be quite transformative, its evaluation is a separate task (Kaur et al. 2002, Nazarenko et al. 1998, Sequeira 2014, Suuster et al. 2011, Tranter et al. 2007). For example, Nazarenko et al. (1998) found that for different soil types the relationship between soil bulk density and humus content is inversely proportional and is both linear and non-linear which is often confirmed by other authors (Chestnykh and Zamolodchikov 2004, Demakov et al. 2017, Makovníková et al. 2017, Manrique and Jones 1991). The obvious influence of the humus content is not only on the bulk density but also on soil aggregation, and physical and hydraulic properties (Makovníková et al. 2017, Meurer et al. 2020).

Detection of the tightness and type of relationships between soil bulk density, humus, and texture (in particular, clay content) is possible when creating appropriate models or pedotransfer functions (Heuscher et al. 2005, Houšková 2002, Jalabert et al. 2010, Kaur et al. 2002, Makovníková et al. 2017, Nazarenko et al. 1998, 2000, Taalab 2013, Tranter et al. 2007, Tranter et al. 2007). Such modeling reduces the time of experimental research and also allows for creation of a spatial continuous model of soil bulk density for agricultural landscapes.

Therefore, the main goal of this study is to develop a methodology for selecting an adequate model of soil bulk density based on a finite set of parameters and creating continuous maps of this indicator for practical needs, in particular, assessment of degradation risks, assessment of carbon reserves in soils and, as a result, ensuring sustainable land use management on different levels.

Methods and Data

The specificity of soil surveys in Ukraine has several features. Field soil mapping of Ukraine in 1957-1961 was intended, as quickly as possible, to make a provisional map of the soil cover at a scale of 1:25 000. Between 1969 and 1991, the second round of soil surveys was undertaken at a field scale of 1:10000. These took a different approach, mapping agro-industrial soil groups (hereinafter, AISG): combinations of soils that exhibit similar morphology and fertility and which we expect to respond to management in much the same way (State Land Cadastre 2022, Solovei 2020). The AISG maps in general depict 222 agro-industrial groups and thousands of individual mapping units. All of them were used in the modeling and such a map provides the required information on the qualitative composition of soils. Of course, such a large number is hard to perceive and, for those unfamiliar with the particularities of the Ukrainian soil classification, and hard to comprehend. Considering our immediate and urgent purpose – development methods of modeling and mapping of the soil bulk density – we have generalised the legend and correlated the mapping units with the World Reference Base for naming soils and creating legends for soil maps (IUSS Working Group WRB 2015), drawing on Dmytruk et al. (2022). This soil survey was almost completed. About 15-18 million hectares of 60 million hectares have never been assessed by systematic soil surveys in scale of 1:10,000; this includes not only the Carpathian and Crimean Mountains, but also forested, built-up, and some cropland areas (Achasov et al. 2015, Cherlinka 2017a, 2017b, 2017c, Cherlinka et al. 2019, 2020), and therefore there is no reliable soil map for these areas. Since 1991, surveys have been only fragmentary (Kanash 2013). Large-scale soil mapping materials (AISG), are urgently needed for a completely peaceful purpose: estimation of soil treatment, fertilizers, and protection against degradation. The available medium-scale soil maps are not up to the job. It is hard to hope that in a state with a war-torn economy, soil surveys will be a top priority.

Therefore, we believe that soil modeling would be satisfactory for filling the "white spots" today. It is worth noting that although Ukraine has built a control system for the state of agrochemical indicators, which is carried out by the State Soil Protection Institute every five years since the 1950s, it pays attention only to the main nutrients, some microelements, pH and humus content. Accordingly, it lacks data on the texture of the soil. And these data can be taken only from AISG maps, which accumulate their soil texture information in the names. Accordingly, it is possible to move from letter indexes to their numerical characteristics of soil texture based on the average values of classes.

The studies were conducted within the Chernivtsi region (Fig. 1a) parts of the Dniester administrative district (Fig. 1b). Input data for humus content modeling (Fig. 1c) obtained by the results of agrochemical certification of soils (Chernivtsi branch of the State Institution "Soils Protection Institute of Ukraine"), and map of agro-industrial groups of soils (Fig. 1d) – in accordance with the maps of the DP "Chernivtsi Research and Project Institute of Land Management". Accordingly, the primary goal is to create a 1:10,000 scale model AISG map of the area of interest. The basic idea is to use the reference points of the terrain and the classifying soils assigned to them (Lagacherie et al. 2001). The analysis of the digital elevation model (DEM) allows to allocate a certain number of geomorphological parameters that are related to soil taxon (or AISG), and apply them as predictors (independent variables). The literature presents successful examples of constructing dependencies and their application for predictive soil maps (Cherlinka 2017a, Malone et al. 2016, Kempen et al. 2009, Debella-Gilo and Etzelmüller 2009, Hengl 2009). The application of this approach is also justified by the fact that it can be linked to the model SCORPAN (McBratney et al. 2003), which, in turn, follows from the classical hypothesis V.V.Dokuchaev about the problems of predictive soil mapping (Florynsky 2012). Of course, for the ideal variant of constructing a predicative soil map, a complete set of SCORPAN parameters needs to be acquired. However, in practice, this is not always possible for various restrictions on the quantity and quality of input data.

In order to process the data, the instrumental capabilities of the available software were used: cartographic representation – QGIS (QGIS Development Team 2022), preparation of morphometric parameters maps – GIS GRASS (GRASS Development Team 2022), construction of a predictive AISG map and regressions analysis/visualisation – the language of statistical computations R-statistic (R Development Core Team 2022). For calculating DEM derivatives the Shuttle Radar Topography Mission (SRTM) data fragments were processed. For geomorphological analysis, the SRTM v4 dataset of the study area (NASA JPL 2013) was loaded, resampled to a resolution of 50 m, and denoised using the Sun *et al.* (2007) algorithm according to the recommendations of Stevenson *et al.* (2009). The resulting denoised DEM and derivatives were used to build a model of the spatial distribution AISG. Basic morphometric characteristics for this purpose: slope and aspect of the slopes (module r.slope.aspect); land surface curvatures: profile & plan – geometric, longitudinal, minimum & maximum – non-geometric curvatures (Minár et al. 2020) – module r.param.scale; data of solar radiation – module r.sun; relief form in r.geomorphon. It is worth noting that for modeling it is promising to use a much larger set of curvatures, but with caveats and remarks described in detail in the work Minár *et al.* (2020). Additional maps of hydrological indicators were also generated: the topographic wetness index in r.topidx; flow accumulation and flow direction in r.terraflow; the length of the flow flux in r.flow and distance to them – the module r.stream.distance. The basis of constructing a predictive model for the distribution of AISG lay a Random Forest algorithm (Wright and Ziegler 2015) with the proposed Dobos and Hengl (2009) and proven Cherlinka (2017b) methodology for creating a training sample. To evaluate the quality of the model, we used Cohen's Kappa coefficient (Landis and Koch 1977), which in this case shows the degree of correspondence between the original and the predicted data. The interpolation of carbon and clay content data was carried out by the algorithm of regularized splines with tension (Mitášová and Mitáš 1993) in GIS GRASS.

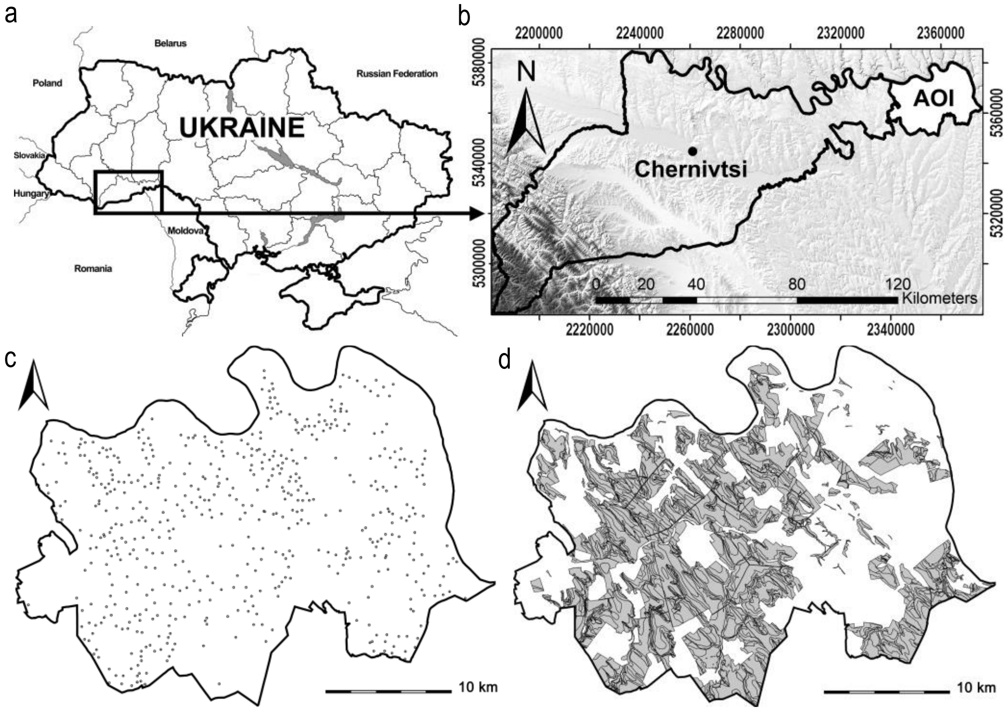

Fig. 1. *Geographical location of the area of interest (AOI) within Ukraine (a) and Chernivtsi region (b); distribution of dataset points (c) and the availability of data large-scale soil surveys (d) ; *SRTM data was used for the background; Coordinate system: Pulkovo 1942 / CS63 zone X2 (EPSG:7826)*

Characterizing the structure of the soil cover, we find that the dominant soils of soils are gray forest soils, dark gray forest soils, and podzolic Chernozems. The structure of the soil cover is quite complicated and field studies are really covered with 51.4% of the area of the district (Fig. 1d). At the same time, there are many locations where large-scale soil studies were not carried out in general, but there are intensively used in agricultural production, which is also characteristic of the study area (Fig. 1c, d).

Empirical data for bulk density (***bd***), soil texture (***clay***), and humus (***hum***) content for pedotransfer modeling were obtained from two sources: part of the dataset provided by National Scientific Centre "Institute for Soil Science and Agrochemistry Research named after O. N. Sokolovsky" for provision of (Laktionova et al. 2012) – 130 values, and some dataset (Cherlinka 2001) – 144 values, 274 in summary. Soil samples were taken from the 0-30 cm layer at the end of summer-autumn, when the influence of tillage has already been eliminated and the soil density is considered to return to an equilibrium state (Dmitriyev and Makarov 1994, Nazarenko et al. 2000, Makovníková et al. 2017). Bulk density was determined by the cutting ring method according to Kachinskiy (DSTU ISO 11272:2001, European analog – ISO 11272:2017; soil texture – by pipette (DSTU 4730:2007), humus content according to the Turin's method (oxidimetric) in modification by Simakov (DSTU 4289-2004). It should be emphasized that Ukraine uses its custom scale of particle sizes, and due to the peculiarities of our database (not all fractions are represented), we will use only one fraction of physical clay with particle sizes < 0.01 mm, which we will call here and, in the future, just *clay*. The studied sample covers all types of soils of this territory involved in agricultural production. Descriptive statistics of the used database show that the averaged studied indicators are close to the soil parameters of modern agricultural landscapes of Ukraine, which are characterized by a fairly high density of the arable layer and a low humus content (Table 1).

Tab. 1. *Statistical indicators of soil bulk density, humus and clay of the database used*

Indicators	Bulk density [g·cm^{-3}]	Humus [%]	Clay [%]
Arithmetic Mean	1.33	2.64	35.70
Standard Error of the Mean	0.01	0.12	0.87
Confidence Level for Mean	0.02	0.24	1.72
Median	1.34	2.30	36.30
Mode	1.35	2.10	52.60
Standard Deviation	0.19	2.00	14.50
Sample Variance	0.04	4.01	209.00
Kurtosis Excess	1.37	10.70	-0.09
Skewness	-0.72	2.33	-0.15
Range	1.11	15.80	67.70
Minimum	0.62	0.04	2.07
Maximum	1.73	15.90	69.80
Count	274		

The created database (Fig. 2a) was used to check pedotransfer models presented in the literature (Medvedev et al. 2004, Demakov et al. 2017, Chestnykh and Zamolodchikov 2004) and to develop our own. Subsequently, the selected pedotransfer model was used to build a cartographic model of the soil bulk density. The density plot is related to a normal distribution only for clay content, for soil bulk density the distribution is intermediate between normal and asymmetric, and for humus content, it is clearly skewed (Fig. 2b). To evaluate the accuracy of the simulation, we use Sum Squared Error (SSE) is an accuracy measure where the errors are squared, then added. It is used to determine the accuracy of the forecasting model when the data points are similar in magnitude. The lower the SSE the more accurate the forecast. With this accuracy statistic, we choose which forecasting model best fits our data:

$$\mathrm{SSE}=\sum_{i=1}^{n}(Y_i-\hat{Y}_i)^2,$$

where n is count of predictions or data points, Y_i is the vector of observed values of the variable being predicted and $\hat{Y}_i$ being the predicted values.

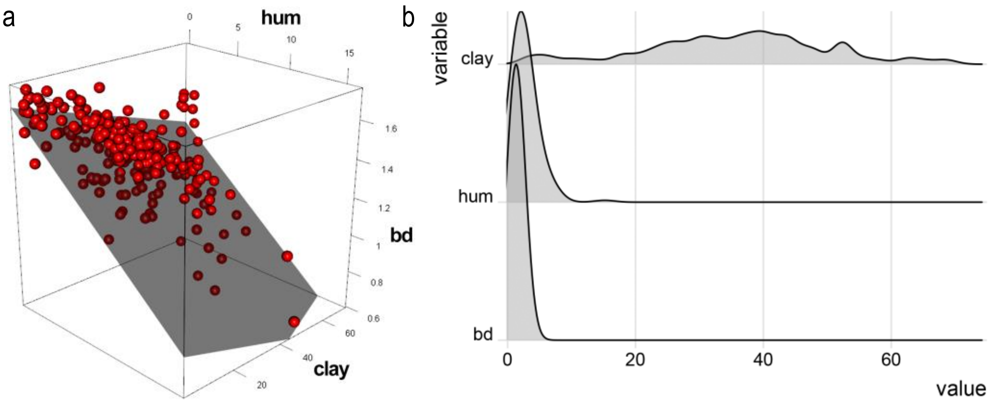

Fig. 2. *Empirical data (a) for bulk density (bd, g·cm^{-3}), soil texture (clay, %) and humus content (hum, %) for pedotransfer modeling and their density plot (b)*

Results and discussion

The set tasks (modeling and mapping of the soil bulk density), based on the current situation with soil surveys in Ukraine, were solved according to the following algorithm: 1) modeling of the map of agro-industrial soil groups (hereinafter, AISG); 2) creation of a raster map of clay content in soils based on the obtained AISG map; 3) creation of a raster map of humus content based on agrochemical soil surveys with the involvement of interpolation or modeling techniques; 4) selection of the optimal equation (pedotransfer function) of the dependence of soil bulk density on the humus and clay content; 5) implementation of the received formula in the GIS environment and construction of a map of the spatial continuous distribution of soil bulk density.

First stage

As already shown (Fig. 1d), existing soil maps do not cover the entire study area, therefore, to fill these gaps, predictive modeling with a Cohen's Kappa coefficient of 89.5% was performed (Fig. 3a). According to the ranges given by Landis and Koch (1977), the predicative results obtained by us refer to the best case, that is, they show almost complete convergence with the original ones (κ=0.81-0.99). This allows us to assess the quality of the predicative map as quite satisfactory for further work. However, we believe that there is still some potential to increase the overall κ, in particular by more precisely selecting model predictors and expanding their number by including Earth remote sensing data, maps of anthropogenic sediments, etc. Filling the gaps in the existing cartographic materials with predictive data does not exclude the need for a large-scale soil survey of such areas in the future for more accurate field verification of soil types.

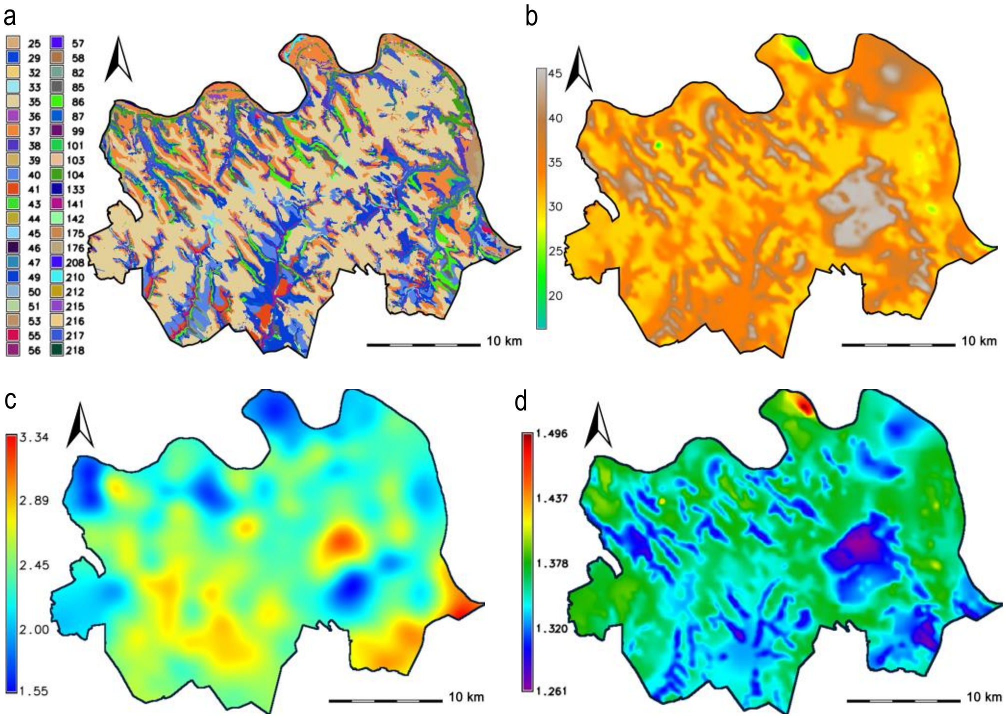

Fig. 3. *Predicted map of agro-industrial groups of soils (a, the number indicates the AISG code, the index of clay content are not specified), clay content map, % (b), humus content, % (c), and predicted bulk density map, g·cm^{-3} (d)*

Second stage

The AISG model map (Fig. 3a) is the basis for the clay content map (Fig. 3b). Modeling clay content is non-trivial, as actual laboratory measurements of clay content in soils are not carried out in the monitoring system of Ukraine. Therefore, to obtain such information, we used AISG ciphers (AISG number and letter index), which correspond to the specific granulometric composition of soils (texture) according to Kachinskiy's (DSTU 4730:2007). Accordingly, for each of the AISG's, we chose the median clay content in Kachinskiy's binomial classification, where physical clay (hereinafter, clay – the content of particles with a size < 0.01 mm, and physical sand – particles > 0.01 mm). These data (Fig. 3d) were later used by us to construct maps and calculations.

Third stage

The basis for calculating the value of the bulk density was the creation of a map of the humus content in the soil, which is one of the factor characteristics. The easiest way to create such a model is to use numerical interpolations (Li and Heap 2008, Tan et al. 2020, Liu et al. 2019). and other modeling techniques (Odeh et al. 2006, Mendonça-Santos et al. 2010, Hengl 2009). In general, the use of model options for forecasting the map of humus content looks more attractive. However, to demonstrate the proposed technology for reproducing soil bulk density values, we used a relatively simple interpolation option based on regularized splines with tension (Mitášová and Mitáš 1993, Hofierka et al. 2002). At the points where soil samples were taken and the humus content at the laboratories was determined (Fig. 1c), we created a humus content map for the studied territory by interpolation (Fig. 3c). It should be noted that in the presence of a high-resolution map of humus content, this stage can be omitted, but, for example, for Ukraine, the most detailed national map (Vyatkin et al. 2018) has a resolution of only 1 km/pixel, which is clearly insufficient for use in regional or more detailed scale.

Fourth stage

At this stage, we select the optimal equation for the dependence of soil bulk density on humus and clay content. That is, at first, we checked the developed author's pedotransfer models of the soil bulk density function using our custom database, and also developed our own. The best of the tested functions was to become the basis for modeling the continuous soil bulk density map. We took into account only equations in which the construction of the soil bulk density model was based on indicators identical to our database – humus and clay content (Medvedev et al. 2004, Demakov et al. 2017, Chestnykh and Zamolodchikov 2004), and the main idea was the assumption of the possibility of successful selection by these authors of regression equations empirically. The dependence of soil bulk density (bd) on the humus (hum) and clay (clay) content was tested according to equations (1-4, the continuous numbering of equations is given) according to Medvedev et al. (2004), (5-9) according to Demakov et al. (2017) and (10-12) according to the studies of Chestnykh and Zamolodchikov (2004).

$$bd=1.724+0.035\cdot hum+0.0006\cdot hum^2 \quad (1) \qquad bd=1.5564-0.0046\cdot clay \quad (2)$$
$$bd=1.66024+0.01021\cdot clay+0.00006\cdot clay^2 \quad (3) \qquad bd=1.27804+1.64749\cdot clay^{-1} \quad (4)$$
$$bd=1.417-0.057\cdot hum \quad (5) \qquad bd=1.13+0.37\cdot \exp(-0.649\cdot hum^{1.629}) \quad (6)$$
$$bd=1.13+0.37\cdot \exp(-0.196\cdot hum^{1.904}) \quad (7) \qquad bd=1.13+0.47\cdot \exp(-0.27\cdot hum^{1.251}) \quad (8)$$
$$bd=0.35+1.35\cdot \exp(-84.98\cdot 10^{-4}\cdot hum^{0.5}\cdot (37\cdot \exp(-62.27\cdot 10^{-6}\cdot clay)) \quad (9) \qquad bd=0.268+9.556/(hum+7.391) \quad (10)$$
$$bd=0.672+4.392/(hum+4.786) \quad (11) \qquad bd=1.064+0.246/(hum+0.276) \quad (12)$$

Checking our custom database according to equations (1-4) showed that they give significantly different results from empirical ones. Note that in the work of Demakov et al. (2017), the soil bulk density distribution diagram has a very similar character to ours (Fig. 2b), and the verification of the five dependencies (5-9) given by the authors indicates that equation (9) with the inclusion of clay as an active factor gives quite acceptable results. In particular, the range of predicted bd data is 0.74-1.62 g·cm^{-3} (SSE=9.32), which is much closer to the range in the available database of 0.62-1.73 g·cm^{-3}. Although clay is present in formula (9), its influence is quite insignificant, which is consistent with the conclusion of Demakov et al. (2017), who believe that the main factor that determines the variability of the soil bulk density is the humus content, with an increase in which the value of the density naturally decreases.

Chestnykh and Zamolodchikov (2004) give a series of dependences of soil bulk density on humus content (10-12) for different types of soils in the format bd=b_0+b_1/(hum+b_2). Equation (11) has a more universal character since significantly more calculated values are close to their empirical counterparts with SSE=5.18, which is the best of all (1-12) dependencies tested according to the literature, although the range of calculated data bd is 0.88-1.58 g·cm^{-3}, which is the second result after equation (9). As shown by previous studies (Chestnykh and Zamolodchikov 2004, Demakov et al. 2017, Medvedev et al. 2004, Nazarenko et al. 1998, Nazarenko et al. 2000), the dependence of soil density on humus, parameters of the soil absorption complex, of other factors, as a rule, has a non-linear character, which is often difficult to approximate with a certain function. Therefore, it is proposed (Dyakonov 1987, Harrell 2015) to carry out linearizing transformations of curvilinear dependencies into linear ones, which makes the selection of regression parameters much easier. We performed sixteen linearizing anamorphoses (Table 2) on the input data (bd, hum, and clay) after Dyakonov (1987).

Tab. 2. *Linearizing transformations (according to Dyakonov, (1987) of nonlinear dependencies into linear ones*

№	Type of equation	Linearizing transformations		№	Type of equation	Linearizing transformations	
		X	Y			X	Y
13.	y=A+B*X	x=x	y=y	21.	y=A*X^{B}	x=lg(x)	y=lg(y)
14.	y=1/(A+B*X)	x=x	y=1/y	22.	y=A+B*lg(X)	x=lg(x)	y=y
15.	y=A+B/X	x=1/x	y=y	23.	y=A+B*ln(X)	x=ln(x)	y=y
16.	y=X/(A+B*X)	x=x	y=x/y	24.	y=A/(B+X)	x=x	y=1/y
17.	y=A*B^{X}	x=x	y=lg(y)	25.	y=A*X/(B+X)	x=1/x	y=1/y
18.	y=A*exp(B*X)	x=x	y=ln(y)	26.	y=A*exp(B/X)	x=1/x	y=ln(y)
19.	y=A*10$^{(B*X)}$	x=x	y=lg(y)	27.	y=A*10$^{B/X}$	x=1/x	y=lg(y)
20.	y=1/(A+B*exp(-X))	x=e^{-x}	y=1/y	28.	y=A+B*(X^{n})	x=x^{n}	y=y

The verification of the pedotransfer functions of dependence of the soil bulk density on the humus and clay content presented in Table 2 was carried out alternately for each of the 16 equations. In the case of the dependence of bd on hum, the comparison of the lower and upper limits of the predicted values with the empirical results gives the best results for dependence 24, for which they are 0.68 and 1.56 g·cm^{-3} at SSE=99.02, and the correlation coefficient between the predicted and empirical data is 0.73. The dependences of soil bulk density on the clay have a similar character, and the best agreement between empirical and calculated data is given by equations (13, 17-19) and (24) with the dominance of the latter: the lower and upper limits of the predicted values are 1.05 and 1.67 g·cm^{-3} at SSE=93.41 and the correlation coefficient between predicted and empirical data is 0.64. The obtained data show that the bulk density variability is determined to a lesser extent by the clay than by humus content, which is consistent with the conclusions of Demakov et al. (2017).

Taking into account the fact that the approximation of paired dependences of soil bulk density either on the content of humus or on clay by linearizing transformations does not give correlation coefficients higher than 0.73 (and it only for humus, and clay the best of them is only 0.64), we selected a number of equations in which soil bulk density, humus and clay content are simultaneously related:

$$bd=1.6300524–0.0510298 \cdot hum–0.0047251 \cdot clay \quad (29)$$

$$bd=-3.886+422.512/(86.139+hum)+45.979/(68.260+clay) \quad (30)$$

$$bd=-0.7868+0.7339 \cdot 4.392/(hum+4.786)+666.9338/(666.9338+clay) \quad (31)$$

$$bd=1.672+1.068 \cdot 10^{-2} \cdot hum–1.371 \cdot 10^{-2} \cdot hum^2+6.914 \cdot 10^{-4} \cdot hum^3–1.071 \cdot 10^{-2} \cdot clay+6.184 \cdot 10^{-5} \cdot clay^2+2.990 \cdot 10^{-7} \cdot clay^3 \quad (32)$$

$$bd=1.685–5.791 \cdot 10^{-2} \cdot (hum)+6.943 \cdot 10^{-4} \cdot (hum^2)-8.062 \cdot 10^{-3} \cdot (clay)+5.038 \cdot 10^{-5} \cdot (clay^2) \quad (33)$$

$$bd=0.90185–0.09514 \cdot (log(hum/(100–hum)))–0.09514 \cdot (log(clay/(100–clay))) \quad (34)$$

Among the block of equations (29-34), the simplest of them is linear (29); (30) – where used the linearizing transformation (24) for humus and clay with appropriate coefficients (this type of equation is also used by Chestnykh and Zamolodchikov (2004); (31) – a construction that consists of the part of the equation of Chestnykh and Zamolodchikov (2004) for humus and selected free term and other coefficients for the physical clay content according to dependence (24); (32-33) are variants of polynomial dependences, and (34) is a variant of regression using logarithms.

Visual analysis (Fig. 4) of selected dependencies shows that the use of logarithmic functions (34) gives unsatisfactory results of matching empirical and predicted data. To facilitate the analysis of the coincidence of predicted data (X-axis) with empirical data (Y-axis), the figure displays the ideal trend line (1:1 line) with identical empirical and calculated values, the point will lie on this line, and as the discrepancies increase, the point will move away from this line: if the predicted values are overestimated relatively empirical data, the array of points will shift under this line, and vice versa; in the case of a relatively uniform error, the points will be located evenly on both sides of the line) which, under such conditions, passes from the origin of coordinates at an angle of 45 degrees. Despite the visual similarity of the results of calculations according to formulas (29-33), the absolute leader among them and all other tested dependencies (1-28) is equation (32) with R=0.792 and SSE=3.75. We propose it for further use, although it should be noted that equation (30) is also quite promising.

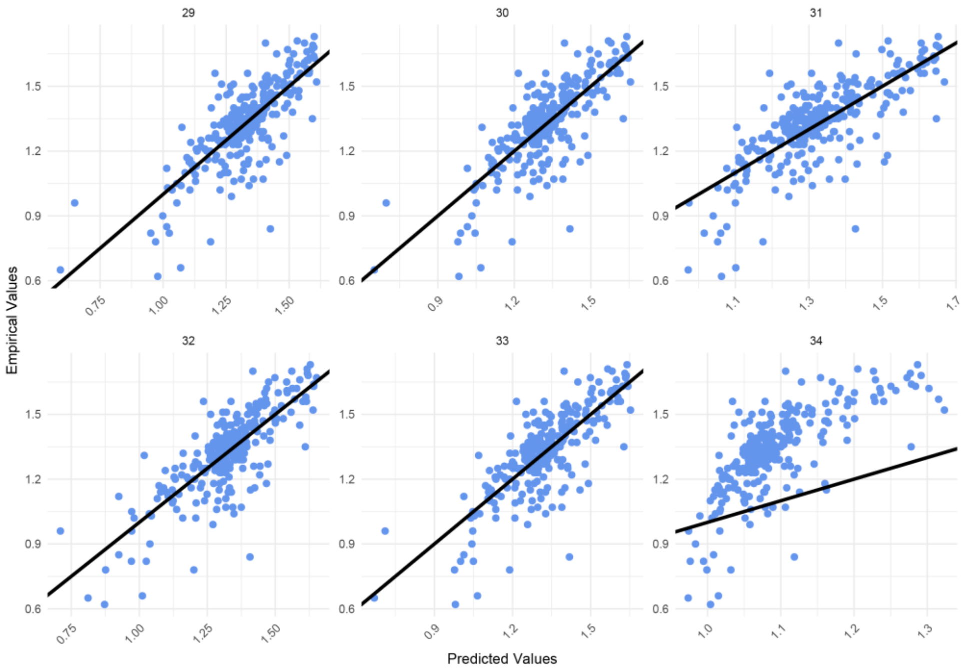

Fig. 4. *Scatter plots for dependence of soil bulk density on the humus and clay content (equations 29-34); the 1:1 line is shown black*

The fifth stage

The final stage of building a map of the continuous spatial distribution of soil bulk density involves the implementation of the selected tested equation (32) in GRASS GIS using elements of map algebra (Shapiro and Westervelt 1992). From the obtained results (Fig. 3d), first of all, we note that the predicted soil bulk density map has a range of data from 1.26 to 1.50 $g \cdot cm^{-3}$ with prevailing values from 1.30 to 1.38 $g \cdot cm^{-3}$. This map is consistent with the data by some authors (Balyuk et al. 2010, Medvedev 1997b, Medvedev et al. 2004) regarding agrophysical soil degradation in Ukraine. The combination of agrotechnological factors and the development of the processes of planar soil erosion contributed to a sharp decrease in humus reserves in the soil profile, especially in the arable layer, and the associated deterioration of the bulk density of the soil.

Therefore, the result of the proposed process is a map of the bulk density, which would otherwise be impossible to obtain quickly without expensive instrumental surveys. This is an undeniable advantage of the proposed method. At the same time, the list of factors that can affect the quality of the final bulk density models to a greater or lesser extent should be indicated. First of all, it is the reliability of the selected regression dependence formula. It, in turn, depends on the dataset of the bd, hum & clay content. The greater the range of data covered by such a sample, the better the equation can be chosen. Here, we see great prospects for future research, so in this case, it will be also possible to choose equations for different types of soils.

The second important set of factors influencing the results is the quality of the spatial modeling of humus (organic carbon) content. As we indicated above, better results can be obtained using geostatistical methods or modeling than using the interpolation method we used. However, it is quite suitable for the demonstration of the proposed method. In future articles, we plan to show more clearly the variations in the quality of the humus (organic carbon) content map depending on the method used.

And the last factor that has a great influence on the final results is the clay content map, the quality of which is directly determined by the resolution of the digital elevation model and predictors set, the source of the DEM, as well as the used prediction algorithms. A detailed review of the described impacts was carried out by us in previous works (Cherlinka 2017c, Cherlinka et al. 2020): the main results of which show that for 1:10000 scale maps, a model resolution of 5 m gives the best results, and LIDAR DEM can have better results, but in the absence of such data it has not yet been possible to verify this. It was found that reducing the resolution to 50 m leads to the loss of small details of the soil cover. At the same time, for the majority of practical tasks, and one of the main ones, where we currently see the greatest perspective – the modeling of a soil organic carbon sequestration potential map (Peralta et al. 2022) – chosen by us resolution is the most appropriate (the optimum between the quality of the results and time necessary for calculations).

Summarizing the above, the proposed workflow allows you to quickly and with minimal financial costs obtain predicted values of soil bulk density for large areas (including the scale of the whole country). At the same time, it is worth approaching each of the stages responsibly, since critical mistakes at each of them (which are not easy in themselves) can give radically different results from those in reality. When bulk density monitoring becomes possible, we recommend that the obtained model values be checked by instrumental methods during field studies. It is especially important to do this in particularly critical of bulk soil density areas, as there are high risks of the final loss of soil cover productivity in conditions of increased anthropogenic load. The resulting model maps of bulk soil density have all the prerequisites to become the basis for risk assessment and development of sustainable land use strategies both in the conditions of an individual field and for some regions or countries.

Conclusions

The analysis of 34 different models, including linearizing transformations, allowed choosing a basic polynomial regression model of dependence between soil bulk density and the humus and clay content ($bd=1,672+1,068\cdot10^{-2}\cdot hum-1,371\cdot10^{-2}\cdot hum^2+6,914\cdot10^{-4}\cdot hum^3-1,071\cdot10^{-2}\cdot$ $\cdot clay+6,184\cdot10^{-5}\cdot clay^2+2,990\cdot10^{-7}\cdot clay^3$). At the same time, the high predictive potential of the pedotransfer function of type $y=b_0+b_1/(x+b_2)$ is confirmed, which provides stable, coordinated with empirical results, what are noted by other authors as well (Chestnykh and Zamolodchikov 2004).

The simulation of soil bulk density was tested in a test area using the database of the humus and clay content. Five stages os the modeling were defined:

1. Creating a prognostic of agro-industrial soil groups data layer using several predictors and Random Forest algorithm.
2. The clay content data layer is modeled using the AISG data layer.
3. The results of agrochemical research are used for modeling the data layer of the humus content in soils by the means of interpolation (or another method of spatial prediction).
4. Estimate the reliability of the empirical dependence of soil bulk density and the humus and clay content.
5. Implement the selected empiric dependence into GRASS GIS to generate a model of the spatial distribution of soil bulk density.

At the same time, parameters for improving the quality of soil bulk density models have been established. First of all, this is the data amount was increased in bd, hum & clay to improve the reliability of the regression model, and in the best case – and the selection of the equation for different types of soils. Next, the quality of spatial modeling of humus (organic carbon) content was improved using geostatistical methods and modeling. The last parameter that has a great influence on the final results is the clay content data layer, the quality of which is directly determined by numerical factors (resolution of DEM and predictors set, source of DEM, predictive algorithms). For highly detailed maps at the scale of a single field, DEM and predictors with a resolution of 5 m or less should be used. We plan to investigate all of the above in further research, including LIDAR as the main source of altitude data.

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Authors´ affiliation

Vasyl Cherlinka
Pavol Jozef Šafárik University in Košice,
Faculty of Science, Institute of Geography,
Jesenná 5, 04001 Košice, Slovakia,
EOS Data Analytics,
Mountain View CA, USA
vasyl.cherlinka@upjs.sk

Yuriy Dmytruk
Podilskyi State University,
Department of ecology and general biological disciplines,
Khmelnytskyi region, Kamianets-Podilskyi,
st. Shevchenko 12, Ukraine, 32316
dmytruk.yur@gmail.com

Liubov Cherlinka
Yuriy Fedkovych Chernivtsi National University,
Institute of Biology, Chemistry and Biotechnology,
Department of Ecology and Biomonitoring, Chernivtsi,
Lesya Ukrainka str., 25, Ukraine, 58012
cherlinka.liubov@chnu.edu.ua

Mykhailo Gunchak
Soil Protection State Institute of Ukraine,
Chernivtsi branch, vul.Heroyiv Maydanu 194-A,
Chernivtsi, Ukraine, 58029
chernivtsi@iogu.gov.ua

Volodymyr Sobko
Soil Protection State Institute of Ukraine,
Khmelnytskyi branch, Khmelnytskyi region,
Kamianets-Podilskyi, vul.Timiryazyeva 114,
Ukraine, 32300
khmelnitsky@iogu.gov.ua