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Development of ternary diagrams for estimating water retention properties using geostatistical approaches

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ABSTRACT

Most pedotransfer functions (PTFs) have adopted soil texture information as the main predictor to estimate soil hydraulic properties, whether inputs are defined in terms of the relative proportion of different grain size particles or texture-based classifications. The objective of this study was to develop ternary diagrams for estimating soil water retention (θ) at −33 and −1500 kPa matric potentials, corresponding to the field capacity and wilting point, respectively, from particle size distribution using two geostatistical approaches. The texture triangle was divided into a 1% grid of soil texture composition resulting in 4332 different soil textures. Measured soil water retention values determined in 742 soil horizons/layers located in Portugal were then used to develop and validate the hydraulic ternary diagrams. The development subset included two-thirds of the data, and the validation subset the remaining samples. The measured soil water content values were displayed in the ternary diagram according to the coordinates given by the particles size distribution determined in the same soil samples. The volumetric water content values were then predicted for the entire ternary diagram using two different geostatistical interpolation algorithms (ordinary kriging and the empirical best linear unbiased predictor). Uncertainty analysis resulted in a root mean square error below 0.040 and 0.034 $cm^3\ cm^{-3}$ when comparing the interpolated water contents at −33 and −1500 kPa matric potential values, respectively, with the measured ones included in the validation dataset. The estimation variance calculated with both methods was also considered to access the uncertainty of the predictions. The available water content of Portuguese soils was then derived from $\theta_{-33\ kPa}$ and $\theta_{-1500\ kPa}$ ternary diagrams developed with both approaches. The hydraulic ternary diagrams may thus serve as simplified tools for estimating water retention properties from particle size distribution and eventually serve as an alternative to the traditional statistical regression and data mining techniques used to derive PTFs.

1. Introduction

Modern hydrologic modeling studies require a quantitative and precise understanding of soil hydraulic properties. That information is essential for a wide range of applications, such as research on soil and water conservation, irrigation scheduling, solute transport, virus and bacterial migration, plant growth, and plant stress. However, classic methods for direct measurement of soil hydraulic properties (Dane and Topp, 2002) are known to be costly, time consuming, and impractical for large-scale applications in which many samples are required to quantify the spatial and temporal variability of those properties. Hence, pedotransfer functions (PTFs) have been developed as an alternative to classical methods to indirectly estimate soil hydraulic properties from basic soil physical and chemical properties (Bouma, 1989; McBratney et al., 2002; Pachepsky and Rawls, 2004; Vereecken et al., 1989), thus overcoming some of the limitations mentioned earlier, especially when the objective is to characterize soil hydraulic properties at large scales.

Most of the available PTFs use soil-texture-based information as the main predictor to estimate the hydraulic behavior of soils. This popular option is justified by the fact that soil texture characteristics are among the most easily measured soil properties, and also by the assumption that soil texture is the dominant soil variable in determining hydraulic properties, while other soil variables, such as bulk density or organic matter content, have a secondary effect (Twarakavi et al., 2010). The simplest texture based PTFs were developed to provide estimates of average soil water retention properties or hydraulic parameters for different texture classes (e.g., Al Majou et al., 2008; Bruand et al., 2003; Ramos et al., 2013; Schaap and Leij, 1998; Wösten et al., 1995). More complex functions have also been developed by relating the particle size limits of the soil constituents to soil hydraulics using multiple regression analysis or data mining tools (e.g., Gupta and Larson, 1979;

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Haghverdi et al., 2012; Nemes et al., 2006; Saxton et al., 1986; Schaap et al., 2001). Although the hierarchical approaches followed in many of those studies showed that the accuracy of PTFs improved considerably when other variables (usually bulk density), rather than soil texture information alone, were used also as predictors, texture based PTFs have been considered to also provide reasonably accurate estimates of soil hydraulic properties for many research and technical applications (Vereecken et al., 2010).

Soil texture is normally represented in a ternary diagram, function of sand, silt and clay percentages, where the limits of the texture classes vary according to the texture classification system used. However, the soil texture triangle has also had more applications than simply grouping texture information data, namely it has also been used as a tool to estimate soil hydraulic properties. Saxton et al. (1986) divided the soil texture triangle into grids of 10% sand and 10% clay content increments to develop texture based PTFs for generalized predictions of soil hydraulic properties in each grid cell. Later, Saxton and Rawls (2006) updated the previous work to further include the effect of organic matter, bulk density, gravel, and salinity in their model and provide a broadly applicable predictive system. The developed model has been successfully applied to a wide variety of analysis, particularly those related to agricultural hydrology and water management, since estimates do not involve complex mathematical methods, and the texture triangle serves as a familiar tool to users for estimating the soil water characteristics. Twarakavi et al. (2010) also focused on the relations between the texture triangle and soil hydraulic properties. Those authors estimated soil hydraulic properties throughout the entire soil texture triangle as a function of sand, silt, and clay contents using the ROSETTA PTFs (Schaap et al., 2001) such that the various soil texture possibilities (i.e., combinations of sand, silt, and clay percentages) were considered. They then concluded that although the soil texture triangle was qualitatively very similar to the soil hydraulic triangle, differences existed especially for soils where capillary forces dominate the flow throughout the soils. Bormann (2007) took those studies one step forward and performed water balance calculations for the entire space of the soil texture triangle, after dividing it into 1% grid cells and applying Rawls and Brakensiek (1985) PTFs for obtaining the soil hydraulic properties.

Following those studies on the prediction of soil hydraulic properties for the entire space of the soil texture triangle, we propose a novel geostatistical approach to obtain the spatial distribution of water retention values (the field capacity and wilting point) available in a soil database (Gonçalves et al., 2011). Our work presents the application of two geostatistical methods, one using ordinary kriging (Goovaerts, 1999, 2001) and the other using the empirical best linear unbiased predictor (EBLUP) based on residual maximum likelihood (REML) estimation of the spatial variance model as proposed by Lark et al. (2006). This second method includes the texture PTF as a trend model. Although there are countless applications of these methods in soil science, as far as we know these estimators have never been used as PTFs to actually derive soil hydraulic properties from basic soil data. To proceed with this study, three very basic concepts were established:

(i) Soil texture and soil water retention properties available in the database were assumed as being determined in the same sample. This is usually not the case in most PTFs where the predictors used in their development, although measured in the same soil horizon, are not always determined directly on the soil samples used for measuring the hydraulic properties. As referred by Vereecken et al. (2010), this becomes more important as the spatial and temporal variability of additional soil information increases and the information content is not related anymore to the samples on which the hydraulic properties were determined. Thus, taking into account the size of the database used in this study, the error resulting from this assumption was not considered to be relevant.

(ii) Soil texture was considered the main predictor to estimate soil hydraulic properties. As mentioned earlier, this is the main assumption sustaining all texture based PTFs since these two soil properties normally exhibit a high correlation.

(iii) The spatial continuity of soil hydraulic properties along the soil texture triangle can be described by means of a variogram. Taking into account that soil texture is the main soil property considered when grouping soils having similar water retention curves (Bruand et al., 2003; Ramos et al., 2013; Wösten et al., 1995), and that the soil texture triangle and the soil hydraulic triangle can be relatively similar (Twarakavi et al., 2010), we assumed that there could be a spatial dependence of soil hydraulic properties, at least within the limits of each soil texture class.

The objective of this study is thus to develop ternary diagrams for estimating point specific water retention values (the field capacity and wilting point) of Portuguese soils using two geostatistical approaches: ordinary kriging (OK), and the empirical best linear unbiased predictor (EBLUP). The available water capacity was later computed from both ternary diagrams derived from each approach.

2. Material and methods

2.1. Soil dataset

The ternary diagrams were developed for estimating the field capacity and wilting point of Portuguese soils from particle size distribution. The field capacity and wilting point were here assumed to correspond to the water retention values at −33 and −1500 kPa, respectively (Romano and Santini, 2002). The data was extracted from the PROPSOLO soil database (Gonçalves et al., 2011), which gathers all information on soil hydraulic and pedological properties from soil profiles obtained from research projects and academic studies performed at the Portuguese National Institute of Agronomic and Veterinarian Research (formerly Estação Agronómica Nacional). This database contains practically all of the existing knowledge on the soil hydraulic properties of Portuguese soils.

The data included information on soil texture and water retention properties of 742 horizons/layers studied in 346 soil profiles located in Portugal between 1977 and 2012 (Fig. 1). It comprised 331 topsoil (0–30 cm depth) and 411 subsoil (>30 cm depth) horizons. The soil reference groups (FAO, 2006) represented were Fluvisols (36.4%), Luvisols (29.5%), Vertisols (9.8%), Cambisols (8.7%), Calcisols (6.6%), Anthrosols (4.0%), Arenosols (1.4%), Podzols (0.9%), Regosols (0.9%), Ferralsols (0.6%), Leptosols (0.6%), and Planosols (0.6%).

The data was randomly divided into two subsets, a development set composed of two-thirds of the data (495 horizons/layers), and a validation set with the remaining one-third of the data (247 horizons/layers). Table 1 presents the main physical and chemical properties of the two datasets. The particle size distribution was obtained using the pipette method for particles having diameters <2 μm (clay) and between 20–2 μm (silt), and by sieving for particles between 200 and 20 μm (fine sand) and between 200 and 2000 μm (coarse sand). These textural classes follow the Portuguese classification system (Gomes and Silva, 1962) and are based on the International Soil Science Society (ISSS) particle limits (Atterberg scale). The dry bulk density (ρ_b) was obtained by drying volumetric soil samples (100 cm^3) at 105 °C for 48 h. The gravimetric water content at −33 kPa matric potential was determined on undisturbed soil samples (100 cm^3) using suction tables (Romano et al., 2002; used in 494 horizons/layers) or the pressure plate apparatus (Dane and Hopmans, 2002; used in 212 horizons/layers). The gravimetric water content at −1500 kPa matric potential was also determined on undisturbed soil samples (100 cm^3) using the pressure plate apparatus. Then, the volumetric water content for each horizon/layer and each matric potential was computed from the gravimetric water contents and the bulk density of the corresponding horizon/layer.