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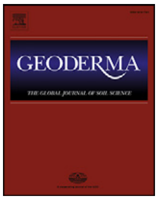

Implementation of a sigmoid depth function to describe change of soil pH with depth

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ABSTRACT

Soil pH controls the availability of the majority of plant nutrients, if not all, and determines the growth environment for plant roots. Profile depth functions have been used to represent the vertical distribution of soil attributes and to predict them at continuous depths. This paper proposes a new model to predict pH for a whole soil profile. Soil properties including pH are often similar within the plow layer from mixing during tillage and other agricultural operations. Similarly, soil pH below the root zone tends to be uniform due to low disturbance, leaving a transition zone from the bottom of the tillage layer to the bottom of the root zone due to depth-dependent root density and related soil processes. Keeping this physical description of agricultural field soil profile in mind, a closed form equation (model) was developed similar to a sigmoid curve. The model has 4 parameters including 1) soil pH at the top of a soil profile, 2) soil pH at the bottom of a soil profile, 3) hillslope parameter representing steepness of the curve that is determined by the length of the root zone, and 4) inflection point representing almost the midpoint of the transition zone or root zone. A total of 32 soil cores down to about 1.1 m depths were collected from an agricultural field of Macdonald farm, McGill University. The sub-samples were taken at every 10 cm and analyzed for soil pH in soil: water suspension in the laboratory. The measured pH was used to test the fitting performance of the sigmoid model. Additionally, a global dataset with 432 profiles with various soil classes, drainage types, land use, and altitude was also used to test the generality of the new model. The performance of this model was compared with the results of the commonly used 3rd order polynomial regression function and the equal-area quadratic spline function. Good performance of the sigmoid model with explicit physical explanation showed promise in predicting soil pH at depths. The spline function had the highest accuracy but lacked a general trend in its shape and parameters. The polynomial function had good accuracy and displayed a non-monotonic trend, which can also be used as a substitute for some profiles with complex variability.

1. Introduction

Soil pH is an important soil quality index and controls the plant nutrient availability, growth environment of plant roots, soil microbial activities, and many chemical processes that take place in soil (Aciego Pietri and Brookes, 2008; Kahlert et al., 2004). Agricultural management decisions are often constrained to surface soil pH measurements due to the convenience and ease of sample collection. However, as the plant roots can reach subsoil and even deep soil, the measurement of soil pH at depths is important for understanding the rhizosphere environment, and chemical and biological activities. Various soil forming factors (Jenny, 1941), such as parent material, organism, and climate, combined with management activities, like fertilizer and manure application, and tillage, contribute together to the variability of soil pH. Quantitative information on the spatial variability of soil pH, sometimes displayed as digital soil maps, plays an essential role in site-specific agricultural management such as lime requirements, and soil quality assessment. Additionally, 3D digital soil mapping combining horizontal maps and profile depth functions becomes increasingly popular and important for understanding three-dimensional spatial variability and its relationship to other soil properties (Liu et al., 2013).

Profile depth functions are based on the premise that soil properties vary continuously with depths in a profile (Russell and Moore, 1968). The variability has been modelled by various depth functions, ranging from a freehand curve created by Jenny (1941), to more sophisticated models, such as exponential decay functions (EDFs) (Minasny et al., 2006), polynomial functions (Veronesi et al., 2012), power functions (Liu et al., 2016), and equal-area quadratic spline functions (EAQSFs)

Abbreviations: 3D, three dimension; EDF, exponential decay functions; EAQSF, equal-area quadratic spline functions; SOC, soil organic carbon; SOM, soil organic matter; EC, electrical conductivity; RMSE, root mean squared error.

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(Bishop et al., 1999). The EAQSFs, fitted by a set of local quadratic polynomials for each horizon, describe a smooth curve through horizon mid-points (McBratney et al., 2000). Spline functions were reported to have the highest accuracy due to higher flexibility and feasibility (Webster, 1978). The EAQSF has been widely and successfully used to model the vertical distribution of various soil properties, including soil organic carbon, available water capacity, soil texture, bulk density, soil salinity, and soil pH (Adhikari et al., 2014; Bishop et al., 2015; Lacoste et al., 2014; Malone et al., 2009; Odgers et al., 2012; Taghizadeh-Mehrjardi et al., 2014). However, without an explicit mathematical formula and a consistent set of parameters, EAQSF is simply a numerical and graphical fitting of horizon data, which changes its shape from profile to profile. Such function individually fits the profile data well but lacks a general trend and the physical explanation of soil-landscape relationship (Liu et al., 2016). Therefore, more effective depth functions with definite mathematical formulas, and clear and general tendency should be searched for specific soil properties.

The EDFs have been used to model the vertical distribution of soil organic carbon content (SOC) basing the fact that higher SOC is present in the topsoil and gradually decreases in the profile (Minasny et al., 2006). Later the EDFs have been modified by involving the integral form (Mishra et al., 2009), segmenting the functions with a constant presenting plow layers (Kempen et al., 2011; Meersmans et al., 2009), and creating a normalized form (Wiese et al., 2016) to take into account practical issues and represent site-specific profiles. However, the monotonic and steady decreasing trends of the EDFs limit their application for other soil properties. In recent years, more and more mathematical models are proposed to delineate the vertical distribution of various soil properties, including a 6th order polynomial regression functions to represent soil compaction (Veronesi et al., 2012), a linear function with Tikhonov regularization (TR) to describe soil EC (Li et al., 2013), and another power function to describe SOC (Liu et al., 2016). Moreover, Minasny et al. (2016) reviewed several common types of parametric and nonparametric depth functions, including uniform, gradational, exponential, wetting front, abrupt, peak, and MiniMax; some of which only have graphical fitting and lack mathematical formulas. Even though these depth functions fit well, the generality of these functions still need further exploration, and the physical explanation of the parameters needs improvement to represent the effect of pedological process and management activities.

Every soil property has its unique vertical distribution which could be modelled by specific depth function (Jenny, 1941). However, soil pH has not been widely recognized for its vertical variability and modelled by explicit equations. Yet few papers used data or graphs to qualitatively show the vertical trend of pH values. For example, Chi et al. (2010) reported an increasing soil pH with depth in reclaimed rice land and soybean land. The EAQSFs have also been used to model the vertical distribution of soil pH for digital soil mapping (Adhikari et al., 2012; Bishop et al., 1999; Odgers et al., 2015). However, the EAQSF fits soil profile individually and lacks generality. Moreover, considering the physical condition of agricultural fields, three types of variability in soil pH may persist with depth: 1) a relatively uniform condition in the plow layer due to the mixing effect of tillage and other agricultural operations, 2) a relatively uniform condition in the bottom layer due to non-disturbance and possible consistent groundwater effect, and 3) a transition layer in between. Soil pH should be fitted with a more general and appropriate function that can better describe the variability with depth.

The goal of this study was to develop a sigmoid-based model representing change of soil pH with depth and test its applicability. More specifically, the objectives were: 1) to develop a sigmoid-based model using soil profiles from a specific agricultural field (using a local dataset); 2) to apply this model to a global soil pH dataset and to quantify its performance; as well as 3) to compare the sigmoid-based model with the polynomial regression and a spline method, as commonly used alternatives.

2. Materials and methods

2.1. Study area

A field experiment was conducted in Field 26 (11 ha) of Macdonald Farm, McGill University, Quebec, Canada (45.4°N and 73.9°W) (Fig. 1). The landscape of the farm locates on two rolling plateaus formed by thousands of years' carving of Ottawa River, resulting in various soil types and providing a good test bed for model validation. Soil types of Field 26 are highly variable and range from the deep organic deposit (peat) over the shallow organic deposit to mineral soils with dominant textures including sand, light sandy loam, ill-drained sandy loam, loam, silt loam, and clay loam. Soils in Field 26 are classified into multiple soil series including Muck, ST-Zotique, Soulanges, ST-Damase, Uplands, Chicot, Farmington, Chateauguay, and Macdonald following the Canadian Soil Classification System. The elevation of Field 26 ranges from 6.88 to 9.22 m above sea level and the long-term (30 years) average annual air temperature is 6.2 °C and average annual precipitation is 979 mm. Field 26 was under corn-soybean rotation and the crop previous to sample collection was soybean.

2.2. Sample collection and analysis

A total of 32 georeferenced soil cores (Fig. 1) down to about 1.1 m depth were collected using a truck-mounted hydraulic soil profiler (Veris® P4000 soil profiler, Veris technologies Inc., Salina, KS, USA) following a modified nested grid sampling design to obtain a good spatial coverage in November 2014. The soil cores were subsampled at every 10 cm layer. Two soil profiles were dug only to 30 cm restricted by rocks occurring at a shallow depth. A total of 284 samples were sealed in Ziploc bags and transported to the laboratory for analysis.

Air-dried and ground (particle size < 2 mm) samples were used for soil pH determination in a soil-water solution of 1:2 soil to water ratio (1:4 for organic soil). Since the samples were taken at 10-cm depth intervals, the measured pH values represented the average values of 10 cm soil horizons and marked as the pH value at mid-point of each soil horizon.

2.3. Sigmoid model

A sigmoid-based model was adopted in this research as follows:

$$f(x) = s + \frac{d-s}{1+\left(\frac{x}{\alpha}\right)^{-k}} \tag{1}$$

where $f(x)$ was the soil pH, and x was the soil profile depth (cm), s and d represented the soil pH at the top and bottom of soil profiles, respectively, α was the depth of inflection point (i.e., the middle of the transition zone), and k was the steepness of the curve related to the thickness of the expected transition soil layer. A possible approach to estimating s and d is to impose the two parameters in the sigmoid function by measured values of soil pH at the top and bottom of soil profiles.

2.4. Depth functions

The sigmoid model was compared with the commonly used 3rd order polynomial regression function and the EAQSF.

For 3rd order polynomial regression function used in this study was:

$$f(x) = a + b \times x + c \times x^2 + d \times x^3 \tag{2}$$

where a, b, c, and d were four parameters of the polynomial function. The 3rd order polynomial function was chosen in this study because similarly to the sigmoid, it has a single deflection point. The sigmoid and 3rd order polynomial functions were fitted by minimizing RMSE