Peak functions for modeling high resolution soil profile data

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A B S T R A C T

Parametric and non-parametric depth functions have been used to estimate continuous soil profile properties. However, some soil properties, such as those seen in weathered loess, have anisotropic peak-shaped depth distributions. These distributions are poorly handled by common parametric functions. And while nonparametric functions can handle this data they lack meaningful parameters to describe physical phenomena in the depth distribution of a property such as a peak, an inflection point, or a gradient. The objective of this work is to introduce the use of asymmetric peak functions to model complex and anisotropic soil property depth profiles. These functions have the advantages of providing parameters, which quantify or describe pedogenic processes. We demonstrate the application of the Pearson Type IV (PIV) and the logistic power peak (LPP) functions to high resolution soil property depth profiles measured by diffuse reflectance spectroscopy in a claypan soil landscape of Northeastern Missouri, USA. Both peak functions successfully fit clay, silt, and pH data for an example soil profile from a summit landscape position (R² = 0.90 for pH and 0.98 for silt and clay). The LPP function was further demonstrated to fit clay depth distribution for a shoulder, backslope, footslope, and a depositional landscape position (R² = 0.98, 0.96, 0.96, 0.91). Relationships between the fitted parameters of these profiles were useful to describe landscape trends in their morphological features and show promise to continuously describe pedogenic processes in three dimensions. Peak functions are a useful companion to high-resolution soil profile data collected by sensors and their combined use may allow more intensive mapping and better explanation of soil landscape variability.

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1. Introduction

Several methods have been proposed to approximate soil property depth distributions with empirical functions, including: linear and polynomial functions, exponential and logarithmic functions (Cook and Kelliker, 2006; Dwyer et al., 1988), and orthogonal polynomials (Colwell, 1970). However, some soil profiles, such as those seen in weathered loess, have anisotropic peak-shaped depth distributions for certain soil properties. Anisotropy refers to the skewed depth variation of soil profile properties occurring mainly due to the gravitational vector of profile weathering and development (Hole, 1961). Modeling a peaked and anisotropic soil profile with a parametric function is problematic, in part due to the sparse and discrete nature of soil profile data. This is the case for soils formed in weathered loess landscapes where the processes of lessivage and eluviation/illuviation have led to the anisotropic profile distribution of clay (Fig. 1), silt, cations, pH, phosphorous, bulk density, and available water capacity, among other soil properties (Myers et al., 2007). The empirical functions that have been utilized are limited in their capability to smoothly fit such peaked and anisotropic soil profile data.

Non-parametric functions often have more flexibility to model complex features of depth profiles. Some non-parametric techniques useful for modeling soil profile properties are local regression (Cleveland and Devlin, 1988; Myers et al., 2007), generalized additive models (Hastie and Tibshirani, 1990), splines (Webster, 1978), and pycnophylactic or area-preserving splines (Bishop et al., 1999; Ponce-Hernandez et al., 1986). However, unlike parametric functions, these non-parametric techniques cannot quantitatively describe critical structures in a soil depth profile, such as a gradient, a relative minimum or maximum, or an inflection point.

1.1. From horizons to high resolution: the role of sensors

The measurement of soil profile properties by discrete intervals or genetic horizons has been the de facto mode of operation in soil science for two main reasons. First, soils often have clear horizons that
appear uniform in their texture, color, or structure. Secondly, field sampling and lab analysis are very costly to implement and horizon-based sampling offers a reasonable compromise between expense and information. Colwell (1970) noted that although soil properties are generally portrayed as discrete step functions, their distributions are continuous and may not strictly correlate with the discrete depth interval chosen. For instance, a horizon designated due to a color change may not have any change in texture or other functional soil property. Discretizing soil profiles also reduces the amount of information available to reconstruct the underlying continuous depth functions of a soil property. However, with the increased use and commercialization of soil sensors, rapid and high resolution measurements of soil property depth distributions are possible at many more locations than reference lab procedures.

Soil property sensors on mobile penetrometer platforms can make soil profile measurements in situ. If successfully calibrated, sensors can estimate soil properties at many more locations than reference lab procedures, and at much finer depth resolution. Examples of such penetrometer based sensing technologies include: cone index (CI) (Grunwald et al., 2001; Perumpral, 1987; Richards, 1941), shaft friction sleeve (Lunne et al., 1997), bulk apparent soil electrical conductivity (ECa) (Drummond et al., 2000), acoustic cone penetrometer (Houlsby and Ruck, 1998; Villet et al., 1981), water content by time or frequency domain waveguides (Kosugi et al., 2009; Sun et al., 2004; Topp et al., 2003), visible spectrum video or digital cameras (Lieberman and Knowles, 1998; Rooney et al., 2001a,b), and near infrared (NIR) or visible/near-infrared (VNIR) diffuse reflectance spectroscopy (DRS) (Hummel et al., 2004; Kweon et al., 2009). Several of these penetrometer technologies may be employed in combination to rapidly and comprehensively characterize soil profiles (Rooney et al., 2002). However, mathematical techniques are needed to provide meaningful interpretation of the resulting high resolution soil profile data.

1.2. Asymmetric peak functions

Peak functions have been used to analyze the signals produced in analytical techniques such as chromatography (Foley, 1987) and voltammetry (Huang et al., 1995; Torres-Lapasió et al., 1997). Several peak functions are potentially useful for modeling soil profile data. Comprehensive lists of candidate functions can be found in Abramowitz and Stegun (1964), Systat (2002), and Romanenko et al. (2006). Many peak functions are related by common components, can be generalized to a mother function, or are part of a family of functions, such as extreme value functions. Some peak functions are asymmetric, exhibiting separate behavior on either side of a maxima or minima. This behavior provides, for instance, a different shape for a soil property depth function above or below a critical feature such as the peak clay content in a series of argillic horizons. Thus, these functions are good choices for modeling the depth-dependent properties of some anisotropic soil property depth profiles. Of these functions, two are given further examination here, the Pearson IV (PIV) and the logistic power peak (LPP). Our first objective for this research was to evaluate and demonstrate the use of the PIV and LPP asymmetric peak functions to model the depth distribution of high-resolution VNIR-DRS measured clay, silt, and pH in a loess mantled summit profile. Our second objective was to demonstrate the use of the LPP function for modeling a toposequence of five high-resolution clay profiles in the same loess mantled landscape.

2. Materials and methods

2.1. Study area

The soil profiles used to develop sensor calibrations and to demonstrate peak functions in this study were taken from the loess-covered glacial-till landscapes of Northeastern Missouri, USA. This region is known as the Central Claypan Area (USDA-NRCS, 2006). Soils formed here tend to be Alfisols and Mollisols with well-expressed argillic horizons. A relatively thin blanket of loess covers glacial till and varies in thickness by landscape position. The thickest loess deposits occur on summits (1 to 2 m). These aeolian deposits thin or disappear on backslopes depending on the degree of slope and severity of erosion. Abluval argillic horizons – giving rise to the term ‘claypan soil’ – form in the loess, mainly on summits, shoulders, and upper backslopes. Clay content commonly exceeds 60% at its peak value in these horizons. Profiles at footslope and toeslope positions are composed of thick (1 to 2 m) loess-derived colluvial sediments having lower peak clay content, much deeper in the profile (Fig. 1). Pedosediment and glacial till occur below the loess throughout the landscape and a paleosol commonly exists in these secondary parent materials.

The profiles used to demonstrate peak functions occurred in a small watershed on flat to gently rolling landforms at the University of Missouri Greenly Research Center near Novelty Missouri, USA (Lat. 40.0302°, Lon. −92.188°). A representative toposequence of five profiles was chosen to demonstrate the use of peak functions. The profiles occurred along a transect of five landscape positions: 1. summit, 2. shoulder, 3. backslope, 4. footslope, and 5. toe slope. Summit and shoulder sites were in a Putnam silt loam, 1 to 3% slopes (Fine, smectitic, mesic Vertic Albaqualfs). The backslope was in a Kilwining silt loam, 1 to 5% slopes (Fine, smectitic, mesic Vertic Epiqualfs). The footslope and toeslope sites were in an Armstrong loam, 5 to 9% slopes (Fine, smectitic, mesic Aquert Hapludalfs). The locations of these sites are indicated on an elevation contour map of the watershed (Fig. 2a). A cutaway view (Fig. 2b) demonstrates the geomorphic position of the profiles on the landscape and their general parent material and argillic horizon relationships.

2.2. Sensor-measured high-resolution soil profile data

High resolution depth profiles of clay, silt, and pH were measured by calibrated VNIR-DRS. The calibration dataset was collected from 74 sites in four different fields from the Central Claypan Area, including the study site. Soil cores (4.5 cm × 1.2 m) were obtained from each site. These cores were segmented into 2.54-cm increments (n = 3100) providing a precision depth support for sensor and lab measurements. Diffuse reflectance spectra (350 to 2500 nm) were collected from the
air-dry crushed and sieved (<2 mm) core segments (FieldSpec Pro FR, ASD Inc., Boulder, CO). To develop a representative calibration dataset, the scanned core segments were stratified by horizon, horizon boundary, and parent material. A random selection of samples from these strata (n=675) was prepared for reference lab measures and calibration procedures. A further 70/30 random split was applied to produce a calibration (n=430) and an independent testing dataset (n=185). Lab measurements included clay and silt content by hydrometer, and pH in 1:1 soil:water suspension. [See Myers (2008) for a fuller description of this dataset.]

Spectra were dimensionally reduced by decomposition into principal components via robust projection pursuit (Croux et al., 2007). Robust projection minimizes the leverage outliers have on important projection vectors. The three measured soil properties were calibrated to the robust principal components by least angle shrinkage and selection operator (LASSO) regression (Tibshirani, 1996). Best LASSO parameters were chosen to minimize the Mallows $C_p$ statistic which optimized effective degrees of freedom and residual sum of squared deviation of the model. LASSO regression provides an automatic variable selection and weighting (coefficient shrinkage), obviating the need for the arbitrary selection of principal components for regression calibrations. These best models were then applied to the VNIR-DRS measurements of 2.54-cm segments of the five pedons used in this study resulting in high-resolution depth profiles of clay, silt, and pH. The peak functions were subsequently fit to these depth profiles.

### 2.3. The Pearson IV asymmetric peak function

The Pearson family of distributions (Heinrich, 2004; Pearson, 1895, 1901, 1916) can flexibly model a wide variety of peak-shaped data.
The Pearson Type IV (PIV) asymmetric probability density function (1) can handle extensive tails with a minimal number of parameters.

$$y = \alpha + \beta \left( 1 + \left( \frac{x - \ln(e) - \mu}{\delta} \right)^2 \right)^{-e}$$
$$\exp\left( -\eta \left( \frac{x - \ln(e) - \mu}{\delta} \right) + \left( \frac{\eta^2}{\delta^2} \right) \right) \left( 1 + \frac{\eta^2}{\delta^2} \right)^{-e}$$

where \(x\) is a vector of profile depths and \(y\) is a soil property vector. The parameters are the intercept (\(\alpha\)), amplitude (\(\beta\)), peak maximum (\(\alpha + \beta\)), peak center (\(\mu\)), peak width (\(\delta\)), and \(e\) and \(\eta\), which control the shape of the peak. The last three parameters interact to give great flexibility in modeling a range of asymmetric peak shapes. Parameter count can be reduced by excluding the intercept term, thus allowing the \(\beta\) term to contain the entire peak amplitude, and \(\mu\) can quite often be supplied by simple observations or by high-resolution sensor soundings.

2.4. The logistic power peak function

The logistic power peak (LPP) function is given by the following Eq. (2) (Systat, 2002).

$$y = \alpha + \frac{\beta}{\mu} \left( 1 + \exp\left( \frac{x + \delta \ln(e) - \mu}{\delta} \right) \right)^{\frac{-1}{\varepsilon}}$$
$$\exp\left( \frac{x + \delta \ln(e) - \mu}{\delta} \right) \left( 1 + \frac{1}{\varepsilon} \right)^{\frac{-1}{\varepsilon}}$$

where \(x\) is a vector of depths and \(y\) is a soil property vector. Again the \(\alpha\) parameter is the intercept, \(\beta\) is the amplitude, \(\alpha + \beta\) is the magnitude of the peak, \(\mu\) is the peak center, \(\delta\) controls the width of the peak and interacts with \(\varepsilon\) to control the asymmetry of the peak. As with the PIV function, parameter count can be reduced by excluding or providing the \(\alpha\) term, and/or providing \(\mu\).

2.5. Peak function fitting

The PIV and LPP functions were fit to the first 1 m of the high-resolution soil profiles for clay, silt, and pH using the Levenburg-Marquardt non-linear regression algorithm with a median absolute deviation objective function (Systat, 2002). The functions were fit with intercepts and without fixing the peak center parameter. Reasonable starting values were supplied for the \(\alpha\), \(\beta\), and \(\mu\) parameters to improve convergence. Regression weights were applied to reduce the impact of secondary parent materials in the lower portion of the profiles and to focus the fits on the upper limb and peak of the depth function. Regression weights were calculated by Eq. (3).

$$w = 1 - (x / 200)$$

where \(x\) (cm) is the vector of depths (\(x\leq1.200\)) and \(w\) is the vector of regression weights.

3. Results and discussion

3.1. Sensor calibration

Sensor calibration and independent test statistics are summarized in Table 1 and displayed graphically in Fig. 3. Overall, results were acceptable as judged by the root mean squared error (RMSE) and bias in the test dataset predictions. The ratio of the standard deviation of the observed values to the RMSE of the test dataset (ratio of prediction to deviation, RPD), and the ratio of the interquartile range to RMSE (RPIQ) (Bellon-Maurel et al., 2010) indicate reasonably successful calibrations. The RPD and RPIQ statistics characterize the fit of the model relative to the dispersion of the measured data and provide a scale-less measure to compare different models fit on the same dataset and models fit on differing measurement units. Comparing the calibration results against the test dataset results showed some differences in the transferability of the calibrated models. Clay content was estimated equally well for both the calibration and test datasets while silt and pH had less transferable results. Silt and pH had larger test dataset root mean squared error (RMSE) than the calibration results, leading to smaller, but still relatively good RPD. These reductions in fit are possibly due to the indirect nature of the relationship between VNIR-DRS and silt or pH.

The relationship between VNIR spectra and clay content is fairly direct. The smectitic mineralogy of the clay-sized particles in these landscapes strongly absorbs radiation around the 1400, 1900, and 2004 nm wavelengths (Chabrillat et al., 2002). These absorption features are associated with –OH functional groups present in clay-bound water and in the 2:1 mineral structures. The dominantly felsic minerals in the silt from these profiles are not active in the VNIR range and since sand sized particles are generally less than 10%, the successful calibration of silt content to VNIR-DRS is likely due to a strong inverse correlation to clay content (\(r = -0.79\)). Clay content also has an inverse relationship to pH (\(r = -0.65\)) in these profiles due to exchangeable acidity (\(Al^{3+}\) and \(H^+\)) on the weathered clay minerals – a likely mechanism for the successful calibration. Other effects on pH such as organic matter content or surface liming amendments might also have added complexity to the VNIR-DRS relationship. The indirect nature of the calibration between VNIR-DRS and silt content or pH may have resulted in over-fitting to noise features in the calibration dataset that would have been different in the independent test dataset.

### Table 1
Calibration set \((n = 430)\) and independent test set \((n = 185)\) statistics for least angle shrinkage and selection operator (LASSO) regression models of clay, silt, and pH.

<table>
<thead>
<tr>
<th>Property</th>
<th>Population statistics</th>
<th>Calibration statistics</th>
<th>Independent test statistics</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean</td>
<td>St. dev.</td>
<td>R²</td>
</tr>
<tr>
<td>Clay (%)</td>
<td>40.6</td>
<td>11.7</td>
<td>0.91</td>
</tr>
<tr>
<td>Silt (%)</td>
<td>48.5</td>
<td>12.2</td>
<td>0.92</td>
</tr>
<tr>
<td>pH</td>
<td>5.8</td>
<td>0.83</td>
<td>0.92</td>
</tr>
</tbody>
</table>

- RMSE = root mean squared error.
- Bias = mean(y) - mean($\hat{y}$).
- RPD = ratio of performance to deviation (sd(y)/RMSE).
- RPIQ = ratio of performance to interquartile range ((q3(y) – q1(y))/RMSE).
3.2. Clay, silt, and pH depth functions

The PIV and LPP functions were compared for their capability to fit the different peaked forms taken by high-resolution measurements of clay, silt, and pH at the summit landscape position. The two functions are similar in their capability to model this anisotropic soil profile (Fig. 4). Both functions fit the data well, and handle the inverted peaks (negative $\beta$) of silt and pH (Table 2). These inverted peaks are a manifestation of the inverse relationship that silt and pH have with clay content in the profiles of these landscapes. Depth-distribution of clay in the Central Claypan Area controls or is covariate with depth-distribution of a wide array of soil chemical and physical properties such as Ca, Mg, K, cation exchange capacity (CEC), plant available water holding capacity, and bulk density (Myers et al., 2007). This relationship is a result of the strong influence of expanding smectitic clays with moderate CEC and very large surface area. Thus peak functions may be suitable to model these and other properties correlated (either positively or negatively) with clay in similar soils.

While both equations are capable of handling the peaked profile data examined here, the PIV and LPP equations have very different forms and differ in the number of their parameters (PIV = 6, LPP = 5). This leads to differences in both the fit of the functions and interpretation of the parameters. The major difference occurs in the shape parameters of the functions. The PIV function has three parameters that control peak shape ($\alpha$, $\beta$, and $\gamma$), while the LPP function has only two ($\delta$ and $\epsilon$). The additional interacting shape parameter of the PIV function adds complexity in finding good starting values for parameters, obtaining successful parameter estimates, and explaining the physical meaning of the parameters. For example, the PIV function strongly fit to both clay and pH (adjusted $R^2$ of 0.98 and 0.90, respectively), but still had some non-significant ($p > 0.05$) parameter estimates (Table 2).

The more complex nonlinear interactions of the three shape parameters of the PIV function are more difficult to interpret than the two shape parameters of the LPP function (discussed in Section 3.3). The added parameter also increases the probability that multiple solutions could result in the same functional form (equifinality). The more parsimonious LPP function suffers less from these problems and was selected to model the five toposequence profiles, and to serve as a basis for further discussion of pedogenic parameter variation in the profile toposequence.

3.3. Pedogenic relationships to parameters

Peak function parameters are empirical descriptors of peak shape. And while they are empirically derived, their values are intrinsically related to the processes determining peak shape. Our intent is to show that besides fitting soil property depth profiles, parameters of peak functions can quantify and describe pedogenic relationships in the landscape. To demonstrate and discuss this capability, the LPP function was fit to the sensor-measured clay content profiles for all five landscape positions (Fig. 5, Table 3). Landscape trends are evident for three primary depth function features: the amplitude of the peak clay content ($\alpha + \beta$), the depth of peak clay content ($\mu$), and the abruptness of the argillic peak (controlled by $\delta$ and $\epsilon$). Plots of the parameters demonstrate these relationships at the five landscape positions (Fig. 6).

The amplitude of the clay peaks (i.e., clay maximum) seen on Fig. 5 decreased as landscape position changed from summit to toeslope. This trend was highlighted by the downward trend of the sum $\alpha + \beta$ from 60 to 35% descending the landforms 1 to 5 (Fig. 6, lower right panel). Key factors in this relationship were the change in materials and genetic processes from loess accretion and weathering at the summit, erosion and influence of till-derived materials on the backslopes, and colluvial accretion of hillslope sediments at the toeslope (refer to Fig. 2a). The most abrupt argillic horizons having the greatest clay content formed entirely in loess at the summit site. Down-slope positions had a larger portion of silt and sand textured material arising from pedisediment and glacial till within 1-m from the surface. Based on field observations at the time of soil sampling, the coarser pedisediment did not influence the summit position until >1.2 m depth while the shoulder position had pedisediment at
78 cm. The backslope position had pedisediment at 73 cm and glacial till at 101 cm. The footslope position had surface materials of loess-derived colluvial sediments and pedisediments throughout, and the depositional position was fully composed of loess-derived colluvial sediments. This down-slope reduction in clay content was demonstrated in the $\alpha + \beta$ relationship.

Based on visual interpretation of Fig. 5, depth to the clay peak gradually decreases between summit and backslope, then increases sharply between the backslope and toeslope. The plot of $\mu$ on Fig. 6 demonstrates this trend which can be explained primarily by the differential action of erosion and deposition. For instance, loess deposits at the geomorphically stable summit position were less likely to erode and the clay peak was moderately deep ($\mu = 47$ cm). Depth to the clay peak at the shoulder position has decreased due to slight erosion ($\mu = 41$ cm), and the more intensely eroded backslope has the shallowest argillic peak ($\mu = 32$ cm). Over-wash of loess-derived

| Soil property | Function | Adj R² | Fit std. error | F-value | Parameter | Parameter value | Std. error | 90% Confidence limits | t-value | P>|t| |
|---------------|----------|--------|----------------|---------|-----------|-----------------|------------|------------------------|---------|-----|
| Clay          | PIV      | 0.98   | 2.11           | 457.1   | $\alpha$  | 0.38            | 15.10      | -25.18 - 25.94         | 0.980   |
|               |          |        |                |         | $\beta$   | 60.65           | 15.30      | 3.96 - 34.76           | 86.55  | <0.001 |
|               |          |        |                |         | $\mu$     | 44.30           | 1.07       | 41.58 - 42.50          | 46.11  | <0.001 |
|               |          |        |                |         | $\delta$  | 5.59            | 0.71       | 4.19 - 3.33            | 7.85   | <0.001 |
|               |          |        |                |         | $\epsilon$| 0.14            | 0.07       | 1.98 - 0.02            | 0.26   | 0.057  |
|               |          |        |                |         | $\eta$    | -0.36           | 0.19       | -1.86 - 0.69           | -0.03  | 0.71   |
|               | LPP      | 0.98   | 2.41           | 433.7   | $\alpha$  | 19.82           | 0.70       | 28.18 - 18.63          | 21.01  | <0.001 |
|               |          |        |                |         | $\beta$   | 40.38           | 1.17       | 34.66 - 38.41          | 42.35  | <0.001 |
|               |          |        |                |         | $\mu$     | 47.06           | 0.97       | 48.35 - 45.42          | 48.71  | <0.001 |
|               |          |        |                |         | $\delta$  | 4.48            | 0.49       | 9.18 - 3.65            | 5.30   | <0.001 |
|               |          |        |                |         | $\epsilon$| 16.14           | 3.63       | 4.45 - 10.00           | 22.27  | <0.001 |
| Silt          | PIV      | 0.98   | 1.96           | 505.5   | $\alpha$  | 69.51           | 1.01       | 68.02 - 67.82          | 71.21  | <0.001 |
|               |          |        |                |         | $\beta$   | -39.38          | 1.38       | -28.58 - -41.70        | -37.06 | <0.001 |
|               |          |        |                |         | $\mu$     | 44.63           | 0.69       | 64.99 - 43.48          | 45.79  | <0.001 |
|               |          |        |                |         | $\delta$  | 10.57           | 1.18       | 9.39 - 11.83           | 12.57  | <0.001 |
|               |          |        |                |         | $\epsilon$| 0.69            | 0.15       | 4.55 - 0.43            | 0.94   | <0.001 |
|               | LPP      | 0.98   | 1.92           | 660.4   | $\alpha$  | 69.01           | 0.50       | 138.80 - 68.18         | 69.85  | <0.001 |
|               |          |        |                |         | $\beta$   | -39.17          | 0.81       | -48.56 - -40.53        | -37.81 | <0.001 |
|               |          |        |                |         | $\mu$     | 44.88           | 0.59       | 75.72 - 43.88          | 45.88  | <0.001 |
|               |          |        |                |         | $\delta$  | 3.74            | 0.30       | 12.68 - 3.25           | 4.24   | <0.001 |
|               |          |        |                |         | $\epsilon$| 13.02           | 1.62       | 8.01 - 10.29           | 15.76  | <0.001 |
| pH            | PIV      | 0.90   | 0.23           | 78.5    | $\alpha$  | 7.69            | 1.07       | 7.22 - 5.89            | 9.48   | <0.001 |
|               |          |        |                |         | $\beta$   | -2.36           | 1.00       | -2.17 - -4.19          | -0.52  | 0.037  |
|               |          |        |                |         | $\mu$     | 56.02           | 3.35       | 50.37 - 61.67          | 61.67  | <0.001 |
|               |          |        |                |         | $\delta$  | 21.30           | 6.48       | 13.29 - 10.38          | 32.23  | <0.01  |
|               |          |        |                |         | $\epsilon$| 0.56            | 0.80       | 0.70 - 0.79            | 1.90   | 0.490  |
|               | LPP      | 0.90   | 0.22           | 102.3   | $\alpha$  | 7.49            | 2.70       | 20.40 - 50.45          | 59.53  | <0.001 |
|               |          |        |                |         | $\beta$   | 54.99           | 2.70       | 50.45 - 59.53          | 59.53  | <0.001 |
|               |          |        |                |         | $\mu$     | 8.32            | 1.85       | 4.49 - 5.19            | 11.44  | <0.001 |
|               |          |        |                |         | $\delta$  | 14.67           | 4.94       | 2.97 - 6.35            | 22.99  | <0.01  |
colluvial sediment from eroded upslope positions leads to accumulation of silty material at footslope and toeslope positions, and deeper argillic horizons (μ = 43 and μ = 80 cm, respectively).

Another factor in the variation of peak shape parameters is differential intensity of weathering across the landform which caused variation in the argillic peak symmetry. Both the depth and the shape of the argillic peak changes systematically across the toposequence. The leading edge of the peak, found nearer the soil surface, is more abrupt in the summit position compared to the backslope, footslope, and toeslope positions. The peak shape at summit and shoulder is also narrower (smaller width at half-maximum) than the backslope and footslope positions, and much more so than the very broad, truncated peak at the depositional site (Fig. 5). These traits are reected in variation in the δ and ε parameters (Fig. 6).

Fig. 7 demonstrates the relationship of the LPP function’s δ and ε parameters and helps to interpret their pedological meaning. Starting with an initial set of parameters similar to those found from the summit soil (α = 20, β = 30, μ = 50, δ = 5, ε = 15) the δ and ε parameters were systematically changed to show the variation in peak shape from summit to toeslope. The relative differences between the shapes in the rising and falling limbs of the peaks are emphasized by holding α, β, and ε constant at their initial values. Adjusting the ε parameter from 2 to 10 (Fig. 7a) increases the width of the peak and the abruptness of the falling and rising limbs on either side of μ. Varying the δ parameter (Fig. 7b) mainly impacts the decay of the falling limb. Panel c in Fig. 7 emulates the relationships of these two parameters in a clayan soil landscape using parameters similar to those in Table 3. The summit and shoulder locations have the most abrupt argillic transition as well as the steepest gradient on the descending limb. The trend is toward less abrupt argillic peaks and broader tails down the toposequence.

Several interacting factors and processes are connected to the variable abruptness and width of clay peaks across these landscapes and they are empirically described by variation in δ and ε. Important spatially variable processes are the intensity of weathering and leaching, distribution, texture, and age of parent materials, as well as spatiotemporal variation in soil-water content. The Albaqualfs and Epiqualfs at the geomorphically stable summit and shoulder positions have an E horizon formed by the intense weathering and lessivage of aluminosilicate minerals from the surface loess deposits. A concomitant vertical leaching brings weathered minerals and mineral components into the argillic horizon. This effect is concentrated within a perched water table

Table 3

<table>
<thead>
<tr>
<th>Profile</th>
<th>Landscape position</th>
<th>Adj R²</th>
<th>Fit std. error</th>
<th>F-value</th>
<th>Parameter</th>
<th>Parameter value</th>
<th>Std. error</th>
<th>90% Conf. Limits</th>
<th>t-Value</th>
<th>P &gt;</th>
<th>β</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Summit</td>
<td>0.95</td>
<td>2.7</td>
<td>208.3</td>
<td>α</td>
<td>23.09</td>
<td>0.98</td>
<td>21.1</td>
<td>25.1</td>
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<tr>
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<td>Shoulder</td>
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<td>1.5</td>
<td>249.9</td>
<td>β</td>
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<td>1.31</td>
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<tr>
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<td>1.5</td>
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<td>μ</td>
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<tr>
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<td>δ</td>
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See Table 2 for Clay-LPP results in Table 2.
occurring above the clay peak during much of the fall, spring, and winter. Long residence time and lateral movement of this water table may be weathering minerals from the leading edge of the argillic peak thereby increasing the abruptness of the transition from E to Bt ($\delta \approx 3$, $\varepsilon \approx 16$). Additionally, the soil parent materials at the geomorphically stable upland positions have a relatively longer timeline for profile development and weathering. Backslope positions have a more lateral vector of weathering and leaching, their slopes leading to greater runoff and less perching of water. They tend to have a less abrupt E to Bt transition and a more symmetrical argillic peak ($\delta \approx 6$, $\varepsilon \approx 11$). The loess derived colluvial parent materials of the footslope and toeslope positions have been more recently delivered. Formation of argillic horizons has been accompanied by the accretion of silty deposits. Transition into the argillic horizon is gradual, and the peak is nearly at the bottom of the profile ($\delta \approx 9$, $\varepsilon \approx 31$). The values of the $\delta$ and $\varepsilon$ parameters of the LPP function empirically describe the interacting processes controlling the morphology of the profile clay depth distribution.

Another similarity between the distribution of soil properties in weathered loess and both the PIV and LPP functions is the peak width ($\delta$). This parameter quantitatively describes the ‘broadness’ of the peak shape. This might reflect, for instance, variation in the depth of weathering whereby deep well-drained and weathered soil profiles might have deeper and broader argillic peaks. Profiles with shallower soils and restrictive subsoil layers have more compressed argillic peak profiles. This feature can be used to quantitatively express the concepts of weathering intensity and/or profile maturity as described by Bray (1935) and Crompton (1960).

The functions described here and others in the class of asymmetric non-linear functions are complex due to the number of their parameters and the interacting and non-linear relationships between them. However, the parameters quantify the relationships between pedogenic processes and soil morphological patterns in the loess mantled landscapes studied here. The processes of weathering, lessivage, eluviation, illuviation, and neoformation of clay minerals responsible for argillic horizon formation are quantified by the values of the $\delta$ and $\varepsilon$ parameters. The same process linkage is true for the $\alpha$, $\beta$, and $\mu$ parameters as described above. Moreover, the morphological patterns described by the parameters are linked to the landscape as the result of continuous pedogenic processes. Continuous peak

Fig. 6. Scatterplots of the parameter values of the logistic power peak (LPP) function fit to high-resolution clay data for soil profiles from five different landscape positions: 1. summit, 2. shoulder, 3. backslope, 4. footslope, and 5. toeslope.

Fig. 7. Variations of logistic power peak (LPP) parameters $\varepsilon$ and $\delta$ with $\alpha$, $\beta$, and $\mu$ parameters held constant. Functions in panel a have constant $\delta = 15$, and $\varepsilon$ is varied from 2 to 10. Increasing the $\varepsilon$ parameter broadens the entire peak. Functions in panel b have constant $\varepsilon = 5$, and $\delta$ is varied from 15 to 75. Increasing the $\delta$ parameter primarily lengthens the right tail. Functions in panel c have simultaneously variable $\varepsilon$ and $\delta$ that represent smooth variation in these parameters from summit to toeslope. The peak intercept ($\alpha$), amplitude ($\alpha + \beta$), and center ($\mu$) are held constant to highlight the relative differences in clay peak shape at these landscape positions. The onset of the argillic horizon is steepest at the summit and declines rapidly after the peak. The trend going down slope is for less abrupt peaks and a smaller rate of decay in clay content below the peak.
functions of soil profiles might be estimated across a pedogenic gradient by spatial models of the parameters, such as kriging or regression kriging models (Malone et al., 2009; Mishra et al., 2009). Geospatial functions of soil profiles could be easily transferable into efforts to model soil hydrology and crop growth.

3.4. Peak function limitations

There are some limitations to the use of peak functions for modeling soil profile properties. First, they are mainly suitable to model peak-shaped soil property distributions occasionally seen in Molisols, but more commonly seen in Alfisols and Ultisols. On the other hand, these functions can model monotonically decreasing or increasing depth profiles. For example, constraining the peak center (μ) to be 0 or above 0, the falling limb of the peak can fit many monotonically decreasing or increasing forms. This could be useful where a peak is present in some parts of the landscape but is truncated in other areas. This does happen on severely eroded backslopes in the study area, especially where no plow layer is present (see landscape position 3 on Fig. 5). In these situations the argillic peak can lie at the surface and clay content monotonically decreases. However; the PIV or other peak functions would probably not be the best choice where only monotonic depth functions are present.

We have found these functions worked best in upland landscapes with a 0.75 to 2 m loess cap. A moderately deep parent material provides the best situation for peaked distributions of soil properties to form without influence from deeper parent materials with different properties. Overprinting of an argillic horizon on deeper materials can cause fit failures as these materials interfere with the shape of the decaying limb of the peak.

Several numerical limitations need to be overcome as well. The quantity of parameters and the non-linear interactions between them can be difficult to fit. Even when the overall fit is excellent, one or more of the parameters may have large p-values. Finally, perhaps the biggest limitation of these functions is the equifinality of their solutions. Parameter interactions can result in similarly shaped curves with very different parameter values. This issue can be mitigated by providing similar logical starting values for the fitting procedure of related profiles and setting reasonable boundary conditions on the parameters.

High resolution sensor estimates of soil property depth distributions can also mitigate some of the problems described in Section 3.4. Traditional horizon sampled soil profile data are too sparse to fit and would exhibit significant bias at depths with large gradients. The best solution for this problem is to have high-resolution measurements such as collected by soil penetrating sensors. Another solution is to aggregate soil profiles in order to create an ensemble fit with the greater data density needed to solve for the unknown parameters.

Coherent depth translation (Myers et al., 2007) is a technique that affine-shifts the depth scale origin of a family of similar pedons to align specific profile features, such as a clay peak. Using this simple transformation peak functions could also be fit to populations of pedons grouped by their distance in soil property or taxonomic space (McBratney and Minasny, 2007). These procedures could allow the use of peak functions to model legacy horizon-based data libraries.

4. Conclusions

A wide variety of tools will be needed to better quantify soil as the science of pedology advances towards a more continuous view of the landscape than current taxonomic and horizon-based models allow. Peak functions were proposed to be suitable for modeling profile distribution of clay and covariates of clay in loess-derived soils of Northeast Missouri, USA. Much of the Midwestern USA's landscapes have similar loess-till construction and peak functions might be used to model a broader range of soils than studied here. Moreover they might be used to model profile properties in three dimensions as they vary across diverse landscape components. Peak functions can provide simultaneously pedological and numerical descriptions of soil profiles and soil processes. These capabilities warrant further study to better relate variation in fitted parameters to variation in quantifiable pedogenic factors and gradients. Soil sensors are a useful tool to accomplish this objective since they can characterize more locations in the landscape with high-resolution measurements of soil property depth profiles. Peak functions are a useful companion to profile sensors and their combined use may allow more intensive mapping and better quantification and explanation of soil landscape variability. More importantly the soil property data produced might better inform crop, hydrologic, and/or environmental models, and its application in resource management could result in better practices for sustainable use.

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References


Systat, 2002. TableCurve 2D. SYSTAT Software Inc., Evanston, IL.
