Aggregate Representation of Genetic Soil Horizons

D.E. Beaudette, P. Roudier and J.M. Skovlin

## Warning: package 'knitr' was built under R version 3.1.3

# Abstract

Published soil survey reports typically describe soils in terms of aggregate information: soil properties, interpretations, and limitations that are based on a collection of field-described soil profiles. While aggregate soil properties are readily estimated via standard statistical functions (mean, median, etc.), an aggregate representation of horizonation (e.g. genetic or functional horizon designation and depth) is typically difficult to construct. Variation in horizon designation among different soil scientists and different soil description systems, changes in horizon designation standards over time, variable depths at which horizons occur, and the various uncertainties associated with these are all factors that complicate the process of delivering an aggregate representation of horizonation. In this paper we propose alternatives to the typical "representative profile" -- e.g. the selection of a single soil profile to represent a collection. Two possible methods for aggregating a collection of soil profiles into synthetic profiles are presented, describing depth-wise probability functions for each horizon. Both methods rely on an expert-guided description of generalized horizon designation (e.g. a subset of horizon designation labels that convey a reasonable "morphologic story") along with associated rules (regular expression patterns) used to correlate field-described to generalized horizon designation. The first method is based on (1-cm interval) slice-wise evaluation of generalized horizon designation; the second is based on a proportional-odds logistic regression model fit to depth-slices. These methods are demonstrated using USDA-NRCS soil survey data (USA).

# Introduction

Published soil survey reports typically describe soils in terms of *aggregate* information, *ie* soil properties, interpretations, and limitations that are based on a collection of field-described soil profiles. While aggregate soil properties are readily estimated via standard statistical functions (mean, median, etc.), an aggregate representation of *horizonation* (e.g. genetic horizon designation and depth) is typically difficult to construct (Beaudette, Roudier, and O’Geen 2013). Variation in horizon designation "style" among different soil scientists, changes in horizon designation standards over time, variable depths at which genetic horizons occur, and the possible lack of a specific genetic horizon are all factors that complicate the process of delivering an aggregate representation of horizonation. The process of designating horizons by soil scientists can be somewhat subjective; even a second description of the same volume of soil can lead to a slightly different set of horizon designations and depths (Holmgren 1988). In addition to human sources of variability, it is understood that most of the variation between profile descriptions is due to real differences between soils observed at different locations (Wilding, Scafer, and Jones 1964).

The "modal pedon" concept ... not ideal, but widely used:

* problems with the modal concept (Hudson 1990)
* discrete representation of soils (via soil profile) despite continuous gradation (T. Jones 1959)

This complex combination of variability in morphologic horizon designation and depths is rarely acknowledged at the series or component level: boundaries between horizons, expressed as horizon depths, are generally considered as "crisp" numbers, while in actuality they represent "fuzzy" numbers due to the varying distinctness of the horizon boundaries and how abruptly characteristics change at horizon boundaries.

Soil profiles and their corresponding soil horizons represent a record of soil formation and encapsulate significant information about soil morphology. Although new tools and technologies may make continuous-depth measurements of soils possible, horizon designations, have historically been the common pedological language used to annotate observations of changes in soil properties with depth (Hartemink and Minasny 2014; Myers et al. 2011; B. Kempen, Brus, and Stoorvogel 2011).

In order to aggregate properties for soil horizons within a collection of soil profiles, horizons must be systematically correlated into groups of similar soil morphology. The aggregation of horizons then becomes a conceptual profile that is synthesized to represent the central concept of the soil morphology conveyed by the entire suite of soil profiles. The use of generalized horizon labels (GHL) provides a framework for correlating individual soil horizons, however, traditional aggregates only provide a coarse summary of corresponding horizon depths derived for the aggregated conceptual profile. This paper presents a novel approach using a depth-slicing method in the aqp package to determine horizon depth probabilities.

Possible mention of logistic regression in context of this paper: \* ordinal response models in ecology (Antoine and Harrell 2000)

* horizon thickness (Vanwalleghem et al. 2010)
* "red clay" hz presence, logistic regression (Evans and Hartemink 2014)

We demonstrate two possible methods for aggregating a collection of soil profiles into "representative synthetic profiles"; describing depth-wise probability functions for each genetic horizon. Both methods rely on an expert-guided description of generalized horizon designation (e.g. horizon designations that are deemed representative) along with associated rules (regular expression patterns) used to correlate field-described to generalized horizon designation. The first method is based on (1-cm interval) slice-wise evaluation of generalized horizon designation; the second is based on a proportional-odds logistic regression (McCullagh 1980) model fit to depth-slices. Specialized classes for soil profile collections and depth-slicing algorithms are implemented in the [aqp](http://cran.at.r-project.org/web/packages/aqp/index.html) package for R (Beaudette, Roudier, and O’Geen 2013).

# Materials and Methods

## Soil Profile Data

A collection of (63) soil profiles from the Sierra Foothill Region of California were used to demonstrate two approaches for determining aggregate representation of genetic horizon boundaries. This collection of soil profile data represents the work of 13 different soil scientists, with described properties spanning ranges in physical properties (mostly related to bedrock composition) and are included within the **soilDB** package for R (Beaudette and Skovlin 2015). These soils are associated with the [Loafercreek](https://soilseries.sc.egov.usda.gov/OSD_Docs/L/LOAFERCREEK.html) soil series (fine-loamy, mixed, super-active, thermic ultic haploxeralfs); moderately deep soils formed in colluvium and residuum from metavolcanic rocks (greenschist) (Figure 1). The climate is characterized by hot, dry summers and cool, wet winters. Mean annual air temperature is approximately 16 degrees C and mean annual precipitation is about 760 mm. The native vegetation is blue oak and annual grass savannah. Land uses for this soil series include range, vineyards, recreation, and wild life habitat.



Figure 1. Eight photos of the Loafercreek soil series, collected in Tuolumne and Calaveras counties, CA, USA. How would you combine the wide range in morphology from these profiles into an aggregate concept?

The methods described in this paper are based on field descriptions: observations based on (experienced) visual and tactile investigation of the soil profile. Given sufficient laboratory characterization data, these same methods could be refined to use a combination of field and lab data.

## Horizon Generalization

Generalized horizon labels (GHL) represent an expert-guided selection of horizon designations that were consistently observed in the field, and meaningful in terms of soil morphology and management.  
These designations were determined to convey the "morphologic story" or conceptual framework of most-likely horizons typically observed in a suite of soil profiles associated with a specific soil series or map unit soil component. The Official Series Description, or OSD (Soil Survey Staff) of the Loafercreek series typical pedon and range in characteristics defines this soil series concept. In this case, the OSD provided a useful GHL template, however, older OSDs or those based on a very limited set of data may not adequately convey an appropriate morphologic story.

Once a set of GHL have been determined (in the case of the sample dataset: Oi, A, BA, Bt1, Bt2, Bt3, Cr, R), it is neccessary to create and apply a set of rules that map the field-described designations to corresponding GHL. When working with a set of pedons that have been described by a small number of individuals over a short period of time (i.e. consistency in both designation application and standards) it is possible to use a regular expression (REGEX) pattern matching to apply GHL. This process typically requires expert-guided review of: 1) regional patterns in horizonation style, 2) morphologic property differences by groups of field-described designation, and, 3) patterns of horizonation and properties with depth. We used a combination of field-described clay content, rock fragment volume, moist Munsell value, and horizon mid-point to evaluate GHL assignments and determine the final set of REGEX rules. Due to this iterative process, local experience with these soils and their properties are (mostly) preserved within the REGEX rules and corresponding GHL. It should be noted that there are some cases where pattern matching alone is not enough and manual adjustment of GHL on a horizon-by-horizon basis are needed. For simplicity, only REGEX-based assignment of GHL was used in this study.

At present there are limited means of capturing this type of soil horizon "micro-correlation" information developed in the application of GHL to soil horizon data. The authors suggest that future studies maintain a record of orginal horizon designations, generalized horizon labels suitable for aggregation, and the rules used to apply these labels. Such a record would be useful should more data on a soil be collected or laboratory data be included in the horizon data set. A convenient, quantitative evaluation of GHL assignments can be performed using the silhouette width metric (Rousseeuw 1987). This metric, commonly used to assess clustering labels, provides a simple metric that can be used to address the basic question of GHL assignment: "given a set of data and labels, how well do these labels split differences within the data?". A more detailed description of this approach has been documented in chapter (???).

### Aggregation of Generalized Horizon Labels

Aggregation of horizons as defined by GHL was performed using empirical probabilities, estimated along regular depth-slices from 0--150cm (Beaudette, Roudier, and O’Geen 2013). The "sliced" GHL data were then aggregated using proportional odds logistic regression (Figure 2). All computation was performed with the R package for statistical computing (R Core Team 2013).

A sequence of morphologic soil horizon designations can be modeled as an ordinal-scale variable: categorical by definition and ordered along a logical gradient, depth. Within the set of GHL associated with our sample data, "Bt2" horizons always occur after "Bt1" horizons and before "Bt3" horizons. The proportional odds logistic regression model (cumulative link model with logit link) (McCullagh 1980) is a convenient framework for estimating the probability of encountering a GHL, as conditioned by depth. The proportional odds logistic regression (PO-LR) model can be defined as:

where is the estimated probability of encountering GHL , is a set of predictor variables, and a vector of fitted regression coefficients (Harrell 2001). In this study, the PO-LR model was fit to "sliced" horizon data; 1-cm slices of GHL and slice top depth (Figure 2). Restricted cubic spline basis functions (Harrell 2001; Hastie, R.Tibshirani, and Friedman 2009) with 4 knots located at the 5th, 35th, 65th, and 95th percentiles of slice top depth were used to accommodate non-linearity. An empirical index of model stability was calculated by repeatedly re-fitting the PO-LR model to 25 randomly sampled profiles (out of 54 total), 250 times.

## Most-Likely Horizon Boundaries

Continuous estimates of GHL probability with depth are a convenient approach to communicating variability, however, there are still cases where discrete horizon depth information is required. For example, the USDA-NRCS Official Series Description pages are used by a wide range of individuals that may not need this level of detail. We used a simple strategy for converting these depth functions into a discrete set of "most-likely" GHL boundary depths. At each depth slice, the GHL with the highest probability is selected. Most-likely boundary depths are determined by locating upper and lower depths from contiguous sets of slices that share a common GHL. Within a collection of highly similar pedons, the most-likely boundary depths roughly correspond to crossings of the GHL probability depth functions (figure #?).

## Quantification of Uncertainty

We used Shannon Entropy to quantify the relative amount of information present within GHL predictions at any given depth. Shannon Entropy was calculated according to (Bas Kempen et al. 2009):

where is an index of uncertainty associated with predicted probabilities, , of encountering horizons through at some depth. Values range from 0 (maximum information, minimum entropy) to 1 (minumum information, maximum entropy). Entropy values were computed along each 1-cm depth slice from predictions generated by the PO-LR model.

We used Brier scores (Harrell 2001) to quantify agreement between assigned GHL and probabilities of predictied GHL:

where is an index of agreement between predicted probabilities, , and horizons, , over depth-slices through associated with a specific horizon. Larger values suggest less agreement between probabilities and observed horizon labels.

# Results

## Generalized Horizon Labels

A graphical representation of the association between field-described horizon designation and associated GHL is presented as a box and whisker plot in Figure 3. Assignment of GHL to the top (A) and bottom-most (Cr and R) genetic horizons by REGEX pattern matching resulted in the most internally-consistent groups of data. Transitional horizons near the surface (AB, BA, etc.) and lower Bt horizons (2Bt3, Bt4, BCt, etc.) were generally the most variable and thus difficult to place within a GHL by pattern matching.

(not sure what else to add here... ideas?)

The degree of overlap in GHL concepts can be expressed in terms of measured soil properties (in this case a limited set of field-described properties), summarized by GHL (Table 1).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| GHL | Clay (%) | Horizon Mid-Point (cm) | Total RF Volume (%) | Moist Munsell Value | Sillhouette Width |
| Oi | NaN (NA) | 0.69 (0.37) | 0 (0) | NaN (NA) | NaN (NA) |
| A | 15.68 (3.34) | 4.17 (3.19) | 6.51 (7.29) | 3.28 (0.6) | 0.16 (0.17) |
| BA | 17.57 (3.74) | 12.07 (6.16) | 9.71 (6.5) | 3.57 (0.76) | -0.12 (0.1) |
| Bt1 | 21.43 (4.54) | 19.87 (9.29) | 12.67 (12.51) | 3.72 (0.56) | 0.02 (0.14) |
| Bt2 | 25.26 (4.98) | 39.63 (11.27) | 24.27 (21.76) | 4 (0.72) | -0.06 (0.14) |
| Bt3 | 28.61 (6.33) | 60.94 (13.56) | 35.02 (23.9) | 4.37 (0.6) | 0.06 (0.14) |
| Cr | NaN (NA) | 76.96 (16.41) | 0 (0) | 5 (NA) | NaN (NA) |
| R | NaN (NA) | 137 (11.54) | 0 (0) | NaN (NA) | NaN (NA) |
| NA | 19.33 (4.93) | 13 (5.2) | 18.33 (11.55) | 4 (0) | NaN (NA) |

Table 1. Evaluation of GHL via field-described soil properties. Reported values are means with standard deviation in parenthesis. Values marked as "NA" or "NaN" are the result of missing or insufficient data.

## Aggregate Representation of GHL

## ML Horizon boundaries

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Horizon | Top (cm) | Bottom (cm) | Brier | Horizon | Top (cm) | Bottom (cm) | Brier |
| A | 0 | 8 | 0.20 | A | 0 | 9 | 0.26 |
| Bt1 | 8 | 28 | 0.23 | Bt1 | 9 | 28 | 0.23 |
| Bt2 | 28 | 51 | 0.25 | Bt2 | 28 | 50 | 0.23 |
| Bt3 | 51 | 68 | 0.44 | Bt3 | 50 | 67 | 0.39 |
| Cr | 68 | 90 | 0.36 | Cr | 67 | 91 | 0.36 |
| R | 90 | 203 | 0.05 | R | 91 | 151 | 0.08 |

Table 3. Most-likely GHL boundary depths and associated Brier scores, computed from empirical probabilities and PO-LR predictions.

## Model Fit

Tidy representation of model fit here.

|  |  |  |  |
| --- | --- | --- | --- |
| Term | Coef | S.E. | Wald Z |
| y>=A | 2.2050 | 0.2008 | 10.98 |
| y>=BA | -1.6688 | 0.1020 | -16.36 |
| y>=Bt1 | -2.3032 | 0.1064 | -21.66 |
| y>=Bt2 | -6.4802 | 0.1961 | -33.04 |
| y>=Bt3 | -10.5553 | 0.2542 | -41.52 |
| y>=Cr | -13.0341 | 0.2656 | -49.08 |
| y>=R | -15.9055 | 0.2785 | -57.12 |
| hzdept | 0.2513 | 0.0077 | 32.78 |
| hzdept' | -0.3356 | 0.0304 | -11.03 |
| hzdept'' | 0.6957 | 0.0806 | 8.63 |

## Model Stability

Predictions from the 250 models were then combined and visualized below.

# Conclusions

Describing and sampling soil by genetic horizon designations represents an efficient approach that has provided a common pedological language used among soil scientists and classification systems. Processes for aggregating horizonation and deriving an aggregate representation across suites of similar soil profile descriptions of a soil series has been challenging. For this reason, soil series typical profiles have historically been represented by an actual representative profile which is selected to summarize the central concept for that series. Advances in soil morphometrics are poised to change our understanding of what it means to describe soil profiles. Continuous depth functions of soil properties will further our understanding of how soil properties vary with depth, adding rich content to the existing genetic horizon framework.  
Here we demonstrate an approach to deriving.....

Ideas for the conclusion.....the ideas presented in this paper regarding modeling horizon depth probabilities are helping to bridge the soil profile/horizonation concept that is are our existing 'pedological language' with the development of continuous-depth soil morphometric measurements. Hartemink talks about continuous functions of morphometrics decoupling the horizon as a support unit for the soil profile. Each method of describing a soil profile has its purpose. Perhaps we should not be looking to decouple it so much as meld and anchor new continuous measurements within the horizon designation framework, thereby building new knowledge within the framework of our existing knowledge. This is an area in which morphometrics has great potential to add value to soil survey products.

* fact: sampling by **genetic horizon** is efficient and will continue to be important
* we can do better than picking a single, **representative profile**
* soil series representative horizonation could be **defined** by GHL rules, PO-LR model, and properties aggregated by GHL
* variability between descriptions **smoothed** as sample size increases-- *given thoughtful correlation*
* continuous **depth-functions** of genetic, or diagnostic horizons
* **most-likely** horizonation, based on depth-function crossings
* quantitative estimates of **uncertainty**: Brier scores, Shannon Entropy, etc.

## Future Work

* minimum sample sizes, model diagnostics, best-practice guidelines, etc.
* more realistic estimates of SE, e.g. correlation structure via GEE
* pedogenic interpretation of model coefficients

# References

fake text here

Antoine, Guisanm, and Frank E. Harrell. 2000. “Ordinal Response Regression Models in Ecology.” *Journal of Vegetation Science* 11: 617–626.

Beaudette, D.E., and J.M. Skovlin. 2015. *soilDB: Soil Database Interface*. <http://CRAN.R-project.org/package=soilDB>.

Beaudette, D.E., P. Roudier, and O’GeenA.T. 2013. “Algorithms for Quantitative Pedology: A Toolkit for Soil Scientists.” *Computers & Geosciences* 52: 258–268.

Evans, D.M., and Alfred E. Hartemink. 2014. “Digital Soil Mapping of a Red Clay Subsoil Covered by Loess.” *Geoderma* 230–231 (0): 296–304. doi:[http://dx.doi.org/10.1016/j.geoderma.2014.03.013](http://dx.doi.org/http://dx.doi.org/10.1016/j.geoderma.2014.03.013). <http://www.sciencedirect.com/science/article/pii/S0016706114001256>.

Harrell, Frank E. 2001. *Regression Modeling Strategies*. Springer Series in Statistics. New York, NY: Springer.

Hartemink, Alfred E., and Budiman Minasny. 2014. “Towards Digital Soil Morphometrics.” *Geoderma* 230–231: 305–317. doi:[http://dx.doi.org/10.1016/j.geoderma.2014.03.008](http://dx.doi.org/http://dx.doi.org/10.1016/j.geoderma.2014.03.008). <http://www.sciencedirect.com/science/article/pii/S0016706114001177>.

Hastie, T., R.Tibshirani, and J. Friedman. 2009. *The Elements of Statistical Learning*. Springer.

Holmgren, G.G.S. 1988. “The Point Representation of Soil.” *Soil Sci. Soc. Am. J.* 52: 712–716.

Hudson, B.D. 1990. “Concepts of Soil Mapping and Interpretation.” *Soil Survey Horizons* 31: 36–72.

Jones, T.A. 1959. “Soil Classification–a Destructive Criticism.” *J. Soil Sci.* 10: 196–200.

Kempen, B., D.J. Brus, and J.J. Stoorvogel. 2011. “Three-Dimensional Mapping of Soil Organic Matter Content Using Soil Type Specific Depth Functions.” *Geoderma* 162: 107–123. doi:[http://dx.doi.org/10.1016/j.geoderma.2011.01.010](http://dx.doi.org/http://dx.doi.org/10.1016/j.geoderma.2011.01.010). <http://www.sciencedirect.com/science/article/pii/S001670611100019X>.

Kempen, Bas, Dick J. Brus, Gerard B.M. Heuvelink, and Jetse J. Stoorvogel. 2009. “Updating the 1:50,000 Dutch Soil Map Using Legacy Soil Data: A Multinominal Logistic Regression Approach.” *Geoderma* 151: 311–326. doi:[10.1016/j.geoderma.2009.04.023](http://dx.doi.org/10.1016/j.geoderma.2009.04.023).

McCullagh, P. 1980. “Regression Models for Ordinal Data.” *Journal of the Royal Statistical Society, Series B* 42: 109–142.

Myers, D Brenton, Newell R Kitchen, Kenneth A Sudduth, Randall J Miles, E John Sadler, and Sabine Grunwald. 2011. “Peak Functions for Modeling High Resolution Soil Profile Data.” *Geoderma* 166 (1): 74–83.

R Core Team. 2013. *R: A Language and Environment for Statistical Computing*. Vienna, Austria: R Foundation for Statistical Computing. <http://www.R-project.org/>.

Rousseeuw, P.J. 1987. “Silhouettes: a Grapical Aid to the Interpretation and Validation of Cluster Analysis.” *Journal of Computational and Applied Mathmatics* 20: 53–65.

Soil Survey Staff. “Official Soil Series Descriptions.” Edited by Natural Resources Conservation Service, United States Department of Agriculture. <https://soilseries.sc.egov.usda.gov/OSD_Docs/L/LOAFERCREEK.html>.

Vanwalleghem, T., J. Poesen, A. McBratney, and J. Deckers. 2010. “Spatial Variability of Soil Horizon Depth in Natural Loess-Derived Soils.” *Geoderma* 157 (1-2): 37–45. doi:[DOI: 10.1016/j.geoderma.2010.03.013](http://dx.doi.org/DOI: 10.1016/j.geoderma.2010.03.013). <http://www.sciencedirect.com/science/article/pii/S001670611000090X>.

Wilding, L.P., G.M. Scafer, and R.B. Jones. 1964. “Morley and Blount Soils: A Statistical Summary of Certain Physical and Chemical Properties of Some Selected Profiles from Ohio.” *Soil Sci. Soc. Proc.* 28: 674–679.