

UNIVERSITY OF TENNESSEE

MULTIVARIATE DATA MINING AND TECHNIQUES

BZAN 552

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# Predict Physical and Chemical Properties of Soil using Spectral Measurements

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# 1 Introduction

There is an increasingly interest for using infrared spectroscopy for predicting soil functional properties at unsampled locations and to provide data for digital soil mapping [Kuang et al.(2012)Kuang, Mahmood, Quraishi, Hoogmoed, Mouazen, and van Henten]. This technique provides a highly repeatable, rapid and low cost measurement of many soil functional properties [Viscarra Rossel and Lark(2009)], is non-destructive, no harmful chemicals are used, and importantly, several soil properties can be measured from a single scan [Viscarra Rossel et al.(2006)Viscarra Rossel, Walvoort, McBratney, Janik, and Skjemstad]. Therefore, one spectrum can be related to various soil constituents by the multi-parameter feature of this technique.

The diffuse reflectance spectroscopy technique is largely general, quite weak and broad due to overlapping absorptions of soil constituents and their often small concentrations in soil. Therefore, the information needs to be mathematically extracted from the spectra so that they may be correlated with soil properties. Therefore, the analysis of soil diffuse reflectance spectra requires the use of multivariate calibration [Martens(1989)]. In these cases, to be useful quantitatively, spectra must be related to a set of known reference samples through a calibration model. The set of reference samples used in the models need to be representative of the range of soils in which the models are to be used. Partial least squares regression (PLSR) is the most common algorithm used to calibrate spectra to soil properties [Wold et al.(1983)Wold, Martens, and Wold]. However, other approaches have also been used, for example, stepwise multiple linear regression [Dalal and Henry(1986)], principal components regression (PCR) [Chang et al.(2001)Chang, Laird, Mausbach, and Hurburgh], artificial neural networks (ANN) [Daniel et al.(2003)Daniel, Tripathi, and Honda], multivariate adaptive regression splines (MARS) [Shepherd and Walsh(2002)], boosted regression trees [Brown et al.(2006)Brown, Shepherd, Walsh, Dewayne Mays, and Reinsch], PLSR with bootstrap aggregation (bagging-PLSR) [Viscarra Rossel(2007)], support vector machines SVM and penalized spline signal regression [Stevens et al.(2008)Stevens, van Wesemael, Bartholomeus, Rosillon, Tychon, and Ben-Dor].

## 2 Dataset

The data was ordered in the training and test set. In order to assemble the data, the spatially stratified multilevel sampling design was used. The 60,  $10 \times 10$  km sized “Sentinel Landscapes” was chosen excluding true desserts and areas due to security reasons.

The ultimate goal was to obtain a representative multilevel/multistage sample consisting of:

- 60 Sentinel Landscapes
- 16 Sampling Clusters per Sentinel Landscape
- 10 Sampling Plots per Sampling Cluster
- 2 composite Soil samples (topsoil and subsoil) per Sampling Plot

Since some locations were either completely inaccessible by four wheeled drive vehicle and on foot or that had soil depth limitations, the actual total number of soil samples is smaller than planned in this dataset.

All samples are characterized with the MIR spectral measurements. The potential spatial predictors, were obtained from NASA remote sensing data missions.

A 10 percent subsample of all the soils went on to be specified with more reference measurements.

Since reference measurements are too expensive (potentially hundreds of US dollars per sample) and tedious, the other 90 percent of samples have been physically archived for calibrating new analytical methods and/or validating old methods.

This research consists of spectral and reference datasets. The training and test data have been split along Sentinel Landscape levels because we are primarily interested in predicting soil properties at new Sentinel Landscapes.

## 2.1 Definition of Variables

Each soil sample has a unique identifier–PIDN. We have 5 response variable to predict and 3587 explanatory variables.

### Response Variables

- SOC: Soil organic carbon
- pH: pH values
- Ca: Mehlich-3 extractable Calcium
- P: Mehlich-3 extractable Phosphorus
- Sand: Sand content

### Explanatory Variables:

- m7497.96 - m599.76: There are 3,578 mid-infrared absorbance measurements.
- Depth: Depth of the soil sample (2 categories: "Topsoil", "Subsoil")
- BSA: average long-term Black Sky Albedo measurements from MODIS satellite images (BSAN = near-infrared, BSAS = shortwave, BSAV = visible)
- CTI: compound topographic index calculated from Shuttle Radar Topography Mission elevation data
- ELEV: Shuttle Radar Topography Mission elevation data
- EVI: average long-term Enhanced Vegetation Index from MODIS satellite images.
- LST: average long-term Land Surface Temperatures from MODIS satellite images (LSTD = day time temperature, LSTN = night time temperature)

- Ref: average long-term Reflectance measurements from MODIS satellite images (Ref1 = blue, Ref2 = red, Ref3 = near-infrared, Ref7 = mid-infrared)
- Reli: topographic Relief calculated from Shuttle Radar Topography mission elevation data
- TMAP and TMFI: average long-term Tropical Rainfall Monitoring Mission data (TMAP = mean annual precipitation, TMFI = modified Fournier index)

### 3 Visualization of Variables

In first step the visualization of a random number of observations helped to compare the effect of removing CO2 related spectrums, suggested by the Kaggle, also the difference between top soil and subsoil samples.

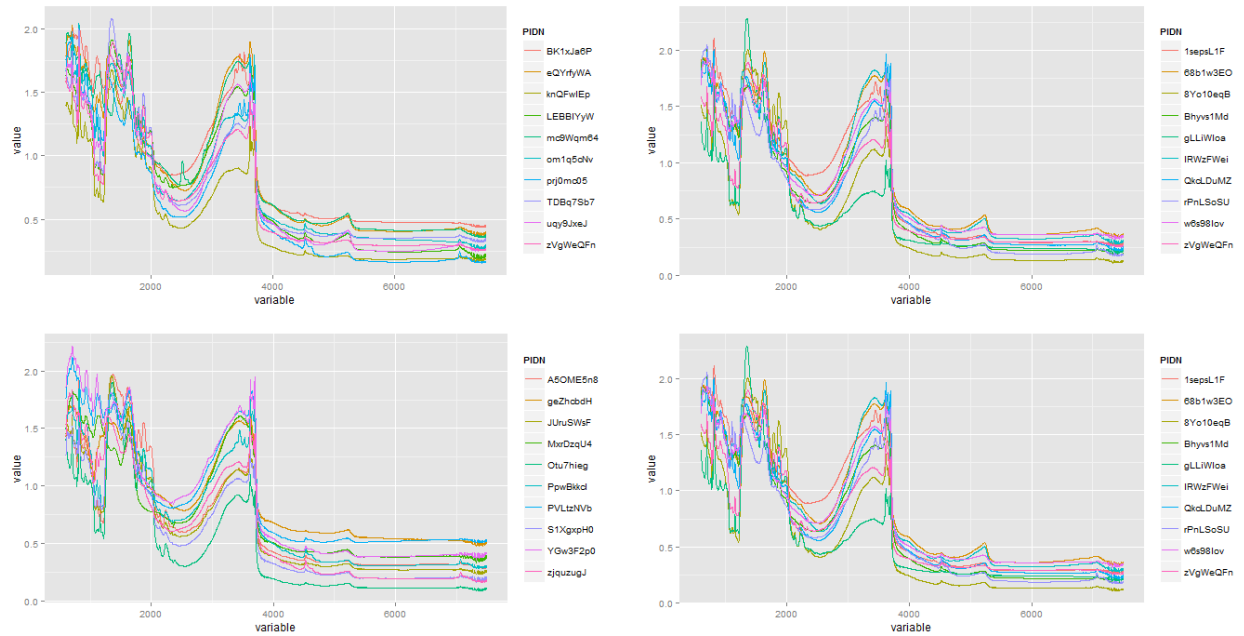


Figure 1: Right: With CO2. Left: W/O CO2. Top: Topsoil. Below: Subsoil

### 4 Preprocessing

Visualization of data helped to see the existence of noise in the data. To remove the noise and smooth the signals the following techniques are used.

- Multiple Scatter Correction:

Multiple Scatter Correction is a math treatment to correct the scatter in the spectra. The scatter is produced for different physical circumstances such as particle size and packaging. Normally scatter makes worse the correlation of the spectra with the constituent of interest.

- First Derivative Transformation:

The goal of using the first derivative is not necessarily to create a transformed data set (or new variables), but rather to smooth out noise in the original spectra. In this project the method helped to:

Reduce baseline offset

Resolve absorption overlapping

Enhance small spectral absorptions

- Discrete Wavelet Transform Technique:

The discrete wavelet transform technique pairs the input values, storing the difference and passing the sum. This has a huge number of applications in science, engineering, mathematics and computer science. Most notably, it is used for signal coding, to represent a discrete signal in a more redundant form, often as a preconditioning for data compression. Practical applications can also be found in signal processing of accelerations for gait analysis, in digital communications and many others.

## 5 Review of Used Algorithms

The performance of different methods was tested for calibrating reflectance spectra to SOC, pH, Ca, P, Sand. These techniques are partial least squares regression (PLSR), random forests (RF), k – Nearest Neighbor, Support Vector Machines and Linear Regression.

- Partial Least Squares Regression (PLSR)

Partial least squares regression (PLS regression) is a statistical method that bears some relation to principal components regression; instead of finding hyperplanes of minimum variance between the response and independent variables, it finds a linear regression model by projecting the predicted variables and the observable variables to a new space. Because both the X and Y data are projected to new spaces, the PLS family of methods are known as bilinear factor models. Partial least squares Discriminant Analysis (PLS-DA) is a variant used when the Y is categorical.

- Random Forest (rf)

In random forests each tree in the ensemble is built from a sample drawn with replacement (i.e., a bootstrap sample) from the training set. In addition, when splitting a node during the construction of the tree, the split that is chosen is no longer the best split among all features. Instead, the split that is picked is the best split among a random subset of the features.

- k-Nearest Neighbor (k-NN)

Neighbors-based classification is a type of instance-based learning or non-generalizing learning: it does not attempt to construct a general internal model, but simply stores instances of the training data. Classification is computed from a simple majority vote of the nearest neighbors of each point: a query point is assigned the data class which has the most representatives within the nearest neighbors of the point.

- Support Vector Machines (SVM)

In machine learning, support vector machines (SVMs, also support vector networks) are supervised learning models with associated learning algorithms that analyze data and recognize patterns, used for classification and regression analysis. Given a set of training examples, each marked as belonging to one of two categories, an SVM training algorithm builds a model that assigns new examples into one category or the other, making it a non-probabilistic binary linear classifier. An SVM model is a representation of the examples as points in space, mapped so that the examples of the separate categories are divided by a clear gap that is as wide as possible. New examples are then mapped into that same space and predicted to belong to a category based on which side of the gap they fall on.

- Linear Regression (lm)

In statistics, linear regression is an approach for modeling the relationship between a scalar dependent variable  $y$  and one or more explanatory variables denoted  $X$ . The case of one explanatory variable is called simple linear regression. For more than one explanatory variable, the process is called multiple linear regression. In linear regression, data are modeled using linear predictor functions, and unknown model parameters are estimated from the data.

## 6 Implementing the Algorithms

Before making any model we used PCA to reduce the dimensions of the data. Principal component analysis (PCA) is a statistical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components. The number of principal components is less than or equal to the number of original variables. This transformation is defined in such a way that the first principal component has the largest possible variance (that is, accounts for as much of the variability in the data as possible), and each succeeding component in turn has the highest variance possible under the constraint that it is orthogonal to (i.e., uncorrelated with) the preceding components.

In next step we used the following R libraries to call the required functions for training and prediction.

- RWeka - Used for PCA
- Wavelets - Used for Discrete wavelet transformation
- caret - Used for training and predicting the model
- pls - Used for training model with partial least squares
- kernlab - Used for training model with SVM
- randomForest - Used for training model with rf

## 7 Algorithm Comparison

The root-mean-square error (RMSE) is a frequently used measure of the differences between value predicted by a model or an estimator and the values actually observed. Basically, the RMSE represents the sample standard deviation of the differences between predicted values and observed values.

$$RMSE = \sqrt{\frac{1}{n} \sum_{j=1}^n (y_j - \hat{y}_j)^2}$$

Figure1 includes the RMSE values gained for each response variable using different models. The best model for predicting each of 5 response variable is the one with the lowest RMSE value.

Variables \ Methods	RMSE Value				
	pls	k-NN	rf	svm	lm
Ca	0.3906	0.5628	0.3547	0.3752	0.4438
P	0.378	0.3638	0.3448	0.401	0.3634
pH	0.3922	0.5402	0.3951	0.3609	0.3714
SOC	0.392	0.5979	0.4049	0.3337	0.3279
Sand	0.4184	0.5188	0.427	0.3927	0.3827

Figure 2: Comparison of RMSE of each model for each response variable

### 7.1 Software Used

Used RStudio Version 0.98.1028 - 2009 –2013 RStudio, Inc.

System Configuration -

- Intel(R) Core(TM) i5-3337U
- 4.00 GB RAM
- 64- bit Operating System, x64-based processor
- Windows 8.1

The code is attached with the document with comments explaining all the steps.

## 8 Conclusion

The best models for predicting response variables are:

Ca - Random Forest

P - Random Forest

pH - Support vector machines

SOC - Linear regression

Sand - Linear regression



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