

Machine Learning Algorithms for Soil Properties Prediction with Treated Vis–NIR Spectrums from the Itatiaia National Park

Yuri Andrei Gelsleichter ^{1*}, Lúcia Helena Cunha dos Anjos ¹, Elias Mendes Costa ¹, Gabriela Valente ¹, Paula Debiasi ¹, Mauro Antonio Homem Antunes ¹, Robson Altiellys Tosta Marcondes ¹

¹ Federal Rural University of Rio de Janeiro, BR-465, km 7 Seropédica-Rio de Janeiro; lanjos@ufrj.br, eliasmccosta@gmail.com, gabivalente.ufrj@gmail.com, pauladebiasi@yahoo.com.br, homemantunes@gmail.com, robson.marcondee@gmail.com

*Correspondence: yurigellichter@gmail.com

Abstract: Visible and near-infrared reflectance (Vis–NIR) techniques are a plausible method to soil analyses. The main objective of the study was to investigate the capacity to predicting soil properties Al, Ca, K, Mg, Na, P, pH, total carbon (TC), H and N, by using different spectral (350–2500 nm) pre-treatments and machine learning algorithms such as Artificial Neural Network (ANN), Random Forest (RF), Partial Least-squares Regression (PLSR) and Cubist (CB). The 300 soil samples were sampled in the upper part of the Itatiaia National Park (INP), located in Southeastern region of Brazil. The 10 K-fold cross validation was used with the models. The best spectral pre-treatment was the Inverse of Reflectance by a Factor of 10⁴ (IRF4) for TC with CB, giving an averaged R² among the folds of 0.85, RMSE of 1.96; and 0.67 with 0.041 respectively for H. Into the K-folds models of TC, the highest prediction had a R² of 0.95. These results are relevant for the INP management plan, and also to similar environments. The good correlation with Vis–NIR techniques can be used for remote sense monitoring, especially in areas with very restricted access such as INP.

Keywords: pedometrics; chemometrics; remote sensing; proximal soil sensing

1. Introduction

Soils of the tropical regions are dominantly highly weathered and with low organic carbon (C) and nitrogen (N) in the upper horizons. However, in the high altitudes of mountain ranges peculiar climate (with low temperature) and endemic vegetation may occur resulting in distinct soil forming processes. In the Southeastern region of Brazil, the Itatiaia National Park (INP) is an example of this conditions, mainly in the INP upper part (plateau) placed above the 2000 m topographic line. The climatic conditions and rock outcrops favored the occurrence of herbaceous graminoid plants, mostly Cyperaceae and Poaceae, arranged in clumps, with fewer incidences of other species [1]. The low temperatures also lead to preservation of C and its incorporation into the soil matrix. Thus, when comparing to most tropical soils the INP soils have a large amount of TC, reaching up to 29.48%; also increasing the N, due to the strong correlation between them.

Among the many environmental functions of the INP soils, the upper part of the park is an important origin and distributor of water, contributing to important watersheds in the region. Especially in the summer, the soils in the INP plateau storage the water from rainfalls [2] and, along the

year, for a long period, the water is slowly released, thus feeding several springs which will contribute to important rivers like the *Paraíba do Sul* and *Rio Grande*, even during dry season.

Remote sense techniques have been applied in a wide range of fields, including soil science. The visible and near-infrared reflectance (Vis–NIR) techniques are fast, non-destructive, environmental-friendly and cost-effective. One of the first studies with soil and reflectance or absorbance was conducted by [3], with the characterization of the vibrational process and spectral signatures of soil minerals. In the consecutive decades, soil properties became more and more a topic of interest for the Vis–NIR study field.

Organic matter and iron oxides have a tendency to absorb the incident radiation, where a low iron content changes the shape of the curve from a horizontal to a positive upward trend [4]. Coarser granulometry and the quartz content tend to increase the reflectance, and the absorption power of incident radiation of organic matter is mainly between 450 and 1000 nm [5]. Correlations among soil attributes and spectral signatures were found by [6]. Spectral behavior of different soil classes is governed mainly by mineralogical composition, organic matter content, and grain size [5]. In a study of spectral behavior of a Brazilian soil in which the organic matter was removed by a chemistry treatment, there was an increase of the reflectance factor by more than 100%, driven mostly by the interaction of organic matter with oxide minerals [7]. Currently, several soil properties and attributes have been predictable by using different methods and algorithms [8].

The most applied technique is the Partial least-squares regression (PLSR), as in the cited studies [9–12]. Other algorithms such as Artificial Neural Network (ANN) were also applied with satisfactory result [13,14]. Other studies [15–19] compared the prediction capacity of soil properties by spectral data using different algorithms such as Artificial Neural Network (ANN), Random Forest (RF), PLSR and Cubist (CB).

Although raw spectral data can be used for soil property prediction, the application of pre-treatments can enhance this capacity. Some frequently used techniques with good results are the Savitzky-Golay filter [20], the noise reduction [21,22], and the continuum removal [23][12,24].

The motivation to undertake this study comes from the fact that INP plateau has peculiar and distinct environmental conditions from what is dominant in other tropical regions, in Brazil and abroad, consequently, different soil types and properties. The hypothesis of this study is that by applying spectral data analysis it is possible to predict soil properties in regions with difficult access such as INP.

Thus, the main objective of the study was to test and compare the prediction capacity of ANN, PLSR, RF and CB algorithms for the contents of extractable elements aluminum (Al), calcium (Ca), potassium (K), magnesium (Mg), sodium (Na), phosphorus (P), plus pH, total carbon (TC), hydrogen (H) and nitrogen (N) through the Vis–NIR spectral region with various spectral pre-treatments.

2. Materials and Methods

2.1. Study area description

The INP is divided in three sectors, *Mauá* (east), lower part (south) and the upper part (central and northwest) (Figure 1). The study area comprehends the upper part of the park, which is a designation applied to the areas with elevation above 2.000 m. The highest point in the park is the so-called *Pico das Agulhas Negras* with 2,791.6 m of elevation. The INP is located at the border of Rio de Janeiro and Minas Gerais states, and also near São Paulo state border, in the Southern region of Brazil.

The area is comprising by the coordinates 44°34'- 44°42'W and 22°16'- 22° 28'S. According to the Köppen classification, the climate is Cwb-type [25–27]. The yearly temperature average is of 11,5°C, and the average during the winter is 8,4°C, reaching below zero sporadically.

INP plateau has an expressive area of Histosols or other shallow soils with an organic horizon, covered mostly by herbaceous graminoid plants, with dominance of Cyperaceae and Poaceae arranged in clumps [1], located in the narrow valleys and talus with lower slopes. The INP plateau dominant geology is formed by alkaline syenites and granite-gneissic rocks [28]. The landscape is mainly formed by high mountains and escarpments with narrow valleys among the rock outcrops.

The INP is the first national park created in Brazil (1937) and it is now a natural conservancy area to preserve the Atlantic Forest biome. Since the eighteenth century, researchers from many countries have been there to study the biodiversity of the mountain complex of *Serra da Mantiqueira*, where the INP is located. The vegetation profile inside the park changes according to the altitude, from dense forest to sparse, until herbaceous graminoid plants [28].

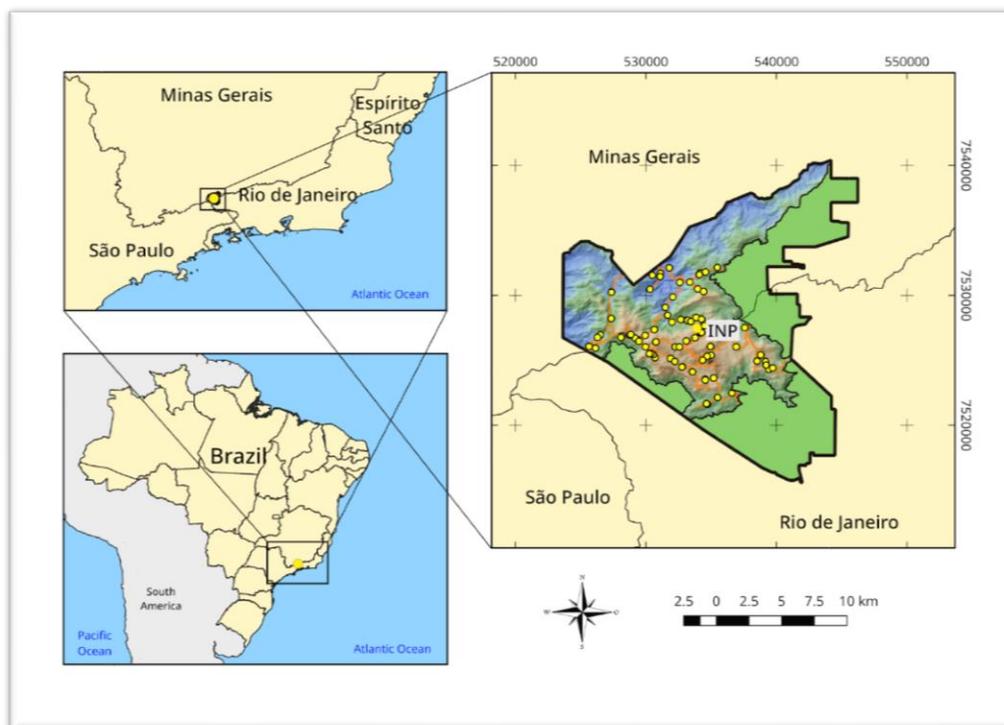


Figure 1. Itatiaia National Park, near the triple border of Rio de Janeiro (RJ), Minas Gerais (MG) and São Paulo (SP) States. To the right, the three sections of the park: *Mauá* (east), lower part (south) and the upper part (central and northwest).

2.2 Soil sampling, analysis and preparations

Soil profiles sampling locations were set by using the Conditioned Latin Hypercube Sampling (cHLS) algorithm [29]. Since the area has a restricted access, due to occurrence of endemic species, environmental protection requirements, steeply relief or lack of trails, the cHLS algorithm was set to place sampling locations near the tracks, with a buffer of 100 m from the paths with highest potential to express the variability of the soils in the landscape.

Initially, 80 points were determined, but 6 fell on rock outcrops. During the excursion 10 random samples were added, set according to the experience of the research team, to cover the range of INP soils variability, thus resulting in a total of 84 profiles (as presented in Figure 1 as yellow dots). Among those 84 profiles, 33 were classified as *Organossolos* according to the Brazilian System of Soil Classification (SiBCS) [30], which is an equivalent of Histosols [31]. From the horizons or layers of the 84 profiles, there were obtained 300 soil samples (96 are from the organic soils). Part of the samples were prepared and analyzed for the contents of Al, H, Ca, K, Mg, Na, N, P, pH and TC according to [32], and another part was set for the spectral readings, as described below.

To minimize the moisture influence in the spectral reading, soil samples were dried in an oven under forced air circulation, at a temperature of 45°C for 48 hours according [6,24,33,34]. Figure 2 presents a summary of these steps.

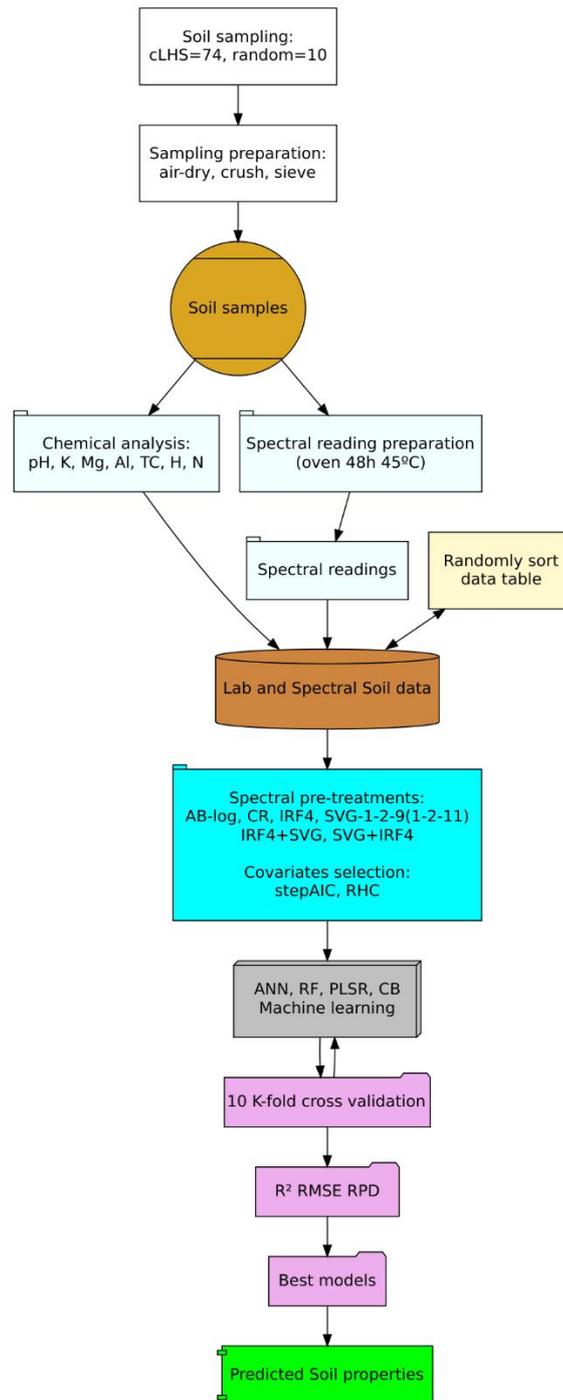


Figure 2. Steps to perform the soil analysis and spectral predictions of soil properties.

For the spectral readings, soil samples were placed into Petry dish of 9 cm of diameter, and they were read by using an ASD FieldSpec 4® spectrometer which the wavelength range Vis–NIR from 350 to 2500 nm, and the bandwidth of 10 nm. All spectral readings were proceeded in a dark room and in the same day. To avoid light source oscillations and consequently variations between readings, a battery powered no break line was connected to the device. The light source was a 70 Watts halogen bulb lamp, positioned 15° from nadir, by the distance of 70 cm. The optical fiber probe sensor was placed 35 cm

from the soil samples with an objective lens of 8° and nadir 0°. To each soil sample, 100 scans were done, rotations of 120° were realized to homogeneous reading. By every 30 minutes or 24 samples reading the optimize and white reference were done according to the equipment manufacturer instructions.

2.3 Data handling, spectral pre-treatment, covariates selection

The spectroradiometer data (format file .asd) was converted in a plain text file, then tie to the contents of Al, Ca, H, K, Mg, Na, N, P, pH and TC data from the wet chemistry laboratory analyses. In order to improve the prediction results, two approaches were adopted. The first was pre-treatments in the spectral data such as Continuum Removal (CR) [23], Savitzky-Golay (SVG) [20] with different settings across the derivative, order polynomial and search window [35], and Inverse of Reflectance by a Factor of 10^4 (IRF4). The IRF4 was obtained dividing 10,000 for each value of the reflectance spectrum. A conversion of spectral data to absorbance by the $-\log_{10}(\text{reflectance})$ [8] (AB-log) was also included as pre-treatment (Table 1) (Figure 3). The second approach was the techniques of dimensionality reduction of spectral covariates, such as Stepwise Algorithm by the Akaike information criteria (stepAIC) which removed 1851 from 2150, keeping only 299 covariates. The second technique was the Removal of High Correlated Covariates (RHCC) by correlation matrix approach removing 480 covariates from the dataset keeping 1686.

Seeking for error in the dataset, we also tested the removal outliers with a Principal Component Analyses Location (PCAL), by removing samples located outside of the standard deviation distance of five percent, which removed 10 samples. A similar approach was used by [15] that accesses the model performance before and after removing the outlier samples.

The best results from the two approaches were combined then reapplied in the algorithms. For example, after apply SVG we performed IRF4 over the result of SVG and vice-versa giving SVG-1-2-11+IRF4; IRF4+SVG-1-2-11 as Table 1. Also was identified noise, which was removed by Noise Removal (350-433 nm) (NR), it was visually identified in the spectral graphs as the initial (83) wavelengths of IRF4 curve (Figure 3).

The dataset (wet chemistry laboratory and spectral combined) was randomly sorted once to avoid biased K-folds selection on the cross-validation approach. Then it was submitted to each pre-treatments and techniques, as defined in Table 1. The data from wet chemistry remained unchanged, in other words, it was not treated or converted in any sort of method, only the spectral data. As a reference the raw data (with no treatment) was also computed across the models.

Table 1. Pre-treatments applied to spectral data from soil samples of the Itatiaia National Park.

Pre-treatment	Abbreviation
Conversion to absorbance $-\log_{10}(R)$	AB-log
Continuum Removal	CR
Inverse of Reflectance by a Factor of 10^4	IRF4
Savitzky-Golay 1st derivative using a 2nd-order polynomial and search window 9	SVG-1-2-9
Savitzky-Golay 1st derivative using a 2nd-order polynomial and search window 11	SVG-1-2-11
Savitzky-Golay 1st derivative using a 2nd-order polynomial and search window 11 + the	SVG-1-2-11 + IRF4
Inverse of Reflectance by a factor of 10^4	

Inverse of Reflectance by a Factor of 10^4 + Savitzky–Golay 1st derivative using a 2nd-order polynomial and search window 11	IRF4 + SVG-1-2-11
Savitzky–Golay 1st derivative using a 2nd-order polynomial and search window 11 + Inverse of Reflectance by a Factor of 10^4 + Noise Reduction (from 434 nm)	SVG-1-2-11 + IRF4 + NR 434
Inverse of Reflectance by a Factor of 10^4 + Savitzky–Golay 1st derivative using a 2nd-order polynomial and search window 11 + Noise Reduction (from 434 nm)	IRF4 + SVG-1-2-11 + NR 434
Savitzky–Golay 1st derivative using a 2nd-order polynomial and search window 11 + Noise Reduction (from 434 nm)	SVG-1-2-11 + NR 434
Inverse of Reflectance by a Factor of 10^4 + Noise Reduction (from 434 nm)	IRF4 + NR 434

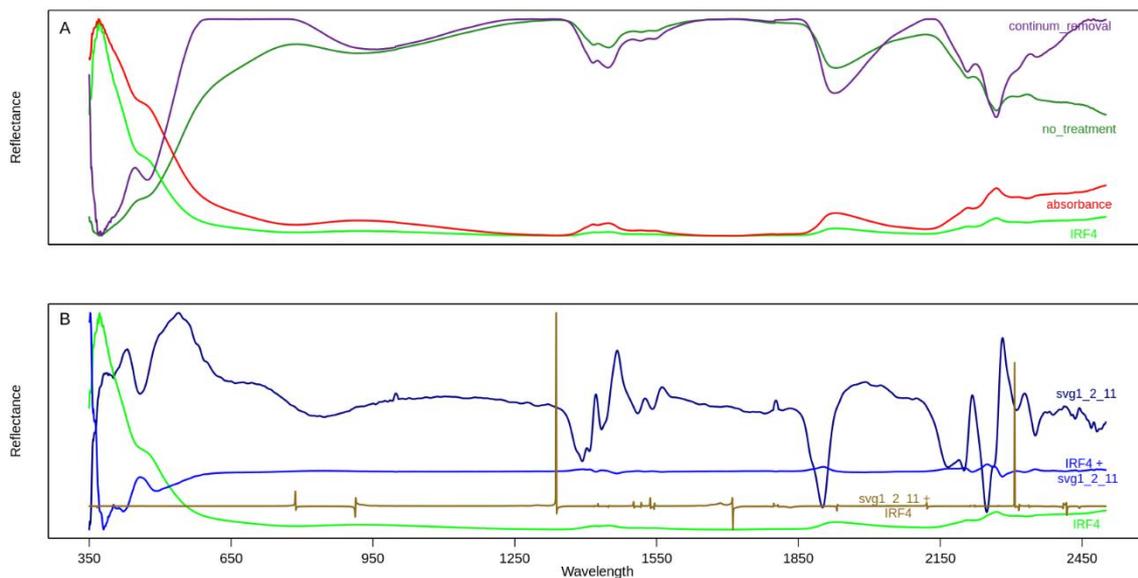


Figure 3. Spectral data: (A) Continuum Removal (magenta); no treatment (raw spectrum) (green); absorbance (red); Inverse of Reflectance by a Factor of 10^4 (light green). (B) Savitzky-Golay first derivative (dark blue); Inverse of Reflectance by a Factor of 10^4 + Savitzky-Golay first derivative (purple); Savitzky-Golay first derivative + Inverse of Reflectance by a Factor of 10^4 (brown); Inverse of Reflectance by a Factor of 10^4 (light green). Each curve fits in its own y (reflectance) scale.

2.4 Artificial Neural Network (ANN)

The initial development of Artificial Neural Network (ANN) was done [36] in 1958, and it was revised by the 80 and 90 decades. In a literature review [8] it was shown that ANN was not commonly applied for prediction of soil properties. PLSR is largely used instead, and Middle Infrared (MIR) is more common in soil analysis than Vis–NIR. One of the first applications of ANN for prediction of soil properties prediction [13] used different bandwidths, 10, 20 50 and 100 nm.

In this study, the ANN algorithm was performed with the dataset scaled between zero (0) and one (1). After that, the predicted data was converted to the original scale to perform the validation. The ANN consists of input data hidden layer (which can be one or more) and output layers. In this case, the hidden layers were defined as a combination of 4 hidden layers containing 13-8-5-3 neurons. In this arrangement every neuron was linked with all neurons of the next layer, but no linkage with others neurons in the same layer (Figure 4).

regression trees [41,42]. The CB follows four steps [41]: i) separation of data to grow a complete tree; ii) creation of a regression model at each node to prepare to pruned and prediction; 3) pruned the tree to evade overfitting problem; 4) smoothing the tree to obfuscate the discontinuities limits caused by the splitting.

2.8 Models performance assessment, cross-validation approach

The dataset was split in 10 K-folds to perform cross validation. Across the 11 pre-treatments, 2 reduction of data dimensionality techniques, PCAL, raw data (no spectral pre-treatment) for the 4 machine learning models (ANN, RF PLSR and CB), and 10 soil properties, a total of 600 models were performed. Considering the models for each of the 10 K-fold performed, we have a total of 6,000 models.

To evaluate the performance of prediction models, the root mean squared error (RMSE), coefficient of determination (R^2) and the ratio of performance to deviation (RPD) were calculated over the average of the K-folds. The coefficients were calculated as an average across the K-folds. RPD is given by the ratio of standard deviation to the RMSECV (root mean square error of cross-validation) or RMSEP (root mean square error of prediction) between measured and predicted values [43]. Three classes of RPD are defined, where $RPD > 2$ are the models that can predict well the soil property in analyze, RPD between 1.4 and 2 as an intermediate, and $RPD < 1.4$ with no prediction ability [9,43]. The models were assessed essentially by the R^2 , RMSE and RPD.

2.9 Software

The software used to proceed the spectral reading was the Rs3®.

The data processing and predictions were proceeding with R [44]. With the packages: base [45] and dplyr [46] for data manipulation; rstudioapi [47] to automatically set working directory; caret [48] to find high correlated covariates; prospectr [49] to visualize spectral data and apply pre-treatments such as Savitzky-Golay and continuum removal; randomForest [50] for Random Forest, Cubist [42,51] for Cubist, pls [52] for PLSR and neuralnet [53] for ANN predictor algorithms; MASS [54] for stepAIC application; ithir [55] for metrics; RColorBrewer [56], hexbin [57], grid [58], and ggplot2 [59] for graphs; DMwR [60] for unscale the data after ANN; and stringr [61] to access the results.

3. Results

3.1. Laboratory measured soil properties

The summary statistics for the soil properties measured using conventional chemistry methods are present in the Table 3 and Figure 5.

Table 3. Descriptive statistics of properties of soils sampled at the INP.

Soil	Unit	N	Mean	SD	Median	Min	Max	Skew	Kurtosis	SE
Al	cmol _c kg ⁻¹	300	2.01	1.48	1.8	0	9.2	1.5	3.57	0.09
Ca	cmol _c kg ⁻¹	300	0,14	0,26	0,09	0	2,55	5,75	42,45	0,02
H	%	300	1.93	0.74	1.88	0.33	4.37	0.47	0.19	0.04
K	cmol _c kg ⁻¹	300	0.14	0.15	0.08	0.01	1.26	3.06	14.64	0.01
Mg	cmol _c kg ⁻¹	300	0.5	0.3	0.42	0	1.67	1.53	2.26	0.02
N	%	300	0.36	0.35	0.25	0	1.85	1.43	1.93	0.02

Na	cmol _c kg ⁻¹	300	0.03	0.05	0.03	0	0.8	10.95	149.19	0
P	ppm	300	7.33	8.47	4.81	0.19	97.51	5.03	43.28	0.49
pH	Unitless	300	4.5	0.4	4.5	3.24	5.72	0.08	0.09	0.02
TC	%	300	5.9	5.62	3.99	0.24	29.48	1.38	1.71	0.32

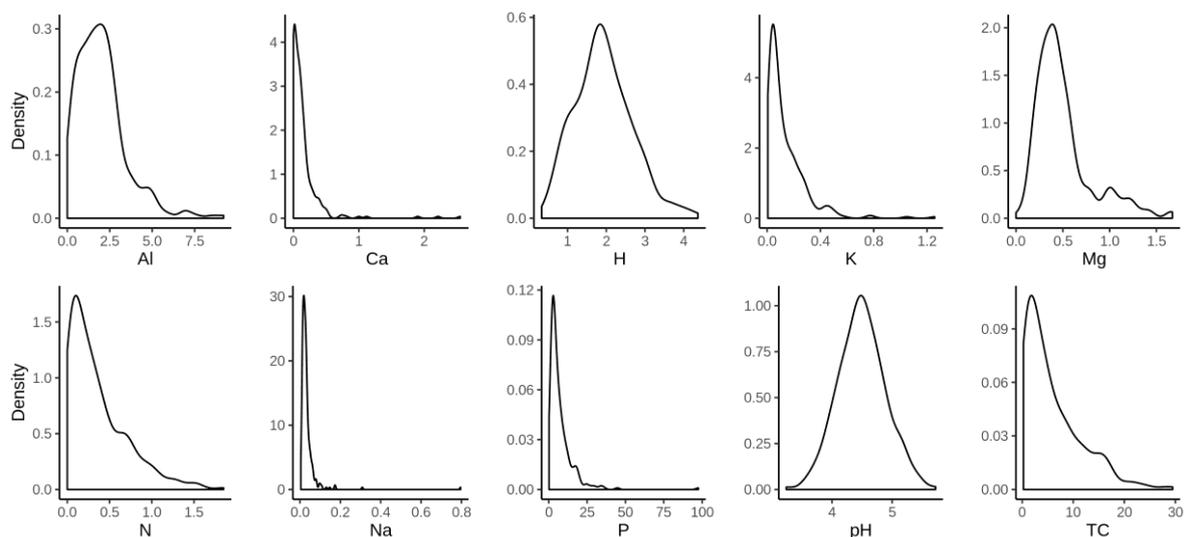


Figure 5. Density plot of properties of soils sampled at the INP.

The number of samples (N) was equal to 300 for all properties. Most of them deviate from normal distribution (Figure 5 and Skew from Table 3), except for pH and H values which presented skew and Kurtosis close to zero.

3.2. Assessment of the models

To evaluate the performance of prediction models, the root mean squared error (RMSE), coefficient of determination (R^2) and ratio of performance to deviation (RPD) were calculated over the average of the K-folds. From the 600 models, the best model associated with the best pre-treatment, was the CB for TC with R^2 of 0.85, RPD of 2.87 (highest), followed by PLSR for N with R^2 of 0.82 and RPD of 2.65, and RF for Al with R^2 of 0.54 and RPD of 1.54 (Table 4). For contents of TC, Al, N, pH the RF presented the best association among the pretreatments giving the best results in 36 cases, compared to 21 cases for CB, 3 for PLSR, and none (0) for ANN. For pH values the pre-treatments significantly increased the performance bringing the R^2 from 0.096 to 0.36, followed by Al from 0.36 to 0.54. In general, the best pre-treatment was IRF4, SVG-1-2-11 and their combination with NR (Table 5). The AB-log was more favorable to TC with a slightly improvement for N and Al values.

The reduction of dimensionality technique was favorable in the case of pH values, with an improvement for Al, but not substantial in all cases. The stepAIC with only 299 wavelengths (covariates) still performed satisfactorily when considered the fact it is using only 14 % of all spectral data. As observed for the N values, in some cases, some pre-treatments decrease the performance of the model, like CR for TC (Table 5). The validation graphs of the properties Al, H, K, Mg, N, P, pH and TC can be observed in the Figure 6, following the models and pre-treatments of Table 4. The 600 models are presented as supplementary materials (Table A1).

Table 4. Outstanding pre-treatment with the associated models for each property of soils sampled at the INP.

Pre-treatments	Model	Soil property ¹	R ²	MSE	RMSE	bias	RPD
IRF4 + SVG-1-2-11 + NR 434	rf	Al	0.536	0.944	0.954	0.037	1.541
IRF4	cb	H	0.672	0.173	0.411	-0.034	1.817
SVG-1-2-11 + IRF4 + NR 434	rf	K	0.275	0.017	0.118	0.003	1.244
SVG-1-2-11	rf	Mg	0.194	0.074	0.267	0.014	1.148
IRF4 + NR 434	plsr	N	0.819	0.018	0.13	-0.005	2.649
SVG-1-2-11 + IRF4 + NR 434	rf	P	0.072	66.896	7.436	0.137	1.07
SVG-1-2-11	rf	pH	0.363	0.096	0.309	-0.005	1.286
IRF4	cb	TC	0.852	3.998	1.958	-0.044	2.867

¹Ca and Na are not shown in the table due to the very poor results.

Table 5. Full group of pre-treatments with the associated models for values of TC, N, Al, pH of soils sampled at the INP.

Pre-treatments	Model	Soil property	R ²	MSE	RMSE	bias	RPD
IRF4	cb	TC	0.852	3.998	1.958	-0.044	2.867
IRF4 + SVG-1-2-11	rf	TC	0.841	4.753	2.112	-0.038	2.65
IRF4 + SVG-1-2-11 + NR 434	rf	TC	0.84	4.749	2.113	-0.027	2.649
SVG-1-2-11	rf	TC	0.836	4.718	2.123	0	2.627
SVG-1-2-9	rf	TC	0.833	4.84	2.147	0.014	2.604
SVG-1-2-11 + NR 434	rf	TC	0.831	4.854	2.143	0.024	2.632
AB-log	cb	TC	0.829	4.717	2.121	-0.14	2.652
SVG-1-2-11 + IRF4	rf	TC	0.826	5.047	2.194	-0.013	2.539
SVG-1-2-11 + IRF4 + NR 434	rf	TC	0.824	5.006	2.183	0.014	2.569
IRF4 + NR 434	plsr	TC	0.824	4.965	2.181	-0.055	2.559
no pre-treatment	cb	TC	0.824	5.128	2.153	-0.059	2.667
CR	rf	TC	0.81	5.581	2.295	0.026	2.442
stepAIC	cb	TC	0.803	5.339	2.266	-0.052	2.466
PCAL	cb	TC	0.793	5.518	2.297	-0.148	2.338
RHCC	cb	TC	0.789	6.179	2.41	-0.166	2.338
IRF4 + NR 434	plsr	N	0.819	0.018	0.13	-0.005	2.649
IRF4 + SVG-1-2-11 + NR 434	rf	N	0.815	0.019	0.137	-0.002	2.466
IRF4 + SVG-1-2-11	rf	N	0.812	0.02	0.138	-0.002	2.446
AB-log	plsr	N	0.798	0.021	0.143	-0.003	2.37
SVG-1-2-11	rf	N	0.797	0.021	0.142	0.003	2.382
SVG-1-2-9	rf	N	0.791	0.021	0.143	0.003	2.37
SVG-1-2-11 + IRF4	rf	N	0.787	0.022	0.146	0	2.321
SVG-1-2-11 + NR 434	rf	N	0.786	0.021	0.144	0.005	2.375

SVG-1-2-11 + IRF4 + NR 434	rf	N	0.777	0.022	0.148	0.002	2.318
RHCC	cb	N	0.769	0.025	0.153	-0.008	2.265
CR	rf	N	0.755	0.026	0.157	0.004	2.166
no pre-treatment	cb	N	0.743	0.028	0.162	-0.009	2.141
IRF4	cb	N	0.731	0.03	0.161	-0.005	2.232
stepAIC	cb	N	0.728	0.028	0.164	-0.009	2.085
PCAL	cb	N	0.701	0.031	0.173	-0.004	1.89
IRF4 + SVG-1-2-11 + NR 434	rf	Al	0.536	0.944	0.954	0.037	1.541
IRF4 + SVG-1-2-11	rf	Al	0.527	0.967	0.965	0.039	1.527
SVG-1-2-11 + NR 434	rf	Al	0.522	0.97	0.966	0.042	1.529
IRF4 + NR 434	cb	Al	0.517	0.935	0.961	0.003	1.514
SVG-1-2-11	rf	Al	0.513	0.987	0.974	0.049	1.52
SVG-1-2-9	rf	Al	0.511	0.981	0.973	0.045	1.516
SVG-1-2-11 + IRF4 + NR 434	rf	Al	0.506	1.028	0.992	0.032	1.485
SVG-1-2-11 + IRF4	rf	Al	0.487	1.071	1.012	0.034	1.459
AB-log	cb	Al	0.431	1.135	1.049	-0.079	1.405
stepAIC	cb	Al	0.423	1.152	1.062	-0.117	1.371
IRF4	cb	Al	0.419	1.078	1.027	-0.078	1.449
CR	rf	Al	0.388	1.225	1.097	0.062	1.322
no pre-treatment	cb	Al	0.362	1.264	1.111	-0.072	1.319
RHCC	cb	Al	0.261	1.402	1.161	-0.076	1.295
PCAL	rf	Al	0.249	1.516	1.218	0.056	1.203
SVG-1-2-11	rf	pH	0.363	0.096	0.309	-0.005	1.286
SVG-1-2-11 + NR 434	rf	pH	0.352	0.098	0.312	-0.007	1.278
SVG-1-2-9	rf	pH	0.352	0.098	0.312	-0.006	1.277
IRF4 + SVG-1-2-11 + NR 434	rf	pH	0.347	0.098	0.311	0	1.284
IRF4 + SVG-1-2-11	rf	pH	0.346	0.098	0.312	0	1.28
SVG-1-2-11 + IRF4 + NR 434	rf	pH	0.329	0.101	0.317	-0.005	1.255
SVG-1-2-11 + IRF4	rf	pH	0.322	0.102	0.319	-0.005	1.249
IRF4	cb	pH	0.22	0.117	0.34	-0.02	1.18
IRF4 + NR 434	cb	pH	0.21	0.118	0.342	-0.007	1.172
CR	rf	pH	0.18	0.124	0.351	0	1.133
AB-log	cb	pH	0.123	0.134	0.362	-0.014	1.115
PCAL	cb	pH	0.097	0.141	0.373	-0.015	1.087
stepAIC	rf	pH	0.097	0.137	0.369	0.004	1.082
no pre-treatment	rf	pH	0.096	0.139	0.37	0.004	1.08
RHCC	rf	pH	0.071	0.141	0.374	0.003	1.067

Scrutinizing inside of the K-folds of TC values (Table 6), it is observed that the R^2 validation coefficient ranges from 0.78 to 0.94. And for the 10th fold the RPD is highest, the best MSE and RMSE stays in the fold 6. For P and K values, the folder 8 shows a huge difference in the coefficients. While the

average of R^2 for P values is 0.072, fold 8 gives 0.35, and for K we have R^2 average of 0.275 and fold 8 of 0.674.

Table 6. The coefficients within the 10 K-folds for TC, P and K.

K-Folds	R^2	MSE	RMSE	bias	RPD
TC.1	0.814	7.209	2.685	0.045	2.36
TC.2	0.899	3.947	1.987	-0.062	3.193
TC.3	0.894	3.203	1.79	-0.433	3.13
TC.4	0.781	7.54	2.746	0.055	2.174
TC.5	0.843	3.005	1.734	0.363	2.571
TC.6	0.9	2.486	1.577	0.047	3.218
TC.7	0.886	2.83	1.682	-0.155	3.018
TC.8	0.87	4.353	2.086	-0.26	2.822
TC.9	0.682	2.794	1.672	0.541	1.804
TC.10	0.946	2.617	1.618	-0.578	4.377
P.1	-0.163	79.717	8.928	-0.819	0.943
P.2	-0.207	37.404	6.116	1.477	0.926
P.3	0.222	34.459	5.87	0.736	1.153
P.4	0.18	56.343	7.506	0.204	1.123
P.5	0.272	24.237	4.923	0.177	1.192
P.6	-0.003	40.109	6.333	0.869	1.015
P.7	-0.023	291.659	17.078	-1.512	1.006
P.8	0.352	34.759	5.896	-0.659	1.264
P.9	-0.023	24.13	4.912	0.71	1.005
P.10	0.108	46.141	6.793	0.185	1.077
K.1	-0.034	0.058	0.24	-0.041	1
K.2	0.27	0.006	0.08	0.006	1.19
K.3	0.141	0.008	0.091	0.033	1.097
K.4	0.35	0.026	0.161	-0.007	1.261
K.5	0.163	0.025	0.158	-0.021	1.112
K.6	0.3	0.006	0.076	0.033	1.215
K.7	0.089	0.006	0.08	0.033	1.066
K.8	0.674	0.005	0.071	-0.001	1.783
K.9	0.576	0.004	0.063	0.024	1.561
K.10	0.225	0.026	0.16	-0.024	1.155

For TC, IRF4 with CB model; for P and K (SVG-1-2-11 + IRF4 + NR 434) with RF model.

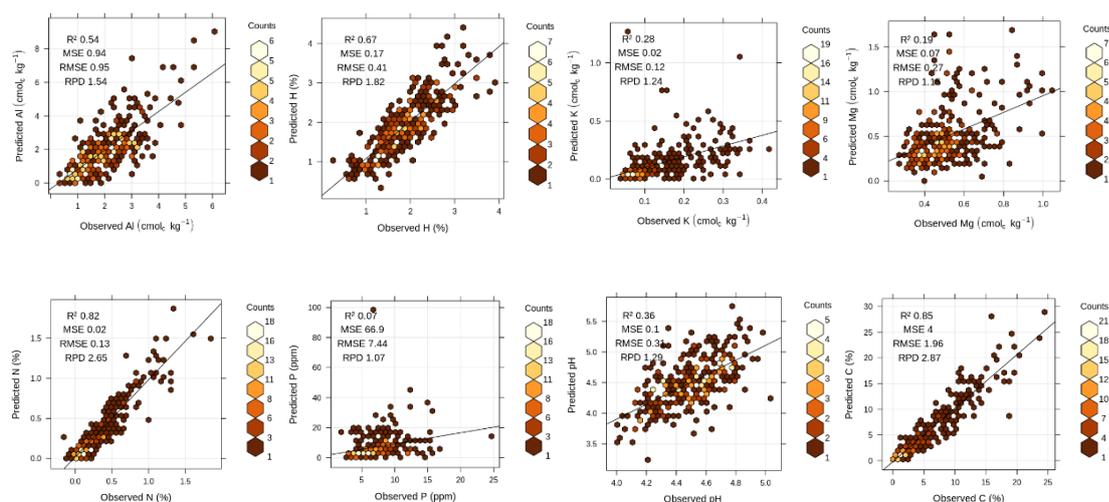


Figure 6. Prediction of Al, H, K, Mg, N, P, pH and TC values with the respective pre-treatment according Table 4.

4. Discussion

The best predicted soil property was the TC, with R^2 0.85, RMSE 1.96, Bias -0.04 and RPD of 2.87 (Figure 6). The other properties showed Bias close to zero with the exception of P with 0.137. From the dimensionality reduction (Table 5) the RHCC, and specially stepAIC demonstrated that the spectral resolution is not the main driver to improve the prediction of soil properties, which is in agreement with [9], but it still allowed the models to reach R^2 0.8, RMSE 2.26, Bias -0.052 and RPD 2.47 for TC with CB model (Table 4). In addition, the RHCC and stepAIC reduced processing time, thus machine power consumption. CR was similar to RF giving R^2 0.81, RMSE 2.30, Bias 0.026 and RPD of 2.44. Differently from [15] the removal of outliers did not improve the prediction; however, it may make a difference in large databases. The PCAL with 5% removed still provided satisfactory results with R^2 0.79 and RPD of 2.33.

The Sawitzky–Golay filter improved the prediction of Al, K, Mg, P and pH [12,35], with the setting of SVG-1-2-11 providing higher coefficients in comparison with SVG-1-2-9. The application of IRF4 benefitted the models and increased the results in 6 of the 8 predicted properties of the Table 4, which are Al, H, K, N, P, and TC.

Close predictions of TC were obtained with ANN and with a bandwidth of 10 nm [13], and the bandwidth had a role in the prediction capacity. Although, the machine learning such as RF and CB showed good prediction capacity, the results using ANN may be further improved with a larger dataset. A review of methods and results [8] show better prediction values [62] in which organic carbon in the VIS–NIR region have a R^2 of 0.89 using PLSR that is widely applied in the literature. In this study we found, overall, that the Cubist model and Random Forest presented the best prediction capacity for TC.

Despite of internal machine learning algorithms variances, the random selection data for calibration/validation the models can produce slightly to considerable different results among the folds, as observed in the properties TC, P, and K (Tables 6). Larger datasets can have this effect dissipated. In the sense of managing the data variability within the dataset, the K-fold cross validation presented consistent coefficients (Tables 4 and 5), since they are given by the average of the coefficients across the folds. Inside the folds (Tables 6) it is possible to observe the models performed very different for each folder. Figure 7 shows the spectral plot of IRF4 K-folds from 1 to 7 and 9 to 10 (orange), with folder 8

illuminated in blue. The spectral behavior of fold 8 show less heterogeneity (from 950 to 2150 nm) which points to a better prediction for P, K inside fold 8 with the machine learning algorithms.

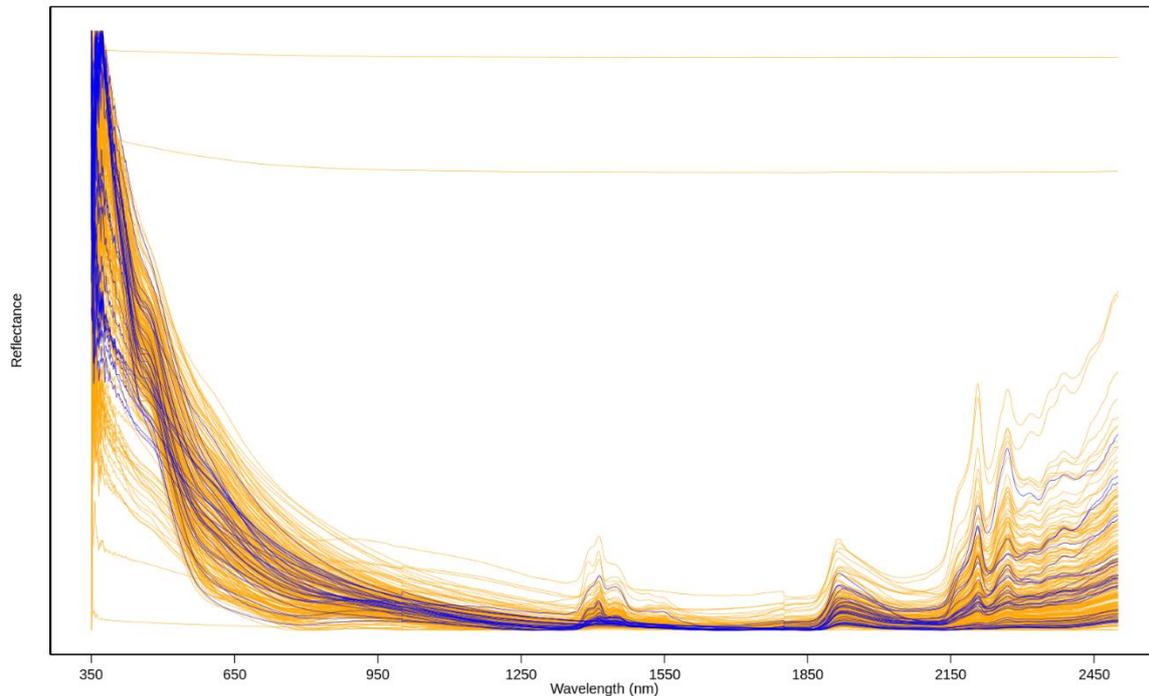


Figure 7. Spectral plots of soil samples from INP, with IRF4 pre-treatment. Fold 8 is in blue.

5. Conclusions

With the usage of Vis–NIR and the prediction algorithms ANN, RF, PLSR, CB, the soil properties TC and N presented the best prediction capacity, followed by H and Al.

As for the pre-treatments, each soil property has the prediction potential increased from a specific spectral pre-treatment. In this way, globally SVG spectral increased the potential of prediction, although, IRF4 outperformed the SVG. The combination of both with NR also showed good response from the algorithms. For some pre-treatment to soil properties, such as CR for TC and IRF4 for N, the pre-treatments decreased the potential of prediction. Without spectral pre-treatment (on raw spectral data), the CB model showed the best prediction capacity, followed by and RF.

IRF4 was the best pre-treatment for N values when combined with NR. And IRF4 was the best for TC (R^2 0.85), also rises the prediction of H, both using CB. Succeeding by PLSR for N, and RF for Al. The most present algorithm among the higher predicted values was RF (5 out of 8).

The K-fold cross validation provides reliable coefficients indicators. The spectral data heterogeneity within the K-folds tend to decrease with the larger datasets, rising the prediction capacity.

Considering that soil carbon is an indicator of soil health, quality and degradation, the results obtained from the applied techniques are relevant for the Itatiaia National Park management plan, and also to similar environments. Those techniques have potential for predicting soil properties in other areas of Atlantic Forest and mountainous landscape, and they are especially important in regions with

limited access. The good correlation with Vis–NIR techniques allows for future monitoring of soil properties, such as organic carbon, by using remote sensing tools.

Funding: This study was funded in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - Finance Code 001; FAPERJ - Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro; Also, Financial Supported by TEMPUS PUBLIC FOUNDATION.

Acknowledgments: To the Federal Rural University of Rio de Janeiro, the Postgraduate Program in Science, Technology and Innovation in Agriculture (PPGCTIA), the team of field campaigns and the team of laboratory analyses. Special thanks to the professors and students involved in this study.

Conflicts of Interest: The authors declare no conflict of interest.

Appendix A

Table A1. The 600 predicted properties across the models and pre-treatments.

Pre-treatments	Model	Soil property	R ²	MSE	RMSE	bias	RPD
AB-log	ann	Al	-0.484	2.631	1.592	0.063	0.944
AB-log	cb	Al	0.431	1.135	1.049	-0.079	1.405
AB-log	plsr	Al	0.382	1.159	1.072	0.031	1.364
AB-log	rf	Al	0.23	1.546	1.227	0.06	1.196
AB-log	ann	TC	0.025	27.364	5.058	0.428	1.154
AB-log	cb	TC	0.829	4.717	2.121	-0.14	2.652
AB-log	plsr	TC	0.819	5.003	2.19	-0.03	2.554
AB-log	rf	TC	0.769	6.714	2.527	0.036	2.213
AB-log	ann	H	0.091	0.473	0.679	-0.027	1.105
AB-log	cb	H	0.625	0.198	0.44	0.001	1.697
AB-log	plsr	H	0.565	0.228	0.471	0.007	1.598
AB-log	rf	H	0.53	0.24	0.486	0.003	1.543
AB-log	ann	N	0.491	0.049	0.208	-0.003	1.761
AB-log	cb	N	0.756	0.028	0.159	-0.005	2.203
AB-log	plsr	N	0.798	0.021	0.143	-0.003	2.37
AB-log	rf	N	0.691	0.032	0.177	0.002	1.935
AB-log	ann	Ca	-0.242	0.111	0.272	0.006	0.949
AB-log	cb	Ca	-0.224	0.088	0.259	-0.043	0.953
AB-log	plsr	Ca	-0.878	0.096	0.29	-0.002	0.787
AB-log	rf	Ca	-0.383	0.076	0.253	0.013	0.919
AB-log	ann	K	0.057	0.021	0.133	0	1.085
AB-log	cb	K	-0.837	0.025	0.136	-0.002	1.25
AB-log	plsr	K	-0.107	0.021	0.135	0.003	1.059
AB-log	rf	K	-0.109	0.022	0.141	0.011	0.998
AB-log	ann	Mg	-0.849	0.166	0.396	0.015	0.794
AB-log	cb	Mg	-0.135	0.101	0.314	-0.05	0.968
AB-log	plsr	Mg	-0.112	0.095	0.305	-0.002	1.002
AB-log	rf	Mg	-0.036	0.093	0.301	0.016	1.013
AB-log	ann	Na	-0.372	0.003	0.038	0	0.933
AB-log	cb	Na	-11.385	0.006	0.061	0	0.773
AB-log	plsr	Na	-3.472	0.004	0.054	0	0.594
AB-log	rf	Na	-1.31	0.003	0.044	0.003	0.874
AB-log	ann	P	-3.714	191.526	10.922	0.551	0.899
AB-log	cb	P	-0.354	85.214	8.583	-1.387	0.939
AB-log	plsr	P	-0.428	83.634	8.805	-0.076	0.869
AB-log	rf	P	-0.057	69.414	7.782	0.043	1.004
AB-log	ann	pH	-0.198	0.183	0.422	-0.011	0.957
AB-log	cb	pH	0.123	0.134	0.362	-0.014	1.115

AB-log	plsr	pH	0.123	0.133	0.362	-0.009	1.108
AB-log	rf	pH	0.095	0.138	0.369	0.005	1.081
CR	ann	Al	-0.063	2.126	1.438	-0.015	1.021
CR	cb	Al	0.381	1.198	1.078	-0.016	1.377
CR	plsr	Al	0.299	1.355	1.146	0.015	1.296
CR	rf	Al	0.388	1.225	1.097	0.062	1.322
CR	ann	TC	0.468	14.341	3.639	-0.07	1.576
CR	cb	TC	0.724	7.494	2.642	0.086	2.188
CR	plsr	TC	0.732	7.021	2.586	-0.05	2.214
CR	rf	TC	0.81	5.581	2.295	0.026	2.442
CR	ann	H	-0.116	0.551	0.736	-0.03	1.02
CR	cb	H	0.522	0.25	0.497	-0.021	1.492
CR	plsr	H	0.455	0.281	0.525	-0.002	1.422
CR	rf	H	0.497	0.265	0.51	0.001	1.46
CR	ann	N	0.642	0.039	0.192	0.009	1.799
CR	cb	N	0.625	0.038	0.19	0.006	1.849
CR	plsr	N	0.686	0.032	0.174	-0.003	2
CR	rf	N	0.755	0.026	0.157	0.004	2.166
CR	ann	Ca	-0.02	0.067	0.233	-0.002	1.012
CR	cb	Ca	-2.34	0.121	0.329	-0.024	0.744
CR	plsr	Ca	-1.748	0.113	0.324	0.001	0.7
CR	rf	Ca	-0.558	0.078	0.262	0.024	0.876
CR	ann	K	-0.136	0.023	0.144	0.002	0.962
CR	cb	K	-0.144	0.02	0.135	-0.009	1.047
CR	plsr	K	-0.066	0.02	0.135	0.002	1.024
CR	rf	K	0.249	0.016	0.116	0.009	1.28
CR	ann	Mg	0.047	0.086	0.29	-0.005	1.044
CR	cb	Mg	-0.364	0.123	0.341	-0.025	0.908
CR	plsr	Mg	-0.235	0.107	0.323	0.004	0.953
CR	rf	Mg	0.107	0.081	0.28	0.019	1.084
CR	ann	Na	-0.643	0.003	0.04	0	0.885
CR	cb	Na	-0.258	0.003	0.037	-0.005	0.99
CR	plsr	Na	-3.951	0.004	0.055	0	0.587
CR	rf	Na	-1.086	0.003	0.04	0.005	0.912
CR	ann	P	-0.165	79.209	8.24	0.177	0.959
CR	cb	P	-0.278	85.186	8.574	-1.374	0.92
CR	plsr	P	-0.702	96.102	9.427	0.189	0.824
CR	rf	P	-0.073	73.08	7.863	0.607	1.016
CR	ann	pH	-0.116	0.168	0.408	-0.002	0.977
CR	cb	pH	0.078	0.14	0.372	-0.018	1.073
CR	plsr	pH	-0.006	0.151	0.383	0	1.061
CR	rf	pH	0.18	0.124	0.351	0	1.133
IRF4	ann	Al	-0.286	2.393	1.518	0.159	0.99
IRF4	cb	Al	0.419	1.078	1.027	-0.078	1.449
IRF4	plsr	Al	0.176	1.67	1.268	0.043	1.168
IRF4	rf	Al	0.231	1.545	1.227	0.063	1.195
IRF4	ann	TC	0.524	14.238	3.624	-0.028	1.57
IRF4	cb	TC	0.852	3.998	1.958	-0.044	2.867
IRF4	plsr	TC	-0.701	60.745	5.01	0.006	1.84
IRF4	rf	TC	0.771	6.601	2.51	0.023	2.22
IRF4	ann	H	0.097	0.458	0.67	-0.043	1.132
IRF4	cb	H	0.672	0.173	0.411	-0.034	1.817
IRF4	plsr	H	-0.1	0.571	0.641	0.041	1.416
IRF4	rf	H	0.532	0.239	0.485	0.006	1.547

IRF4	ann	N	0.546	0.048	0.207	-0.003	1.75
IRF4	cb	N	0.731	0.03	0.161	-0.005	2.232
IRF4	plsr	N	0.375	0.066	0.23	0.006	1.731
IRF4	rf	N	0.685	0.033	0.179	0.003	1.908
IRF4	ann	Ca	-1.231	0.114	0.307	0.018	0.804
IRF4	cb	Ca	-0.307	0.091	0.266	-0.032	0.915
IRF4	plsr	Ca	-2.552	0.285	0.391	0.012	0.759
IRF4	rf	Ca	-0.374	0.076	0.253	0.013	0.923
IRF4	ann	K	-0.848	0.029	0.159	0.001	0.927
IRF4	cb	K	-0.551	0.023	0.13	-0.012	1.316
IRF4	plsr	K	-1.114	0.076	0.189	0.006	0.986
IRF4	rf	K	-0.117	0.022	0.141	0.011	0.993
IRF4	ann	Mg	-0.712	0.149	0.378	0.022	0.823
IRF4	cb	Mg	-0.056	0.095	0.304	-0.054	1.001
IRF4	plsr	Mg	-15.95	2.22	0.741	0.033	0.874
IRF4	rf	Mg	-0.037	0.093	0.301	0.017	1.013
IRF4	ann	Na	-1.626	0.003	0.041	-0.001	0.931
IRF4	cb	Na	-22.349	0.007	0.067	0	0.747
IRF4	plsr	Na	-102.221	0.039	0.118	0.006	0.474
IRF4	rf	Na	-1.345	0.003	0.044	0.003	0.864
IRF4	ann	P	-2.279	189.791	11.801	1.356	0.817
IRF4	cb	P	-0.335	80.372	8.382	-1.304	0.961
IRF4	plsr	P	-8.816	648.131	16.14	0.651	0.722
IRF4	rf	P	-0.062	70.088	7.812	0.052	1
IRF4	ann	pH	-0.328	0.204	0.44	-0.007	0.933
IRF4	cb	pH	0.22	0.117	0.34	-0.02	1.18
IRF4	plsr	pH	-2.228	0.457	0.558	-0.022	0.889
IRF4	rf	pH	0.096	0.138	0.369	0.006	1.081
IRF4 + NR 434	ann	Al	-0.01	1.816	1.329	0.04	1.131
IRF4 + NR 434	cb	Al	0.517	0.935	0.961	0.003	1.514
IRF4 + NR 434	plsr	Al	0.405	1.096	1.039	-0.012	1.431
IRF4 + NR 434	rf	Al	0.218	1.56	1.233	0.049	1.191
IRF4 + NR 434	ann	TC	0.472	12.351	3.401	0.366	1.728
IRF4 + NR 434	cb	TC	0.813	5.562	2.291	-0.204	2.451
IRF4 + NR 434	plsr	TC	0.824	4.965	2.181	-0.055	2.559
IRF4 + NR 434	rf	TC	0.774	6.521	2.493	0.048	2.24
IRF4 + NR 434	ann	H	0.066	0.47	0.672	-0.025	1.136
IRF4 + NR 434	cb	H	0.64	0.188	0.427	-0.026	1.766
IRF4 + NR 434	plsr	H	0.647	0.185	0.426	-0.019	1.745
IRF4 + NR 434	rf	H	0.498	0.257	0.502	0.005	1.503
IRF4 + NR 434	ann	N	0.624	0.04	0.186	-0.001	2.007
IRF4 + NR 434	cb	N	0.682	0.035	0.175	-0.001	2.054
IRF4 + NR 434	plsr	N	0.819	0.018	0.13	-0.005	2.649
IRF4 + NR 434	rf	N	0.697	0.032	0.175	0.002	1.952
IRF4 + NR 434	ann	Ca	-6.843	0.243	0.45	0.052	0.624
IRF4 + NR 434	cb	Ca	-0.704	0.094	0.276	-0.038	0.875
IRF4 + NR 434	plsr	Ca	-1.379	0.109	0.314	0.003	0.725
IRF4 + NR 434	rf	Ca	-0.345	0.075	0.251	0.012	0.934
IRF4 + NR 434	ann	K	-0.257	0.025	0.151	0.005	0.92
IRF4 + NR 434	cb	K	-0.95	0.027	0.15	-0.011	1.045
IRF4 + NR 434	plsr	K	-0.928	0.036	0.174	0.005	0.861
IRF4 + NR 434	rf	K	-0.109	0.022	0.141	0.012	0.999
IRF4 + NR 434	ann	Mg	-29.83	2.272	0.954	0.2	0.687
IRF4 + NR 434	cb	Mg	-0.143	0.101	0.315	-0.065	0.959

IRF4 + NR 434	plsr	Mg	-0.674	0.148	0.375	-0.007	0.828
IRF4 + NR 434	rf	Mg	-0.041	0.093	0.302	0.015	1.01
IRF4 + NR 434	ann	Na	-0.301	0.003	0.038	0	0.951
IRF4 + NR 434	cb	Na	-20.05	0.006	0.057	-0.003	0.902
IRF4 + NR 434	plsr	Na	-8.223	0.005	0.065	-0.001	0.505
IRF4 + NR 434	rf	Na	-1.328	0.003	0.044	0.003	0.854
IRF4 + NR 434	ann	P	-0.928	114.486	9.562	0.385	0.901
IRF4 + NR 434	cb	P	-0.071	75.301	7.954	-1.704	1.001
IRF4 + NR 434	plsr	P	-0.921	109.123	10.099	-0.02	0.763
IRF4 + NR 434	rf	P	-0.04	69.833	7.765	0.03	1.008
IRF4 + NR 434	ann	pH	-0.485	0.223	0.466	-0.024	0.873
IRF4 + NR 434	cb	pH	0.21	0.118	0.342	-0.007	1.172
IRF4 + NR 434	plsr	pH	-0.11	0.169	0.403	0	1.011
IRF4 + NR 434	rf	pH	0.081	0.14	0.372	0.005	1.071
IRF4 + SVG1-2-11	ann	Al	0.1	1.856	1.339	0.049	1.091
IRF4 + SVG1-2-11	cb	Al	0.398	1.166	1.056	-0.084	1.409
IRF4 + SVG1-2-11	plsr	Al	-8.592	21.427	2.541	-0.052	1.064
IRF4 + SVG1-2-11	rf	Al	0.527	0.967	0.965	0.039	1.527
IRF4 + SVG1-2-11	ann	TC	0.579	11.144	3.203	0.396	1.837
IRF4 + SVG1-2-11	cb	TC	0.819	4.896	2.167	-0.125	2.575
IRF4 + SVG1-2-11	plsr	TC	-2.989	148.945	6.607	-0.126	1.78
IRF4 + SVG1-2-11	rf	TC	0.841	4.753	2.112	-0.038	2.65
IRF4 + SVG1-2-11	ann	H	0.273	0.385	0.599	-0.015	1.321
IRF4 + SVG1-2-11	cb	H	0.602	0.207	0.447	0.006	1.702
IRF4 + SVG1-2-11	plsr	H	0.015	0.51	0.632	0.004	1.402
IRF4 + SVG1-2-11	rf	H	0.617	0.195	0.437	-0.004	1.724
IRF4 + SVG1-2-11	ann	N	0.544	0.053	0.208	0.008	1.897
IRF4 + SVG1-2-11	cb	N	0.741	0.027	0.161	-0.011	2.121
IRF4 + SVG1-2-11	plsr	N	-0.543	0.204	0.318	-0.001	1.604
IRF4 + SVG1-2-11	rf	N	0.812	0.02	0.138	-0.002	2.446
IRF4 + SVG1-2-11	ann	Ca	-2.12	0.129	0.319	0.016	0.809
IRF4 + SVG1-2-11	cb	Ca	-2.862	0.157	0.353	0.018	0.736
IRF4 + SVG1-2-11	plsr	Ca	-2.005	0.153	0.354	0.009	0.689
IRF4 + SVG1-2-11	rf	Ca	-0.471	0.079	0.261	0.021	0.881
IRF4 + SVG1-2-11	ann	K	0.084	0.02	0.13	-0.002	1.117
IRF4 + SVG1-2-11	cb	K	0.138	0.02	0.128	-0.007	1.144
IRF4 + SVG1-2-11	plsr	K	-1.611	0.079	0.204	0.005	0.908
IRF4 + SVG1-2-11	rf	K	0.215	0.017	0.12	0.006	1.24
IRF4 + SVG1-2-11	ann	Mg	-0.048	0.095	0.305	-0.001	0.996
IRF4 + SVG1-2-11	cb	Mg	-0.23	0.11	0.325	0.005	0.948
IRF4 + SVG1-2-11	plsr	Mg	-2.735	0.434	0.491	0.007	0.806
IRF4 + SVG1-2-11	rf	Mg	0.145	0.078	0.273	0.015	1.126
IRF4 + SVG1-2-11	ann	Na	-0.315	0.003	0.037	-0.001	0.96
IRF4 + SVG1-2-11	cb	Na	-19.047	0.007	0.064	0.002	0.737
IRF4 + SVG1-2-11	plsr	Na	-434.102	0.156	0.181	0.009	0.504
IRF4 + SVG1-2-11	rf	Na	-0.525	0.003	0.039	0.002	0.936
IRF4 + SVG1-2-11	ann	P	-2.677	151.246	10.146	1.297	0.92
IRF4 + SVG1-2-11	cb	P	-0.024	72.729	7.792	-1.313	1.019
IRF4 + SVG1-2-11	plsr	P	-9.319	673.771	16.989	0.786	0.663
IRF4 + SVG1-2-11	rf	P	0.032	68.528	7.548	0.468	1.072
IRF4 + SVG1-2-11	ann	pH	-0.111	0.171	0.408	0.015	0.988
IRF4 + SVG1-2-11	cb	pH	0.156	0.126	0.353	-0.015	1.138
IRF4 + SVG1-2-11	plsr	pH	-2.977	0.566	0.627	-0.012	0.785
IRF4 + SVG1-2-11	rf	pH	0.346	0.098	0.312	0	1.28

IRF4 + SVG-1-2-11 + NR 434	ann	Al	-0.05	2.094	1.432	0.019	1.018
IRF4 + SVG-1-2-11 + NR 434	cb	Al	0.464	1.112	1.037	-0.058	1.404
IRF4 + SVG-1-2-11 + NR 434	plsr	Al	0.263	1.387	1.165	-0.019	1.28
IRF4 + SVG-1-2-11 + NR 434	rf	Al	0.536	0.944	0.954	0.037	1.541
IRF4 + SVG-1-2-11 + NR 434	ann	TC	0.581	13.967	3.335	0.063	1.91
IRF4 + SVG-1-2-11 + NR 434	cb	TC	0.798	5.648	2.3	-0.212	2.461
IRF4 + SVG-1-2-11 + NR 434	plsr	TC	0.778	6.235	2.463	-0.065	2.229
IRF4 + SVG-1-2-11 + NR 434	rf	TC	0.84	4.749	2.113	-0.027	2.649
IRF4 + SVG-1-2-11 + NR 434	ann	H	0.198	0.418	0.632	-0.04	1.229
IRF4 + SVG-1-2-11 + NR 434	cb	H	0.627	0.194	0.436	-0.006	1.722
IRF4 + SVG-1-2-11 + NR 434	plsr	H	0.498	0.267	0.505	-0.014	1.509
IRF4 + SVG-1-2-11 + NR 434	rf	H	0.605	0.201	0.443	-0.002	1.699
IRF4 + SVG-1-2-11 + NR 434	ann	N	0.59	0.048	0.207	0.008	1.7
IRF4 + SVG-1-2-11 + NR 434	cb	N	0.764	0.024	0.15	-0.016	2.305
IRF4 + SVG-1-2-11 + NR 434	plsr	N	0.781	0.023	0.149	-0.005	2.267
IRF4 + SVG-1-2-11 + NR 434	rf	N	0.815	0.019	0.137	-0.002	2.466
IRF4 + SVG-1-2-11 + NR 434	ann	Ca	-0.457	0.088	0.266	0.011	0.905
IRF4 + SVG-1-2-11 + NR 434	cb	Ca	-1.401	0.121	0.319	0	0.761
IRF4 + SVG-1-2-11 + NR 434	plsr	Ca	-2.694	0.148	0.372	0.01	0.611
IRF4 + SVG-1-2-11 + NR 434	rf	Ca	-0.354	0.077	0.255	0.019	0.903
IRF4 + SVG-1-2-11 + NR 434	ann	K	0.076	0.02	0.131	-0.008	1.08
IRF4 + SVG-1-2-11 + NR 434	cb	K	-0.01	0.02	0.13	-0.006	1.138
IRF4 + SVG-1-2-11 + NR 434	plsr	K	-0.895	0.032	0.173	-0.001	0.806
IRF4 + SVG-1-2-11 + NR 434	rf	K	0.207	0.017	0.12	0.006	1.243
IRF4 + SVG-1-2-11 + NR 434	ann	Mg	-0.079	0.099	0.309	0.012	0.986
IRF4 + SVG-1-2-11 + NR 434	cb	Mg	-0.025	0.093	0.299	-0.014	1.027
IRF4 + SVG-1-2-11 + NR 434	plsr	Mg	-0.557	0.132	0.359	-0.009	0.855
IRF4 + SVG-1-2-11 + NR 434	rf	Mg	0.138	0.078	0.274	0.017	1.122
IRF4 + SVG-1-2-11 + NR 434	ann	Na	-0.582	0.003	0.039	0.001	0.898
IRF4 + SVG-1-2-11 + NR 434	cb	Na	-23.439	0.008	0.074	0.004	0.688
IRF4 + SVG-1-2-11 + NR 434	plsr	Na	-7.947	0.005	0.065	-0.001	0.511
IRF4 + SVG-1-2-11 + NR 434	rf	Na	-0.645	0.003	0.039	0.002	0.932
IRF4 + SVG-1-2-11 + NR 434	ann	P	-0.421	81.295	8.443	-0.064	0.941
IRF4 + SVG-1-2-11 + NR 434	cb	P	-0.078	71.454	7.796	-1.137	1.014
IRF4 + SVG-1-2-11 + NR 434	plsr	P	-1.348	122.642	10.846	-0.262	0.71
IRF4 + SVG-1-2-11 + NR 434	rf	P	0.02	69.58	7.589	0.552	1.075
IRF4 + SVG-1-2-11 + NR 434	ann	pH	-0.059	0.157	0.393	-0.015	1.023
IRF4 + SVG-1-2-11 + NR 434	cb	pH	0.183	0.122	0.347	-0.013	1.154
IRF4 + SVG-1-2-11 + NR 434	plsr	pH	-0.241	0.185	0.427	0.002	0.944
IRF4 + SVG-1-2-11 + NR 434	rf	pH	0.347	0.098	0.311	0	1.284
no pre-treatment	ann	Al	-0.285	2.529	1.557	0.059	0.969
no pre-treatment	cb	Al	0.362	1.264	1.111	-0.072	1.319
no pre-treatment	plsr	Al	0.115	1.64	1.261	-0.042	1.187
no pre-treatment	rf	Al	0.242	1.525	1.218	0.054	1.205
no pre-treatment	ann	TC	0.695	9.024	2.872	-0.095	2.021
no pre-treatment	cb	TC	0.824	5.128	2.153	-0.059	2.667
no pre-treatment	plsr	TC	0.727	6.63	2.548	-0.037	2.189
no pre-treatment	rf	TC	0.771	6.604	2.507	0.032	2.229
no pre-treatment	ann	H	0.27	0.374	0.605	0.031	1.243
no pre-treatment	cb	H	0.631	0.191	0.433	-0.023	1.721
no pre-treatment	plsr	H	0.592	0.212	0.459	0.004	1.611
no pre-treatment	rf	H	0.523	0.244	0.489	0.003	1.533
no pre-treatment	ann	N	0.596	0.041	0.198	0.005	1.769
no pre-treatment	cb	N	0.743	0.028	0.162	-0.009	2.141

no pre-treatment	plsr	N	0.676	0.03	0.172	-0.002	1.975
no pre-treatment	rf	N	0.69	0.032	0.177	0.002	1.917
no pre-treatment	ann	Ca	-3.928	0.143	0.352	0.028	0.747
no pre-treatment	cb	Ca	-0.401	0.092	0.27	-0.035	0.89
no pre-treatment	plsr	Ca	-1.192	0.095	0.297	0.005	0.757
no pre-treatment	rf	Ca	-0.4	0.075	0.253	0.014	0.925
no pre-treatment	ann	K	0.018	0.022	0.137	0.001	1.043
no pre-treatment	cb	K	-0.865	0.025	0.144	-0.004	1.103
no pre-treatment	plsr	K	-0.167	0.02	0.137	0	1.009
no pre-treatment	rf	K	-0.087	0.022	0.14	0.011	1.011
no pre-treatment	ann	Mg	-0.562	0.145	0.365	0.042	0.874
no pre-treatment	cb	Mg	-0.106	0.1	0.312	-0.065	0.97
no pre-treatment	plsr	Mg	-0.116	0.097	0.308	-0.005	0.989
no pre-treatment	rf	Mg	-0.031	0.093	0.301	0.018	1.015
no pre-treatment	ann	Na	-3.777	0.005	0.053	0.003	0.79
no pre-treatment	cb	Na	-10.222	0.006	0.062	0	0.836
no pre-treatment	plsr	Na	-2.819	0.003	0.05	0.001	0.65
no pre-treatment	rf	Na	-1.196	0.003	0.043	0.003	0.878
no pre-treatment	ann	P	-0.966	122.897	10.064	0.517	0.854
no pre-treatment	cb	P	-0.107	75.897	8.019	-1.422	0.993
no pre-treatment	plsr	P	-0.319	77.514	8.345	-0.152	0.938
no pre-treatment	rf	P	-0.051	69.888	7.781	0.048	1.006
no pre-treatment	ann	pH	-0.306	0.195	0.433	0.021	0.942
no pre-treatment	cb	pH	-0.033	0.156	0.393	-0.008	1.014
no pre-treatment	plsr	pH	-0.045	0.157	0.392	-0.008	1.031
no pre-treatment	rf	pH	0.096	0.139	0.37	0.004	1.08
PCAL	ann	Al	-0.029	2.061	1.406	0.004	1.067
PCAL	cb	Al	0.197	1.562	1.233	-0.023	1.203
PCAL	plsr	Al	0.057	1.724	1.293	-0.035	1.166
PCAL	rf	Al	0.249	1.516	1.218	0.056	1.203
PCAL	ann	TC	0.652	8.995	2.952	-0.061	1.8
PCAL	cb	TC	0.793	5.518	2.297	-0.148	2.338
PCAL	plsr	TC	0.717	6.24	2.488	-0.068	2.134
PCAL	rf	TC	0.757	6.528	2.496	0.039	2.146
PCAL	ann	H	0.189	0.394	0.625	-0.022	1.15
PCAL	cb	H	0.538	0.223	0.464	-0.026	1.596
PCAL	plsr	H	0.568	0.213	0.459	-0.001	1.565
PCAL	rf	H	0.521	0.235	0.481	0.004	1.509
PCAL	ann	N	0.423	0.054	0.22	0.02	1.645
PCAL	cb	N	0.701	0.031	0.173	-0.004	1.89
PCAL	plsr	N	0.667	0.029	0.17	-0.004	1.933
PCAL	rf	N	0.664	0.034	0.181	0.004	1.817
PCAL	ann	Ca	-0.777	0.094	0.281	0.007	0.87
PCAL	cb	Ca	-2.497	0.138	0.339	-0.016	0.765
PCAL	plsr	Ca	-1.417	0.101	0.306	0	0.741
PCAL	rf	Ca	-0.409	0.08	0.258	0.011	0.917
PCAL	ann	K	-0.929	0.045	0.187	0.02	0.803
PCAL	cb	K	-1.255	0.029	0.155	-0.005	1.067
PCAL	plsr	K	-0.193	0.021	0.138	-0.001	0.998
PCAL	rf	K	-0.143	0.023	0.143	0.011	0.973
PCAL	ann	Mg	-0.4	0.132	0.354	0.01	0.882
PCAL	cb	Mg	-0.103	0.101	0.314	-0.042	0.981
PCAL	plsr	Mg	-0.144	0.101	0.314	-0.005	0.982
PCAL	rf	Mg	-0.062	0.098	0.309	0.019	1

PCAL	ann	Na	-0.377	0.003	0.038	-0.001	0.967
PCAL	cb	Na	-11.993	0.005	0.058	0	0.79
PCAL	plsr	Na	-3.468	0.004	0.051	0.001	0.644
PCAL	rf	Na	-1.198	0.003	0.043	0.003	0.889
PCAL	ann	P	-0.681	80.899	8.103	0.019	0.938
PCAL	cb	P	-0.436	74.15	7.918	-1.156	0.927
PCAL	plsr	P	-0.433	71.914	7.927	-0.021	0.908
PCAL	rf	P	0.036	60.975	7.013	0.002	1.042
PCAL	ann	pH	-0.511	0.236	0.474	0.021	0.883
PCAL	cb	pH	0.097	0.141	0.373	-0.015	1.087
PCAL	plsr	pH	-0.089	0.169	0.406	-0.008	1.008
PCAL	rf	pH	0.091	0.143	0.375	0.006	1.075
RHCC	ann	Al	-0.298	2.596	1.555	0.137	0.985
RHCC	cb	Al	0.261	1.402	1.161	-0.076	1.295
RHCC	plsr	Al	0.137	1.598	1.245	0.012	1.201
RHCC	rf	Al	0.238	1.524	1.218	0.043	1.205
RHCC	ann	TC	0.755	7.184	2.58	-0.052	2.198
RHCC	cb	TC	0.789	6.179	2.41	-0.166	2.338
RHCC	plsr	TC	0.732	7.045	2.608	-0.067	2.146
RHCC	rf	TC	0.778	6.422	2.476	0.009	2.248
RHCC	ann	H	-0.046	0.533	0.722	0.002	1.036
RHCC	cb	H	0.537	0.241	0.485	-0.001	1.548
RHCC	plsr	H	0.479	0.277	0.519	-0.008	1.444
RHCC	rf	H	0.49	0.261	0.506	0.004	1.485
RHCC	ann	N	0.61	0.039	0.193	0.009	1.809
RHCC	cb	N	0.769	0.025	0.153	-0.008	2.265
RHCC	plsr	N	0.701	0.029	0.169	-0.004	1.995
RHCC	rf	N	0.694	0.032	0.176	0.001	1.935
RHCC	ann	Ca	-0.847	0.104	0.292	0.011	0.839
RHCC	cb	Ca	-0.624	0.079	0.259	-0.044	0.913
RHCC	plsr	Ca	-0.962	0.093	0.291	0.002	0.777
RHCC	rf	Ca	-0.345	0.075	0.252	0.009	0.922
RHCC	ann	K	-1.572	0.038	0.178	0.008	0.862
RHCC	cb	K	-0.515	0.023	0.136	-0.008	1.158
RHCC	plsr	K	-0.406	0.024	0.15	-0.001	0.923
RHCC	rf	K	-0.055	0.022	0.138	0.01	1.024
RHCC	ann	Mg	-0.908	0.149	0.374	0.017	0.862
RHCC	cb	Mg	-0.101	0.099	0.31	-0.059	0.98
RHCC	plsr	Mg	-0.01	0.09	0.296	0.001	1.031
RHCC	rf	Mg	-0.042	0.094	0.302	0.013	1.01
RHCC	ann	Na	-1.259	0.003	0.042	0.001	0.858
RHCC	cb	Na	-7.096	0.005	0.052	-0.002	0.903
RHCC	plsr	Na	-2.357	0.003	0.048	0.001	0.681
RHCC	rf	Na	-1.244	0.003	0.043	0.003	0.874
RHCC	ann	P	-0.286	83.166	8.412	0.254	0.96
RHCC	cb	P	-0.038	72.124	7.746	-1.41	1.04
RHCC	plsr	P	-0.341	83.167	8.569	0.053	0.916
RHCC	rf	P	-0.036	69.63	7.755	0.042	1.014
RHCC	ann	pH	-0.232	0.19	0.424	-0.012	0.969
RHCC	cb	pH	-0.037	0.157	0.394	-0.014	1.012
RHCC	plsr	pH	0.006	0.151	0.378	-0.011	1.096
RHCC	rf	pH	0.071	0.141	0.374	0.003	1.067
stepAIC	ann	Al	-0.191	2.223	1.445	0.16	1.064
stepAIC	cb	Al	0.423	1.152	1.062	-0.117	1.371

stepAIC	plsr	Al	0.253	1.364	1.157	0.015	1.29
stepAIC	rf	Al	0.226	1.553	1.228	0.062	1.197
stepAIC	ann	TC	0.591	10.659	3.041	-0.264	2.037
stepAIC	cb	TC	0.803	5.339	2.266	-0.052	2.466
stepAIC	plsr	TC	0.695	7.5	2.713	-0.037	2.051
stepAIC	rf	TC	0.778	6.502	2.485	0.045	2.246
stepAIC	ann	H	0.315	0.345	0.58	0.034	1.309
stepAIC	cb	H	0.594	0.211	0.454	0	1.648
stepAIC	plsr	H	0.523	0.245	0.49	0.003	1.53
stepAIC	rf	H	0.525	0.243	0.489	0.004	1.532
stepAIC	ann	N	0.666	0.034	0.18	0.008	1.932
stepAIC	cb	N	0.728	0.028	0.164	-0.009	2.085
stepAIC	plsr	N	0.636	0.033	0.181	-0.001	1.884
stepAIC	rf	N	0.706	0.031	0.173	0.003	1.982
stepAIC	ann	Ca	-1.728	0.109	0.311	0.021	0.791
stepAIC	cb	Ca	-0.162	0.074	0.245	-0.046	0.965
stepAIC	plsr	Ca	-0.854	0.087	0.282	0.008	0.796
stepAIC	rf	Ca	-0.516	0.078	0.26	0.015	0.896
stepAIC	ann	K	-0.972	0.041	0.185	0.017	0.8
stepAIC	cb	K	-0.067	0.023	0.133	-0.005	1.194
stepAIC	plsr	K	0.017	0.019	0.13	-0.001	1.065
stepAIC	rf	K	-0.07	0.022	0.139	0.01	1.008
stepAIC	ann	Mg	-1.79	0.209	0.426	0.04	0.799
stepAIC	cb	Mg	-0.038	0.093	0.301	-0.056	1.007
stepAIC	plsr	Mg	-0.062	0.094	0.302	0.006	1.01
stepAIC	rf	Mg	-0.065	0.096	0.305	0.015	0.996
stepAIC	ann	Na	-7.165	0.007	0.059	0.005	0.796
stepAIC	cb	Na	-7.107	0.005	0.052	-0.001	0.916
stepAIC	plsr	Na	-2.888	0.003	0.05	0	0.657
stepAIC	rf	Na	-1.593	0.003	0.045	0.003	0.885
stepAIC	ann	P	-0.931	94.434	8.908	0.019	0.945
stepAIC	cb	P	0	70.808	7.719	-1.66	1.026
stepAIC	plsr	P	-0.416	80.903	8.533	-0.063	0.923
stepAIC	rf	P	-0.056	69.372	7.779	0.098	1.005
stepAIC	ann	pH	-0.43	0.218	0.462	-0.008	0.872
stepAIC	cb	pH	0.014	0.151	0.385	-0.001	1.042
stepAIC	plsr	pH	0.079	0.14	0.371	-0.015	1.086
stepAIC	rf	pH	0.097	0.137	0.369	0.004	1.082
SVG-1-2-11	ann	Al	0.021	1.983	1.379	0.059	1.075
SVG-1-2-11	cb	Al	-0.05	1.994	1.371	0.042	1.106
SVG-1-2-11	plsr	Al	0.137	1.598	1.243	-0.027	1.209
SVG-1-2-11	rf	Al	0.513	0.987	0.974	0.049	1.52
SVG-1-2-11	ann	TC	0.553	12.93	3.348	0.184	1.884
SVG-1-2-11	cb	TC	0.734	7.393	2.655	0.085	2.121
SVG-1-2-11	plsr	TC	0.637	8.938	2.944	-0.11	1.911
SVG-1-2-11	rf	TC	0.836	4.718	2.123	0	2.627
SVG-1-2-11	ann	H	0.11	0.458	0.668	0.022	1.14
SVG-1-2-11	cb	H	0.278	0.367	0.6	-0.009	1.252
SVG-1-2-11	plsr	H	0.495	0.264	0.511	-0.021	1.45
SVG-1-2-11	rf	H	0.587	0.214	0.459	0.008	1.619
SVG-1-2-11	ann	N	0.546	0.039	0.191	0.009	1.893
SVG-1-2-11	cb	N	0.643	0.037	0.189	-0.012	1.826
SVG-1-2-11	plsr	N	0.589	0.039	0.198	-0.008	1.706
SVG-1-2-11	rf	N	0.797	0.021	0.142	0.003	2.382

SVG-1-2-11	ann	Ca	-1.667	0.086	0.264	0	0.964
SVG-1-2-11	cb	Ca	-3.158	0.139	0.359	-0.003	0.685
SVG-1-2-11	plsr	Ca	-1.343	0.103	0.309	0.014	0.736
SVG-1-2-11	rf	Ca	-0.498	0.082	0.264	0.021	0.882
SVG-1-2-11	ann	K	-0.094	0.022	0.14	0.003	0.991
SVG-1-2-11	cb	K	0.174	0.02	0.127	-0.012	1.153
SVG-1-2-11	plsr	K	-0.142	0.019	0.135	0	1.013
SVG-1-2-11	rf	K	0.192	0.017	0.12	0.007	1.17
SVG-1-2-11	ann	Mg	-0.347	0.117	0.335	0.013	0.923
SVG-1-2-11	cb	Mg	-0.286	0.114	0.332	-0.021	0.925
SVG-1-2-11	plsr	Mg	-0.154	0.101	0.315	0.006	0.966
SVG-1-2-11	rf	Mg	0.194	0.074	0.267	0.014	1.148
SVG-1-2-11	ann	Na	-0.35	0.003	0.038	0	0.95
SVG-1-2-11	cb	Na	-1.446	0.003	0.04	-0.003	0.931
SVG-1-2-11	plsr	Na	-7.089	0.005	0.062	0.001	0.516
SVG-1-2-11	rf	Na	-1.357	0.003	0.04	0.004	0.905
SVG-1-2-11	ann	P	-0.104	78.887	8.037	-0.13	1.001
SVG-1-2-11	cb	P	-0.14	78.031	8.118	-1.761	0.985
SVG-1-2-11	plsr	P	-1.088	109.271	10.155	-0.323	0.762
SVG-1-2-11	rf	P	0.021	67.732	7.548	0.471	1.051
SVG-1-2-11	ann	pH	0.062	0.143	0.376	-0.002	1.063
SVG-1-2-11	cb	pH	0.042	0.144	0.378	-0.015	1.053
SVG-1-2-11	plsr	pH	-0.064	0.158	0.395	-0.004	1.016
SVG-1-2-11	rf	pH	0.363	0.096	0.309	-0.005	1.286
SVG-1-2-11 + IRF4	ann	Al	-0.245	2.44	1.531	0.017	0.972
SVG-1-2-11 + IRF4	cb	Al	0.234	1.571	1.229	-0.097	1.2
SVG-1-2-11 + IRF4	plsr	Al	-84.456	141.554	7.007	0.567	0.462
SVG-1-2-11 + IRF4	rf	Al	0.487	1.071	1.012	0.034	1.459
SVG-1-2-11 + IRF4	ann	TC	0.377	13.865	3.596	0.149	1.694
SVG-1-2-11 + IRF4	cb	TC	0.736	7.778	2.694	0.163	2.082
SVG-1-2-11 + IRF4	plsr	TC	-55.531	1742.886	26.977	1.488	0.381
SVG-1-2-11 + IRF4	rf	TC	0.826	5.047	2.194	-0.013	2.539
SVG-1-2-11 + IRF4	ann	H	0.078	0.48	0.689	-0.042	1.077
SVG-1-2-11 + IRF4	cb	H	-0.001	0.517	0.706	0.004	1.077
SVG-1-2-11 + IRF4	plsr	H	-35.454	20.454	3.083	0.356	0.439
SVG-1-2-11 + IRF4	rf	H	0.568	0.224	0.47	0.003	1.58
SVG-1-2-11 + IRF4	ann	N	0.4	0.058	0.232	0.008	1.549
SVG-1-2-11 + IRF4	cb	N	0.61	0.045	0.203	-0.016	1.721
SVG-1-2-11 + IRF4	plsr	N	-57.865	7.296	1.681	0.094	0.381
SVG-1-2-11 + IRF4	rf	N	0.787	0.022	0.146	0	2.321
SVG-1-2-11 + IRF4	ann	Ca	-0.715	0.084	0.268	-0.004	0.891
SVG-1-2-11 + IRF4	cb	Ca	-2.28	0.162	0.329	-0.009	0.849
SVG-1-2-11 + IRF4	plsr	Ca	-36.225	0.955	0.675	-0.041	0.515
SVG-1-2-11 + IRF4	rf	Ca	-0.168	0.073	0.244	0.007	0.958
SVG-1-2-11 + IRF4	ann	K	-0.237	0.023	0.143	-0.006	1.004
SVG-1-2-11 + IRF4	cb	K	-0.421	0.028	0.156	-0.008	0.918
SVG-1-2-11 + IRF4	plsr	K	-30.568	0.577	0.594	-0.038	0.34
SVG-1-2-11 + IRF4	rf	K	0.274	0.017	0.118	0.003	1.242
SVG-1-2-11 + IRF4	ann	Mg	-0.329	0.119	0.338	-0.005	0.907
SVG-1-2-11 + IRF4	cb	Mg	-0.439	0.127	0.35	-0.023	0.879
SVG-1-2-11 + IRF4	plsr	Mg	-13.912	1.212	0.897	-0.098	0.49
SVG-1-2-11 + IRF4	rf	Mg	0.135	0.078	0.276	0.002	1.098
SVG-1-2-11 + IRF4	ann	Na	-0.507	0.003	0.04	-0.001	0.888
SVG-1-2-11 + IRF4	cb	Na	-19.333	0.006	0.061	0.001	0.777

SVG-1-2-11 + IRF4	plsr	Na	-202.6	0.097	0.233	0.022	0.281
SVG-1-2-11 + IRF4	rf	Na	-0.4	0.003	0.038	0.001	0.965
SVG-1-2-11 + IRF4	ann	P	-0.341	86.279	8.572	0.011	0.939
SVG-1-2-11 + IRF4	cb	P	-1.191	133.208	10.364	-0.715	0.828
SVG-1-2-11 + IRF4	plsr	P	-14.752	820.441	24.617	-0.47	0.414
SVG-1-2-11 + IRF4	rf	P	0.06	67.103	7.467	0.158	1.063
SVG-1-2-11 + IRF4	ann	pH	-0.137	0.176	0.412	-0.004	0.979
SVG-1-2-11 + IRF4	cb	pH	-0.131	0.17	0.408	-0.008	0.992
SVG-1-2-11 + IRF4	plsr	pH	-70.768	11.581	1.924	0.026	0.458
SVG-1-2-11 + IRF4	rf	pH	0.322	0.102	0.319	-0.005	1.249
SVG-1-2-11 + IRF4 + NR 434	ann	Al	0.033	1.98	1.376	-0.015	1.08
SVG-1-2-11 + IRF4 + NR 434	cb	Al	0.002	1.92	1.355	-0.056	1.105
SVG-1-2-11 + IRF4 + NR 434	plsr	Al	-84.671	141.719	6.988	0.565	0.463
SVG-1-2-11 + IRF4 + NR 434	rf	Al	0.506	1.028	0.992	0.032	1.485
SVG-1-2-11 + IRF4 + NR 434	ann	TC	0.501	13.818	3.609	0.092	1.586
SVG-1-2-11 + IRF4 + NR 434	cb	TC	0.72	8.274	2.788	0.049	2.019
SVG-1-2-11 + IRF4 + NR 434	plsr	TC	-56.013	1760.657	27.079	1.458	0.379
SVG-1-2-11 + IRF4 + NR 434	rf	TC	0.824	5.006	2.183	0.014	2.569
SVG-1-2-11 + IRF4 + NR 434	ann	H	-0.016	0.513	0.707	0.011	1.068
SVG-1-2-11 + IRF4 + NR 434	cb	H	0.131	0.433	0.647	0.054	1.179
SVG-1-2-11 + IRF4 + NR 434	plsr	H	-36.175	20.882	3.112	0.356	0.434
SVG-1-2-11 + IRF4 + NR 434	rf	H	0.541	0.239	0.486	-0.001	1.521
SVG-1-2-11 + IRF4 + NR 434	ann	N	0.193	0.085	0.285	0.02	1.218
SVG-1-2-11 + IRF4 + NR 434	cb	N	0.641	0.04	0.188	-0.01	1.948
SVG-1-2-11 + IRF4 + NR 434	plsr	N	-58.464	7.385	1.687	0.093	0.38
SVG-1-2-11 + IRF4 + NR 434	rf	N	0.777	0.022	0.148	0.002	2.318
SVG-1-2-11 + IRF4 + NR 434	ann	Ca	-2.08	0.123	0.324	0.028	0.788
SVG-1-2-11 + IRF4 + NR 434	cb	Ca	-1.642	0.14	0.321	-0.005	0.82
SVG-1-2-11 + IRF4 + NR 434	plsr	Ca	-36.106	0.951	0.674	-0.041	0.516
SVG-1-2-11 + IRF4 + NR 434	rf	Ca	-0.142	0.072	0.243	0.006	0.965
SVG-1-2-11 + IRF4 + NR 434	ann	K	-0.317	0.025	0.151	-0.007	0.919
SVG-1-2-11 + IRF4 + NR 434	cb	K	-0.61	0.031	0.165	-0.003	0.863
SVG-1-2-11 + IRF4 + NR 434	plsr	K	-31.138	0.587	0.598	-0.039	0.338
SVG-1-2-11 + IRF4 + NR 434	rf	K	0.275	0.017	0.118	0.003	1.244
SVG-1-2-11 + IRF4 + NR 434	ann	Mg	-0.217	0.105	0.321	-0.006	0.948
SVG-1-2-11 + IRF4 + NR 434	cb	Mg	-0.425	0.125	0.346	-0.029	0.892
SVG-1-2-11 + IRF4 + NR 434	plsr	Mg	-14.048	1.224	0.9	-0.097	0.488
SVG-1-2-11 + IRF4 + NR 434	rf	Mg	0.128	0.079	0.277	0.003	1.093
SVG-1-2-11 + IRF4 + NR 434	ann	Na	-0.601	0.003	0.039	0.001	0.892
SVG-1-2-11 + IRF4 + NR 434	cb	Na	-13.51	0.004	0.05	0	0.85
SVG-1-2-11 + IRF4 + NR 434	plsr	Na	-200.571	0.096	0.232	0.021	0.287
SVG-1-2-11 + IRF4 + NR 434	rf	Na	-0.341	0.003	0.038	0.001	0.971
SVG-1-2-11 + IRF4 + NR 434	ann	P	-0.431	94.117	8.963	-0.123	0.896
SVG-1-2-11 + IRF4 + NR 434	cb	P	-0.948	118.427	9.781	-0.759	0.859
SVG-1-2-11 + IRF4 + NR 434	plsr	P	-14.921	831.006	24.737	-0.526	0.412
SVG-1-2-11 + IRF4 + NR 434	rf	P	0.072	66.896	7.436	0.137	1.07
SVG-1-2-11 + IRF4 + NR 434	ann	pH	-0.139	0.172	0.413	0.013	0.963
SVG-1-2-11 + IRF4 + NR 434	cb	pH	-0.121	0.172	0.408	-0.003	0.992
SVG-1-2-11 + IRF4 + NR 434	plsr	pH	-73.21	11.976	1.946	0.026	0.456
SVG-1-2-11 + IRF4 + NR 434	rf	pH	0.329	0.101	0.317	-0.005	1.255
SVG-1-2-11 + NR 434	ann	Al	0.264	1.518	1.203	-0.01	1.233
SVG-1-2-11 + NR 434	cb	Al	0.019	1.915	1.338	-0.022	1.13
SVG-1-2-11 + NR 434	plsr	Al	0.107	1.675	1.271	-0.028	1.182
SVG-1-2-11 + NR 434	rf	Al	0.522	0.97	0.966	0.042	1.529

SVG-1-2-11 + NR 434	ann	TC	0.508	12.849	3.335	0.433	1.804
SVG-1-2-11 + NR 434	cb	TC	0.712	8.06	2.775	-0.008	2.022
SVG-1-2-11 + NR 434	plsr	TC	0.66	8.878	2.933	-0.036	1.91
SVG-1-2-11 + NR 434	rf	TC	0.831	4.854	2.143	0.024	2.632
SVG-1-2-11 + NR 434	ann	H	0.123	0.466	0.676	0.045	1.102
SVG-1-2-11 + NR 434	cb	H	0.178	0.43	0.649	-0.016	1.15
SVG-1-2-11 + NR 434	plsr	H	0.486	0.27	0.513	-0.013	1.456
SVG-1-2-11 + NR 434	rf	H	0.574	0.222	0.468	0.005	1.581
SVG-1-2-11 + NR 434	ann	N	0.513	0.049	0.212	-0.003	1.696
SVG-1-2-11 + NR 434	cb	N	0.621	0.04	0.196	-0.015	1.749
SVG-1-2-11 + NR 434	plsr	N	0.607	0.039	0.195	-0.006	1.752
SVG-1-2-11 + NR 434	rf	N	0.786	0.021	0.144	0.005	2.375
SVG-1-2-11 + NR 434	ann	Ca	-0.144	0.091	0.256	0.006	0.966
SVG-1-2-11 + NR 434	cb	Ca	-3.173	0.139	0.359	-0.003	0.685
SVG-1-2-11 + NR 434	plsr	Ca	-1.555	0.112	0.324	0.02	0.695
SVG-1-2-11 + NR 434	rf	Ca	-0.502	0.083	0.265	0.021	0.881
SVG-1-2-11 + NR 434	ann	K	0.048	0.02	0.133	0	1.057
SVG-1-2-11 + NR 434	cb	K	0.086	0.022	0.132	-0.008	1.113
SVG-1-2-11 + NR 434	plsr	K	-0.291	0.022	0.144	-0.001	0.951
SVG-1-2-11 + NR 434	rf	K	0.186	0.017	0.12	0.007	1.167
SVG-1-2-11 + NR 434	ann	Mg	-0.174	0.105	0.32	-0.014	0.947
SVG-1-2-11 + NR 434	cb	Mg	-0.258	0.114	0.33	-0.021	0.936
SVG-1-2-11 + NR 434	plsr	Mg	-0.083	0.094	0.305	0.012	0.989
SVG-1-2-11 + NR 434	rf	Mg	0.177	0.076	0.269	0.014	1.137
SVG-1-2-11 + NR 434	ann	Na	-2.559	0.005	0.05	0.003	0.827
SVG-1-2-11 + NR 434	cb	Na	-3.351	0.004	0.049	-0.002	0.755
SVG-1-2-11 + NR 434	plsr	Na	-6.623	0.005	0.063	0	0.51
SVG-1-2-11 + NR 434	rf	Na	-2.143	0.003	0.043	0.004	0.837
SVG-1-2-11 + NR 434	ann	P	-0.61	107.351	9.36	0.601	0.897
SVG-1-2-11 + NR 434	cb	P	-0.203	80.812	8.361	-1.931	0.932
SVG-1-2-11 + NR 434	plsr	P	-1.014	109.473	10.118	-0.289	0.763
SVG-1-2-11 + NR 434	rf	P	-0.007	68.8	7.623	0.483	1.042
SVG-1-2-11 + NR 434	ann	pH	-0.009	0.152	0.386	0.006	1.044
SVG-1-2-11 + NR 434	cb	pH	0.032	0.145	0.38	-0.014	1.049
SVG-1-2-11 + NR 434	plsr	pH	-0.064	0.157	0.393	0.005	1.027
SVG-1-2-11 + NR 434	rf	pH	0.352	0.098	0.312	-0.007	1.278
SVG-1-2-9	ann	Al	-0.039	2.059	1.413	0.08	1.038
SVG-1-2-9	cb	Al	0.145	1.694	1.282	-0.062	1.149
SVG-1-2-9	plsr	Al	0.095	1.684	1.28	-0.036	1.165
SVG-1-2-9	rf	Al	0.511	0.981	0.973	0.045	1.516
SVG-1-2-9	ann	TC	0.49	11.863	3.192	0.079	1.985
SVG-1-2-9	cb	TC	0.717	7.869	2.701	-0.087	2.148
SVG-1-2-9	plsr	TC	0.596	9.517	3.046	-0.107	1.845
SVG-1-2-9	rf	TC	0.833	4.84	2.147	0.014	2.604
SVG-1-2-9	ann	H	0.221	0.411	0.629	-0.012	1.208
SVG-1-2-9	cb	H	0.281	0.371	0.602	0.009	1.246
SVG-1-2-9	plsr	H	0.476	0.272	0.519	-0.014	1.426
SVG-1-2-9	rf	H	0.574	0.22	0.466	0.007	1.596
SVG-1-2-9	ann	N	0.599	0.041	0.186	-0.006	2.05
SVG-1-2-9	cb	N	0.694	0.034	0.179	-0.009	1.919
SVG-1-2-9	plsr	N	0.54	0.043	0.206	-0.007	1.635
SVG-1-2-9	rf	N	0.791	0.021	0.143	0.003	2.37
SVG-1-2-9	ann	Ca	-0.728	0.084	0.265	0	0.915
SVG-1-2-9	cb	Ca	-1.905	0.13	0.329	-0.013	0.771

SVG-1-2-9	plsr	Ca	-1.643	0.113	0.325	0.018	0.693
SVG-1-2-9	rf	Ca	-0.337	0.079	0.254	0.016	0.947
SVG-1-2-9	ann	K	-0.11	0.023	0.142	-0.005	1.027
SVG-1-2-9	cb	K	0.223	0.019	0.123	-0.017	1.19
SVG-1-2-9	plsr	K	-0.192	0.02	0.138	0	0.988
SVG-1-2-9	rf	K	0.26	0.016	0.116	0.006	1.225
SVG-1-2-9	ann	Mg	-0.275	0.122	0.332	0.009	0.949
SVG-1-2-9	cb	Mg	-0.289	0.116	0.334	-0.029	0.922
SVG-1-2-9	plsr	Mg	-0.224	0.108	0.325	0.012	0.936
SVG-1-2-9	rf	Mg	0.191	0.074	0.267	0.012	1.146
SVG-1-2-9	ann	Na	-0.54	0.003	0.039	0.001	0.903
SVG-1-2-9	cb	Na	-2.079	0.003	0.045	0	0.862
SVG-1-2-9	plsr	Na	-8.53	0.005	0.066	0.001	0.491
SVG-1-2-9	rf	Na	-1.422	0.003	0.041	0.004	0.845
SVG-1-2-9	ann	P	-0.217	84.147	8.449	0.102	0.94
SVG-1-2-9	cb	P	-0.163	78.572	8.223	-2.042	0.952
SVG-1-2-9	plsr	P	-1.217	116.174	10.524	-0.239	0.73
SVG-1-2-9	rf	P	-0.002	69.391	7.65	0.502	1.036
SVG-1-2-9	ann	pH	-0.125	0.169	0.409	-0.005	0.972
SVG-1-2-9	cb	pH	-0.058	0.16	0.398	-0.011	1.004
SVG-1-2-9	plsr	pH	-0.094	0.164	0.402	0	0.996
SVG-1-2-9	rf	pH	0.352	0.098	0.312	-0.006	1.277

References

1. Fernanda Chaves Soares, P.; Helena Cunha dos Anjos, L.; Gervasio Pereira, M.; Carlos Ruiz Pessenda, L. Histosols in an Upper Montane Environment in the Itatiaia Plateau. *Rev Bras Cienc Solo* **2016**, *40*.
2. Aximoff, I.A.; Alves, R.G.; Rodrigues, R. de C. Campos de Altitude do Itatiaia: Aspectos Ambientais, Biológico e Ecológicos. *Boletim do Parque Nacional do Itatiaia N° 18* **2014**, *74*.
3. Hunt, G.R. Spectral signatures of particulate minerals in the visible and near infrared. *Geophysics* **1977**, *42*.
4. Demattê, J.A.M. Characterization and discrimination of soils by their reflected electromagnetic energy. *Pesquisa Agropecuária Brasileira* **2002**, *37*, 1445–1458.
5. Formaggio, A.R.; Epiphanyo, J.C.N.; Valeriano, M.M.; Oliveira, J.B. Comportamento espectral (450-2.450 nm) de solos tropicais de São Paulo. **1996**, *0*, 467–474.
6. Demattê, J.A.M.; Terra, F. da S.; Quartaroli, C.F. Spectral behavior of some modal soil profiles from São Paulo State, Brazil. *Bragantia* **2012**, *71*, 413–423.
7. Vitorello, I.; Galvão, L.S. Role of organic matter in obliterating the effects of iron on spectral reflectance and colour of Brazilian tropical soils. **1998**, *19*, 1969–1979.
8. Rossel, R.A.V.; Walvoort, D.J.J.; McBratney, A.B.; Janik, L.J.; Skjemstad, J.O. Visible, near infrared, mid infrared or combined diffuse reflectance spectroscopy for simultaneous assessment of various soil properties. *Geoderma* **2005**, *131*, 59–75.
9. Gomez, C.; Viscarra Rossel, R.A.; McBratney, A.B. Soil organic carbon prediction by hyperspectral remote sensing and field vis-NIR spectroscopy: An Australian case study. *Geoderma* **2008**, *146*, 403–411.
10. Adeline, K.R.M.; Gomez, C.; Gorretta, N.; Roger, J.-M. Predictive ability of soil properties to spectral degradation from laboratory Vis-NIR spectroscopy data. **2017**.
11. Viscarra Rossel, R.A. ParLeS : Software for chemometric analysis of spectroscopic data. **2008**.

12. Kopačková, V.; Ben-Dor, E.; Carmon, N.; Notesco, G. Modelling Diverse Soil Attributes with Visible to Longwave Infrared Spectroscopy Using PLSR Employed by an Automatic Modelling Engine. *Remote Sensing* **2017**, *9*, 134.
13. Daniel A,B, K.W.; Tripathi, N.K.; Honda, K. Artificial neural network analysis of laboratory and in situ spectra for the estimation of macronutrients in soils of Lop Buri (Thailand). *Australian Journal of Soil Research* **2003**, *41*, 47–59.
14. Rossel, R.A.V.; Behrens, T. Using data mining to model and interpret soil diffuse reflectance spectra. *Geoderma* **2010**, *158*, 46–54.
15. Dangal, S.; Sanderman, J.; Wills, S.; Ramirez-Lopez, L.; Dangal, S.R.S.; Sanderman, J.; Wills, S.; Ramirez-Lopez, L. Accurate and Precise Prediction of Soil Properties from a Large Mid-Infrared Spectral Library. *Soil Systems* **2019**, *3*, 11.
16. Kuang, B.; Tekin, Y.; Mouazen, A.M. Comparison between artificial neural network and partial least squares for on-line visible and near infrared spectroscopy measurement of soil organic carbon, pH and clay content. *Soil and Tillage Research* **2015**, *146*, 243–252.
17. Morellos, A.; Pantazi, X.-E.; Moshou, D.; Alexandridis, T.; Whetton, R.; Tziotziou, G.; Wiebensohn, J.; Bill, R. Machine learning based prediction of soil total nitrogen, organic carbon and moisture content by using VIS-NIR spectroscopy. *Biosystems Engineering* **2016**, *152*, 104–116.
18. Mouazen, A.M.; Kuang, B.; de Baerdemaeker, J.; Ramon, H. Comparison among principal component, partial least squares and back propagation neural network analyses for accuracy of measurement of selected soil properties with visible and near infrared spectroscopy. *Geoderma* **2010**, *158*, 23–31.
19. Nawar, S.; Mouazen, A.; Nawar, S.; Mouazen, A.M. Comparison between Random Forests, Artificial Neural Networks and Gradient Boosted Machines Methods of On-Line Vis-NIR Spectroscopy Measurements of Soil Total Nitrogen and Total Carbon. *Sensors* **2017**, *17*, 2428.
20. Savitzky, Abraham.; Golay, M.J.E. Smoothing and Differentiation of Data by Simplified Least Squares Procedures. *Analytical Chemistry* **1964**, *36*, 1627–1639.
21. Gholizadeh, A.; Borůvka, L.; Saberioon, M.; Vašát, R.; Gholizadeh, A.; Borůvka, L.; Saberioon, M.; Vašát, R. A Memory-Based Learning Approach as Compared to Other Data Mining Algorithms for the Prediction of Soil Texture Using Diffuse Reflectance Spectra. *Remote Sensing* **2016**, *8*, 341.
22. Maleki, M.R.; van Holm, L.; Ramon, H.; Merckx, R.; de Baerdemaeker, J.; Mouazen, A.M. Phosphorus Sensing for Fresh Soils using Visible and Near Infrared Spectroscopy. *Biosystems Engineering* **2006**, *95*, 425–436.
23. Clark, R.N. *Spectroscopy of rocks and minerals, and principles of spectroscopy*; 1999; Vol. 3; ISBN 0471294055.
24. Terra, F.S.; Demattê, J.A.M.; Viscarra Rossel, R.A. Spectral libraries for quantitative analyses of tropical Brazilian soils: Comparing vis-NIR and mid-IR reflectance data. *Geoderma* **2015**, *255–256*, 81–93.
25. Alvares, C.A.; Stape, J.L.; Sentelhas, P.C.; de Moraes Gonçalves, J.L.; Sparovek, G. Köppen's climate classification map for Brazil. *Meteorologische Zeitschrift* **2013**, *22*, 711–728.
26. Modenesi, M.C. Depósitos de vertente e evolução quaternária do planalto do Itatiaia. *Revista do Instituto Geológico* **1992**, *13*, 31–46.
27. Santos, R.F. dos; Pires Neto, A.G.; Csordas, S.M. O Parque Nacional do Itatiaia. *Fundação Brasileira para o Desenvolvimento Sustentável* **2000**, 09–19.
28. Barreto, C.G.; Campos, J.B.; Roberto, D.M.; Roberto, D.M.; Schwarzstein, N.T.; Alves, G.S.G.; Coelho, W. Plano de Manejo: Parque Nacional do Itatiaia - Encarte 3. *Relatório Técnico Instituto Chico Mendes* **2013**, 215.
29. Minasny, B.; McBratney, A.B. A conditioned Latin hypercube method for sampling in the presence of ancillary information. *Computers & Geosciences* **2006**, *32*, 1378–1388.

30. Santos, H.G. dos; Jacomine, P.K.T.; Anjos, L.H.C. dos; Oliveira, V.Á. de; Lumbreras, J.F.; Coelho, M.R.; Almeida, J.A. de; Cunha, T.J.F.; Oliveira, J.B. de *Brazilian soil classification system 5th edition revised and expanded*; 2018; ISBN 9788570358219.
31. IUSS Working Group WRB *World Reference Base for Soil Resources*; 2015; Vol. 43; ISBN 9789251083697.
32. Teixeira, P.C.; Fontana, G.K.D.A.; Teixeira, W.G. *Manual de metodos de analises*; 2017; ISBN 9788570357717.
33. Terra, F.S.; Demattê, J.A.M.; Viscarra Rossel, R.A. Proximal spectral sensing in pedological assessments: vis–NIR spectra for soil classification based on weathering and pedogenesis. *Geoderma* **2018**, *318*, 123–136.
34. Demattê, J.A.M.; Terra, F. da S. Spectral pedology: A new perspective on evaluation of soils along pedogenetic alterations. *Geoderma* **2013**.
35. Vasques, G.M.; Grunwald, S.; Sickman, J.O. Comparison of multivariate methods for inferential modeling of soil carbon using visible/near-infrared spectra. *Geoderma* **2008**, *146*, 14–25.
36. Rosenblatt, F. The Perceptron: A probabilistic model for information storage and organization in the brain. *Psychological Review* **1958**, *65*, 386–408.
37. Breiman, L. Random forests. *Machine Learning* **2001**, *45*, 5–32.
38. Lawrence, R.L.; Wood, S.D.; Sheley, R.L. Mapping invasive plants using hyperspectral imagery and Breiman Cutler classifications (randomForest). *Remote Sensing of Environment* **2006**, *100*, 356–362.
39. Liu, Y.; Sun, X.; Ouyang, A. Nondestructive measurement of soluble solid content of navel orange fruit by visible–NIR spectrometric technique with PLSR and PCA-BPNN. *LWT - Food Science and Technology* **2010**, *43*, 602–607.
40. Quinlan Bassar, J.R. *LEARNING WITH CONTINUOUS CLASSES*; World Scientific, 1992;
41. Nguyen, H.; Bui, X.-N.; Tran, Q.-H.; Mai, N.-L. A new soft computing model for estimating and controlling blast-produced ground vibration based on Hierarchical K-means clustering and Cubist algorithms. *Applied Soft Computing* **2019**, *77*, 376–386.
42. Rulequest Research Rulequest, data mining with cubist Available online: <https://rulequest.com/cubist-info.html> (accessed on Jul 15, 2019).
43. Chang, C.W.; Laird, D.A. Near-infrared reflectance spectroscopic analysis of soil C and N. *Soil Science* **2002**, *167*, 110–116.
44. R Core Team R: A Language and Environment for Statistical Computing 2018.
45. R Core Team foreign: Read Data Stored by “Minitab”, “S”, “SAS”, “SPSS”, “Stata”, “Systat”, “Weka”, “dBase”, ... 2018.
46. Wickham, H. dtplyr: Data Table Back-End for “dplyr” 2017.
47. Allaire, J.J.; Wickham, H.; Ushey, K.; Ritchie, G. rstudioapi: Safely Access the RStudio API 2017.
48. Jed Wing, M.Kuhn.C.; Weston, S.; Williams, A.; Keefer, C.; Engelhardt, A.; Cooper, T.; Mayer, Z.; Kenkel, B.; the R Core Team; Benesty, M.; et al. caret: Classification and Regression Training 2018.
49. Stevens, A.; Ramirez-Lopez, L. prospectr: Miscellaneous functions for processing and sample selection of vis-NIR diffuse reflectance data 2014.
50. Breiman, L.; Cutler, A.; Liaw, A.; Wiener, M. randomForest: Breiman and Cutler’s Random Forests for Classification and Regression 2018.
51. Kuhn, M.; Quinlan, R. Cubist: Rule- And Instance-Based Regression Modeling 2018.
52. Mevik, B.-H.; Wehrens, R.; Liland, K.H. pls: Partial Least Squares and Principal Component Regression 2016.
53. Fritsch, S.; Guenther, F. neuralnet: Training of Neural Networks 2016.
54. Ripley, B. MASS: Support Functions and Datasets for Venables and Ripley’s MASS 2019.

55. Malone, B. *ithir: Soil data and some useful associated functions*. 2018.
56. Neuwirth, E. *RColorBrewer: ColorBrewer Palettes* 2014.
57. Carr, D.; Lewin-Koh, N.; Maechler, M. *hexbin: Hexagonal Binning Routines* 2018.
58. Murrell, P. *gridBase: Integration of base and grid graphics* 2014.
59. Wickham, H.; Chang, W.; Henry, L.; Pedersen, T.L.; Takahashi, K.; Wilke, C.; Woo, K. *ggplot2: Create Elegant Data Visualisations Using the Grammar of Graphics* 2018.
60. Torgo, L. *DMwR: Functions and data for "Data Mining with R"* 2013.
61. Wickham, H. *stringr: Simple, Consistent Wrappers for Common String Operations* 2018.
62. Chang, C.-W.; Laird, D.A.; Mausbach, M.J.; Charles R. Hurburgh, J. Near-Infrared Reflectance Spectroscopy–Principal Components Regression Analyses of Soil Properties. *Soil Science Society of America Journal* **2001**, 480–490.