Master Degree Internship :

Development of prediction models for C, N, Fe and Al in volcanic soils in Costa Rica using Infrared spectroscopy

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Colaborators : Aurélie CAMBOU (IRD), Gilles CHAIX (CIRAD),
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Introduction : do you know Costa Rica ?

Costa Rica : a small country in Central America, well known for its nature and a model of eco-tourism...

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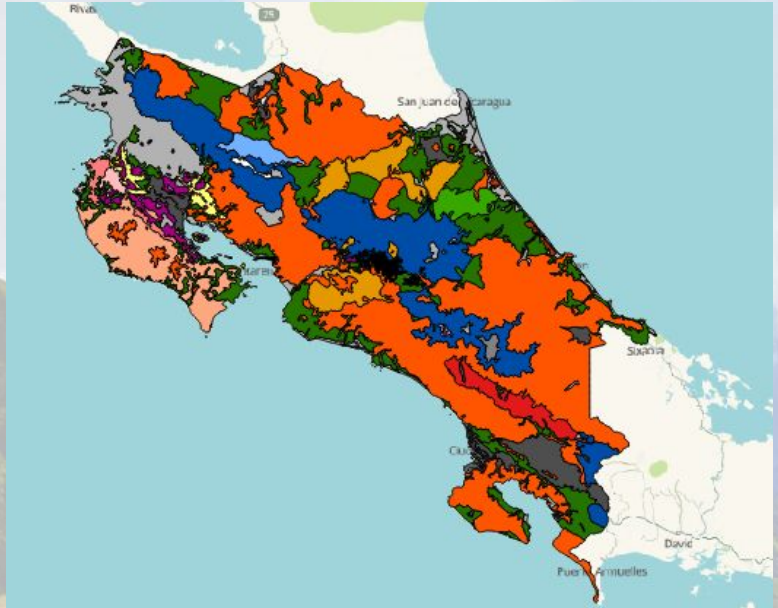
Costa Rica : a small country in Central America, well known for its nature and a model of eco-tourism...

…But Costa Rica is also a country with intense agriculture (very fertile volcanic **andosols** and **ultisols**), and is the country in the world with the highest use of herbicides per km² *



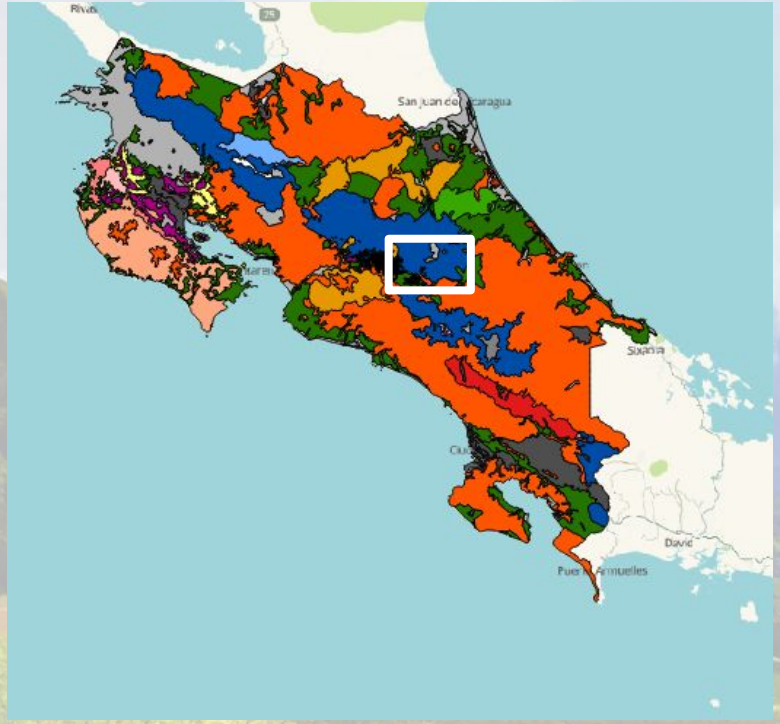
Costa Rica soil suborden maps : SuelosCR built by the UCR

* technically, it is third after the Maldives and Trinity and Tobago, but they both account for less than 0.1% of world global pesticide use (1500 tonnes/year), meanwhile Costa Rica is the 34th country in the world using most pesticides, with 12 811 tonnes/year. source : FAOSTAT

Introduction

The region of the Irazu and Turrialba volcano at the North of Cartago, is the most intensively cultivated, and supplies to the whole country.

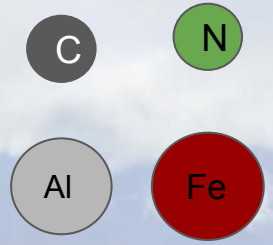
photo credit : Julien Demenois



Introduction

Classic monitoring of agricultural soil implies **laboratory analysis** of C,N, Al and Fe
-> time consuming, expensive and produces waste

photo credit : Julien Demenois



OBJECTIVE : Being able to assess C,N,Al and Fe from soil thanks to **infrared spectroscopy** (cheaper and faster) for a better monitoring of soil characteristics in the region.

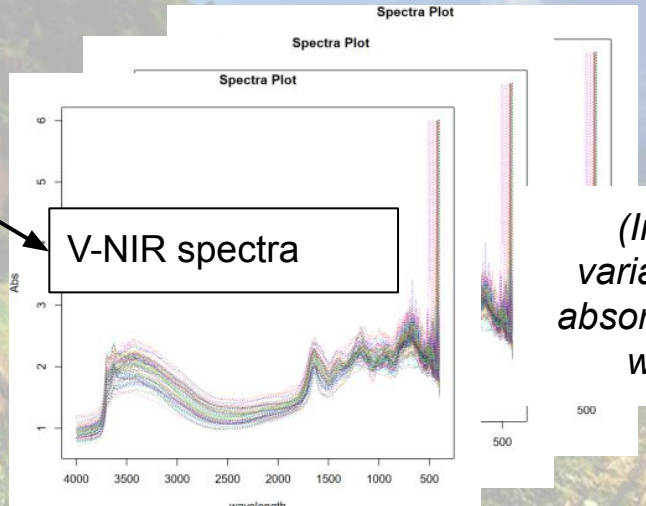
Quick reminder : How to develop a prediction model

Field samples

(Independant variables: altitude, temperature, precipitation, depth)

laboratory analysis

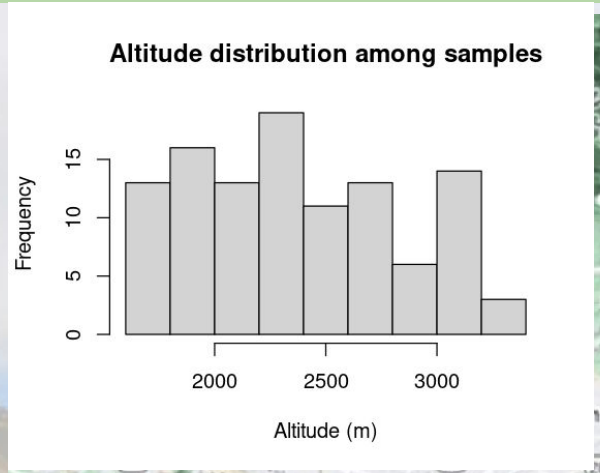
(Target variables : C, N, Fe, Al)



V-NIR spectra

(Independent variables: value of absorbance for each wavelength)

Sampling the Irazu volcano south flank…



At each point, several samples were taken at different depths

Spectroscopy and laboratory measurements

VNIR spectra (500nm - 2500nm) acquired with the FOSS DS2500 provided by CINA

MIR spectra (2000 - 25000 nm) acquired with a PERKIN ELMER provided by CICA (currently analysed)

C I N A

Laboratory analysis : lab provided by CIA (UCR)

SOC : **dry combustion** using C / N analyser (Dumas method)

Al / Fe : **selective dissolution** extraction by **ammonium oxalate**

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Final dataset

The dataset is made of:

· A total of **108** samples, from 39 locations, with 2 to 10 horizons sampled at each location

· Environmental data : Soil type, soil subtype, altitude, land use, mean annual temperature, mean annual precipitation

· Laboratory measurement of Al, C, N and Fe for each sample

· V-NIR Spectra measurement for each sample

· MIR spectra measurement for each sample (not analysed yet)

Final dataset

A priori problems :

- 108 samples isn’t that much to make a PLSR model
- some of the data are strongly correlated (samples from the same hole…)

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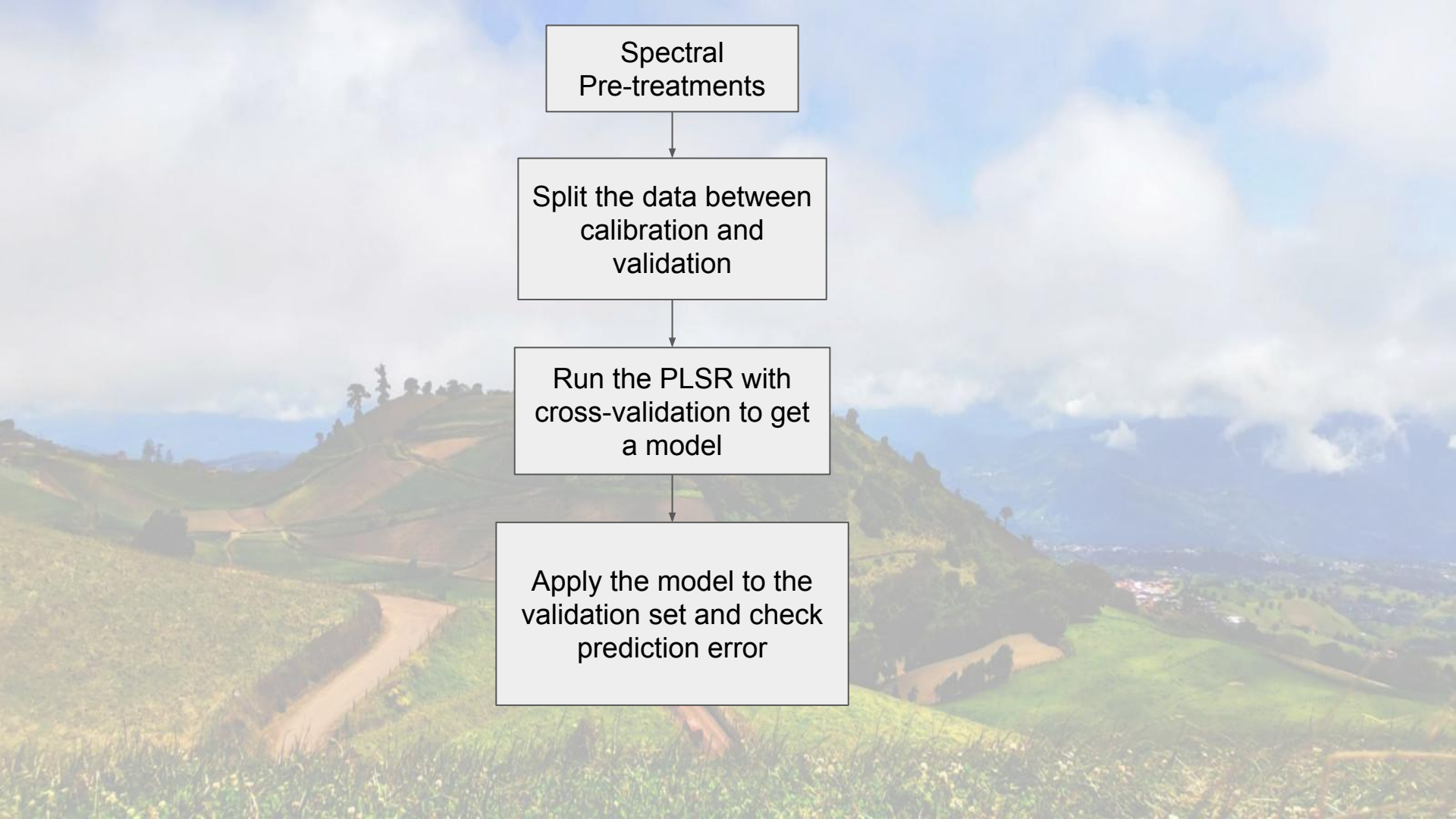
Idea to make a better model :

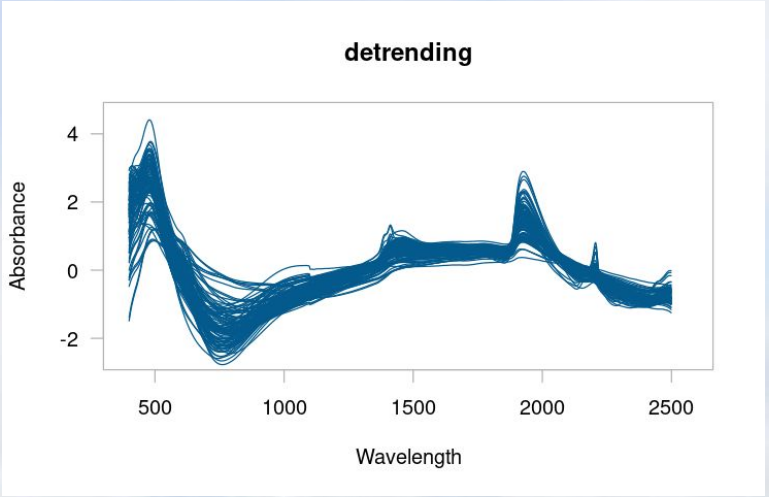
- use VNIR *and* MIR data (separately or together with spiking)
- **add environmental variables** (altitude, depth) as extra covariables

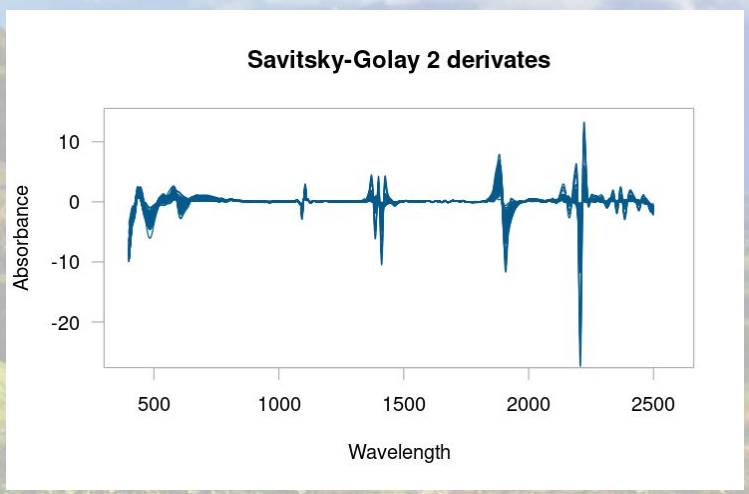
Calibrating the model


Spectral Pre-treatments
Split the data between calibration and validation
Run the PLSR with cross-validation to get a model
Apply the model to the validation set and check prediction error

Spectral Pre-treatments

for each element, 7 different pretreatments were tested (none, detrend, SNV, SavGol1/2, SNV+SavGol1/2)





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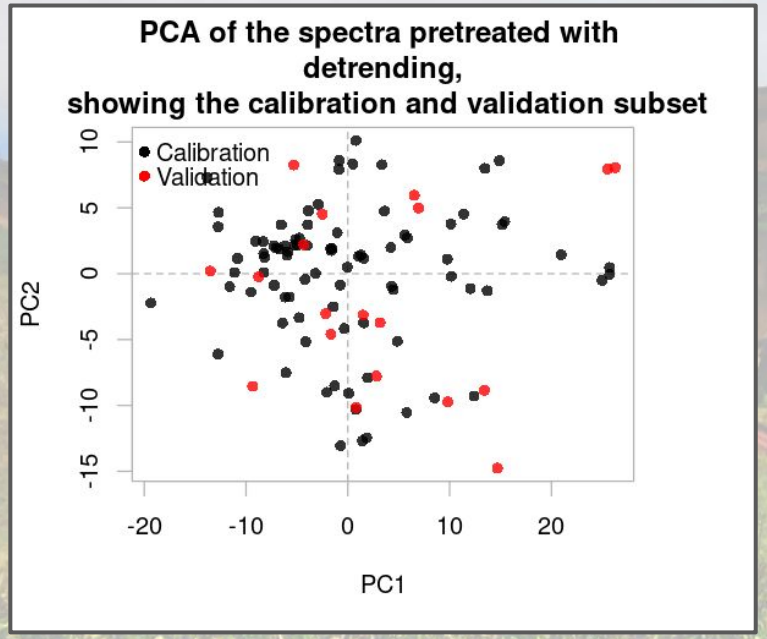
We used a custom Duplex sampling algorithm, enabling us to keep in a same group the samples from the same geographic point -> independence between calibration and validation



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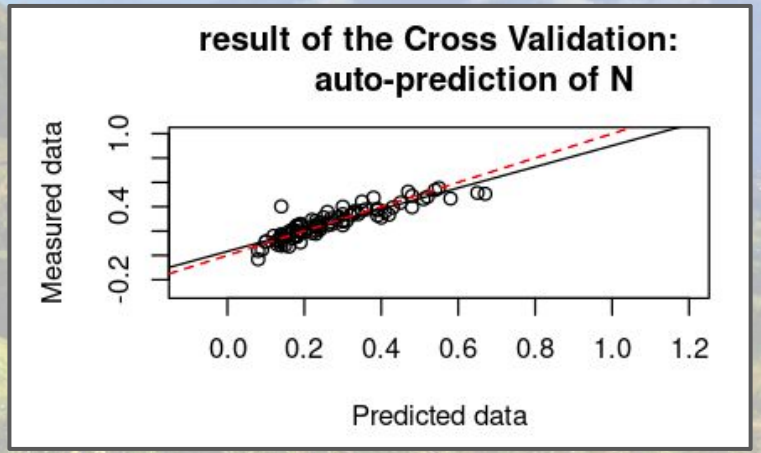
Run the PLSR with cross-validation to get a model

The PLSR was run with R package ***rnirs*** and used 3 group of cross-validation sampled with the K-foldings method, with 10 replicates.

We selected at this step the number of Latent variables (LV) for which the RMSECV was the lowest.



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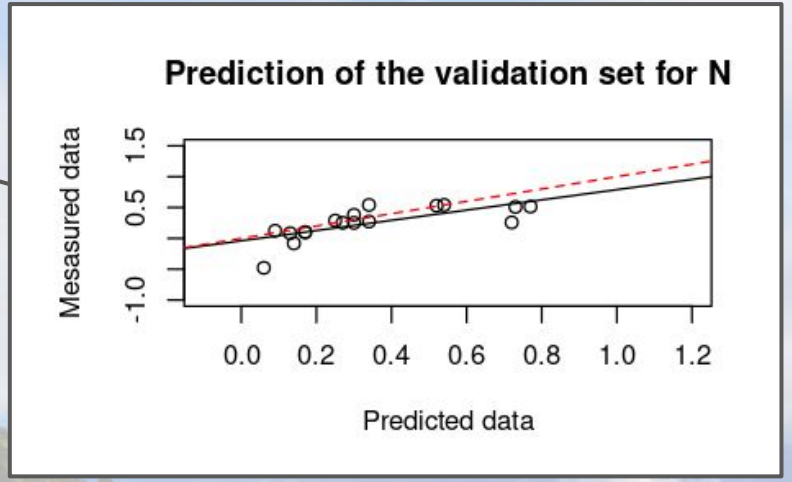

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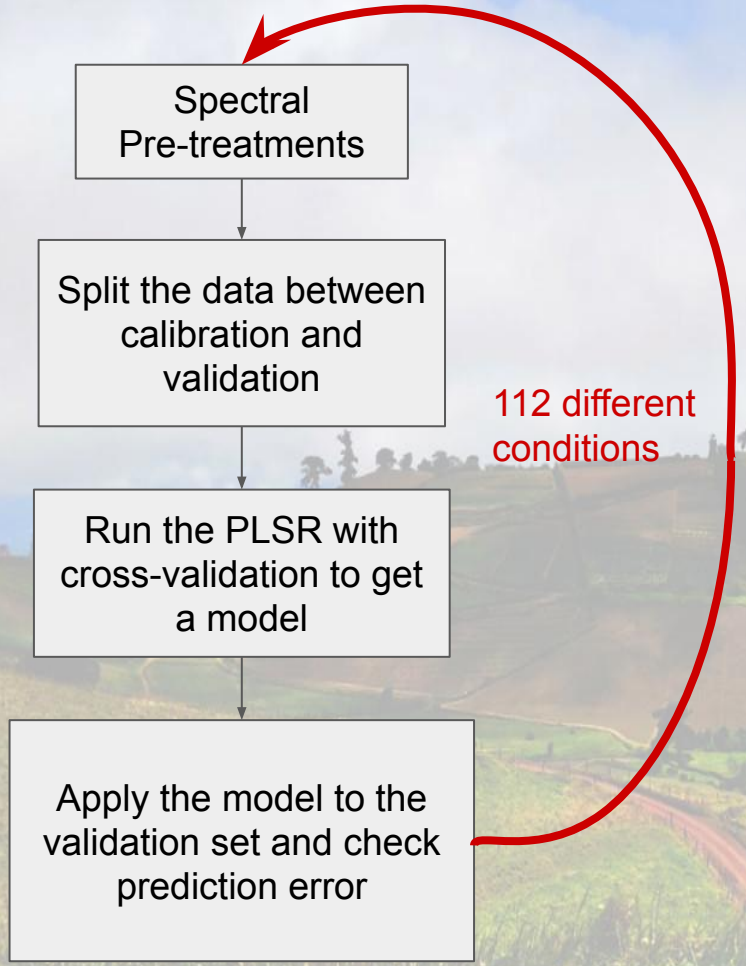
For each element and each pretreatment, we looked at the RPD of the prediction of the validation. If **RPD>1.6**, we accept the model.



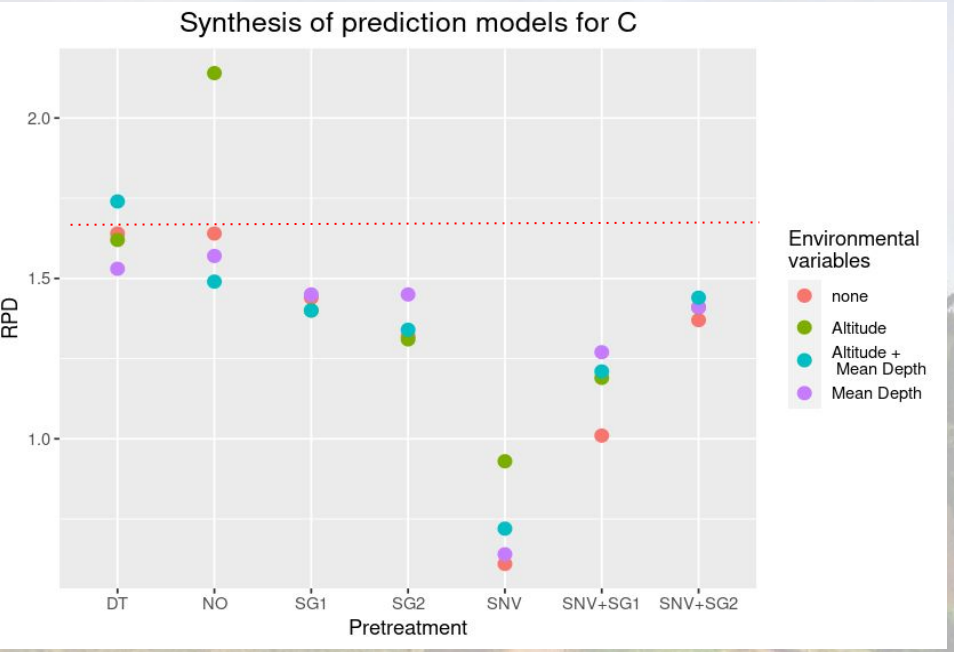
For each element (C, N, Fe, Al) :

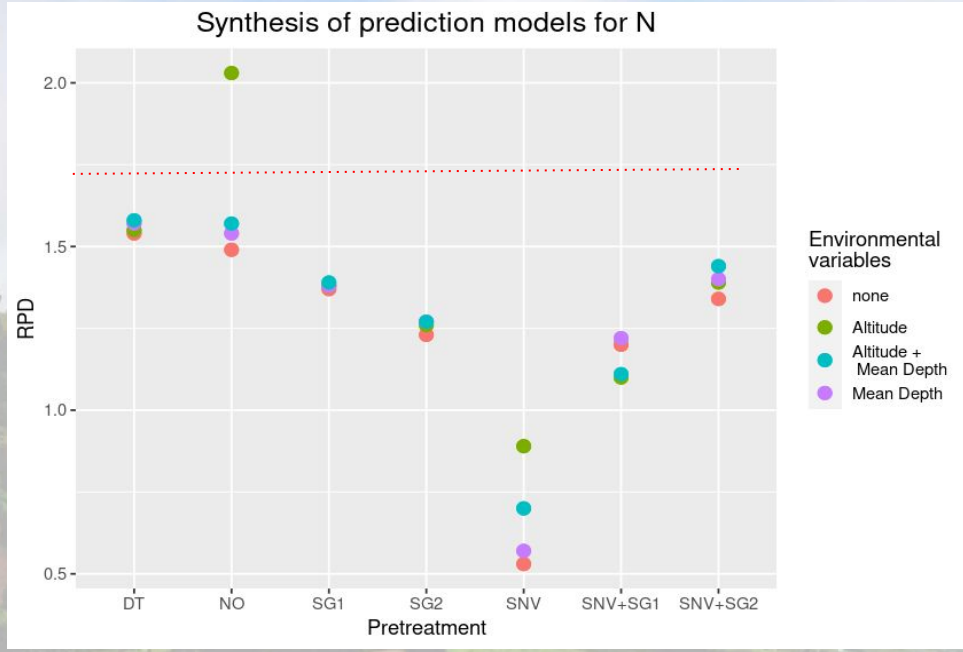
For each of the 7 pretreatments :

For each combination of environmental variables : without, with Altitude, with depth, with altitude+depth

-> 112 PLSR models (28 per element) were run

Synthesis of the results

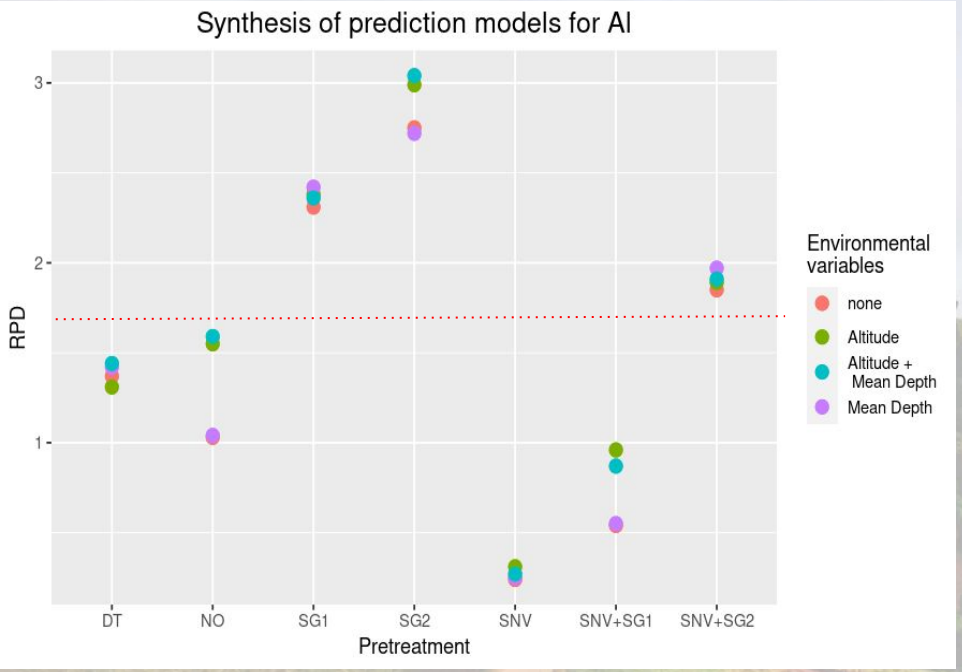


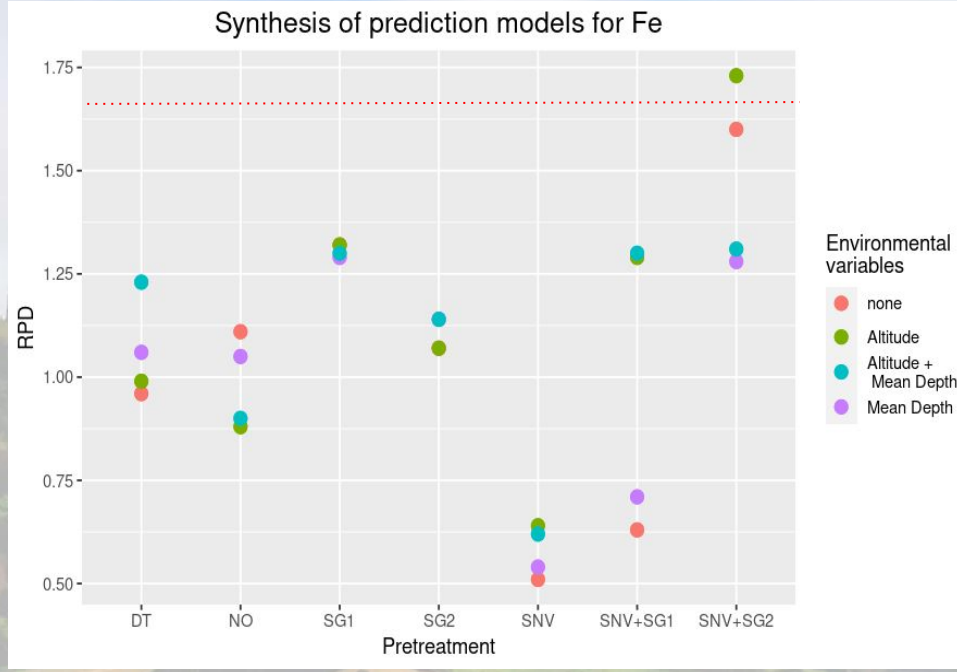


RPD = SDcal / RMSEP

The prediction for C and N is better with lighter/no pretreatments, and improved when we add field covariables

Synthesis of the results : prediction of Al and Fe

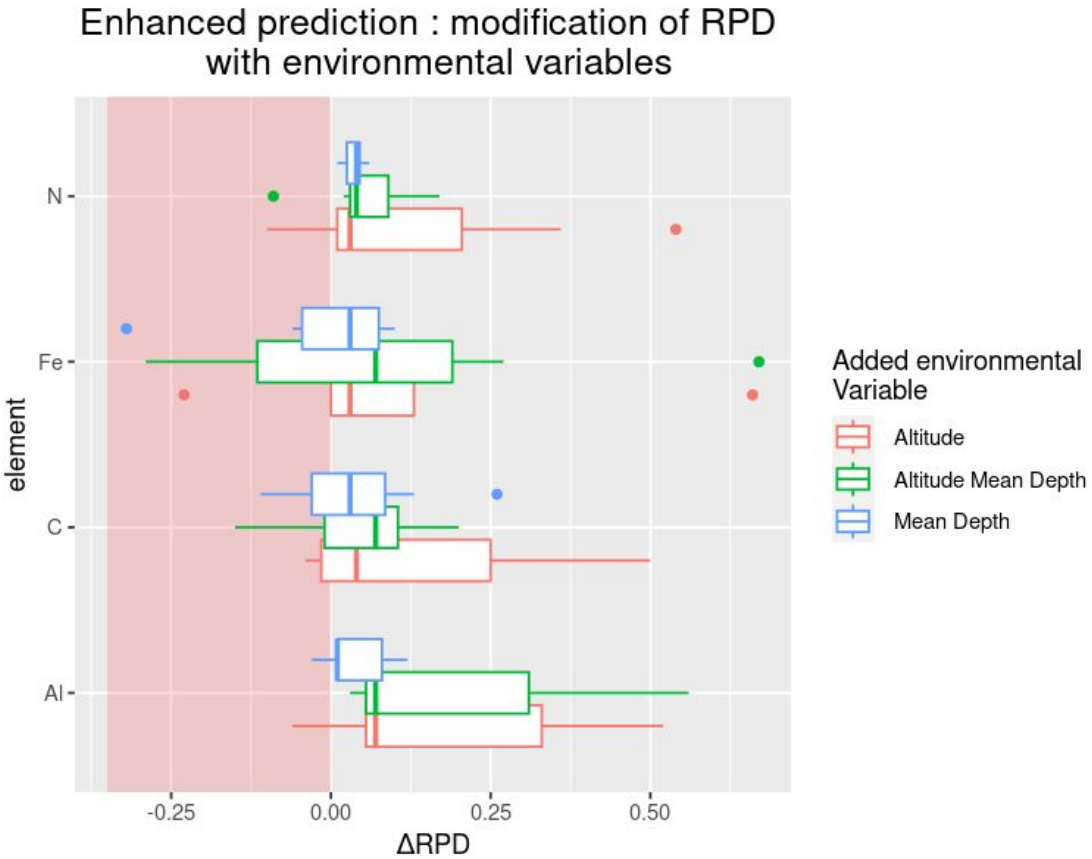




RPD = SD_{cal} / RMSEP

Fe was poorly predicted in almost every situation. Adding environmental variables on heavily-treated spectras seems helping.

Summary



· Adding environmental variables increased the prediction performance of most PLSR models

· For C, N and Al, we encountered some models with a good (RPD>1.6) prediction performance.

· Fe was poorly predicted, but with heavy pre-treatment and environmental variables, we managed to reach the RPD threshold

Limitations and further investigations

· Selection Cal/Val **after** the pretreatments

=> overfitting +

we don’t have the same Cal and Val groups for each model : can we really compare the different RPD with themselves ?

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Solution

· making the cal/val selection **before** the pretreatments to have the same groups

and/or

· making the cal/val selection based on the explanatory variables (y growing) rather than on the spectra

That’s it!
Thanks for your attention!

photo credit for the background : Cintya Solano (UCR)