



International Workshop

“Soil Spectroscopy: the present and future of Soil Monitoring”

FAO HQ, Rome, Italy, 4-6 December 2013

Spectral data fusion for quantitative assessment of soils from Brazil

Dr. Fabrício da Silva Terra

Dr. José Alexandre Melo Demattê

Dr. Raphael Viscarra Rossel



Introduction:

Brazil has territorial area
8,514,887 km²

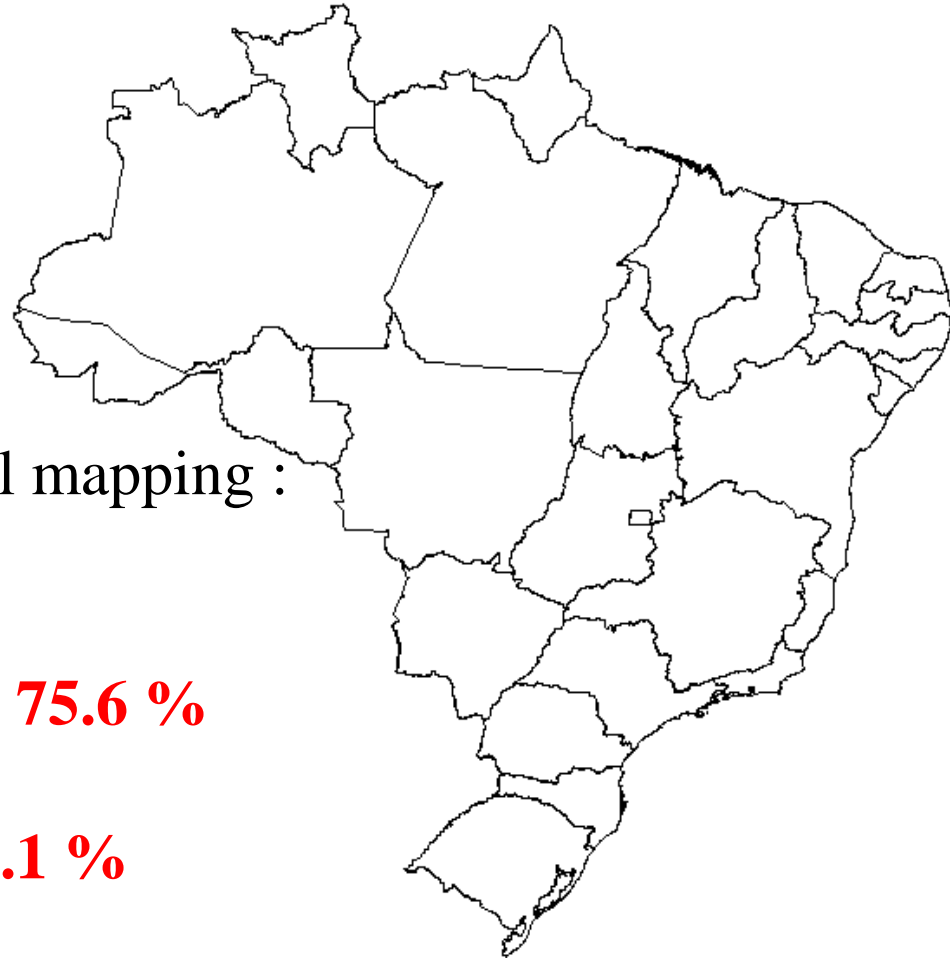
➤ Brief overview of Brazilian soil mapping :

Mapping at:

1:750,000 to 1:2,500,000 **75.6 %**

1:100,000 to 1:750,000 **17.1 %**

≥ 1:100,000 and ≥ 1:20,000 **only 0.25%**
(semi-detailed and detailed)



Santos and Santos (2007)

Introduction:

➤ Expansion and intensification of agriculture, and the growing environmental concern ...

➤ Necessity of soil monitoring

➤ For this...

Soil maps with scales suitable for our purposes.

... in other words:

We need to expand those **0.25 %**

(semi and detailed soil mapping)

And to do this ...

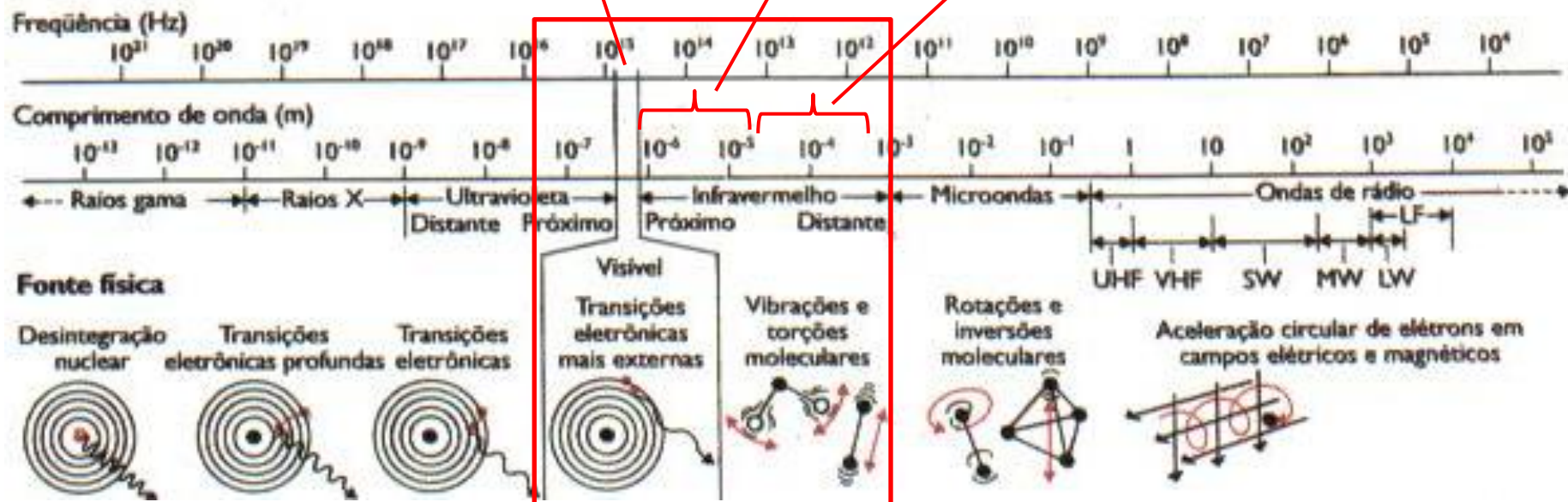
- Lots of field work, soil surveys, soil sampling and analyses are needed: expensive, time consuming and wasteful



Introduction:

- In this sense... Soil Reflectance Spectroscopy): efficient alternative in evaluating soils and their attributes.
- What is the **most appropriate** spectral range in quantitative assessment?
- Can **spectral fusion** increase predictive efficiency?

Vis: 350-700 nm **NIR: 700-2500 nm** **MidIR: 2500-25000 nm**



Aims:

- To **compare** the predictions of clay content (CC), soil organic carbon (SOC) and sum of bases ($\text{SB} = \text{Ca}^{2+} + \text{Mg}^{2+} + \text{K}^{+}$) based on **individual** and **combined** spectral ranges from visible to near-infrared (VisNIR: 350 to 2500 nm) e from mid-infrared (MIR: 4000 to 400 cm^{-1})

Soil database

- **1259** soil samples

Soil classes

(FAO – WRB)

Leptosols

Ferralsols

Nitisols

Gleysols

Cambisols

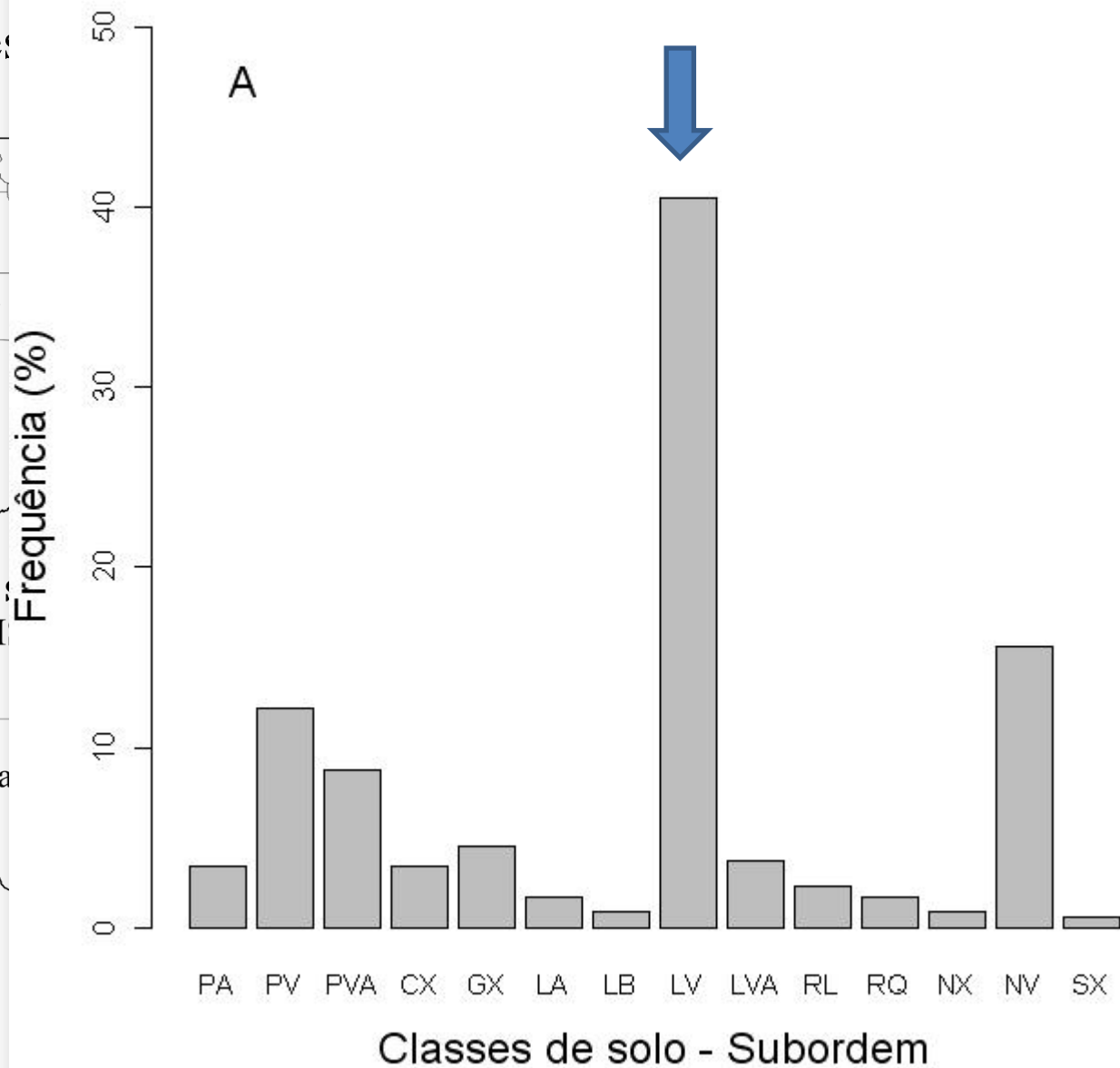
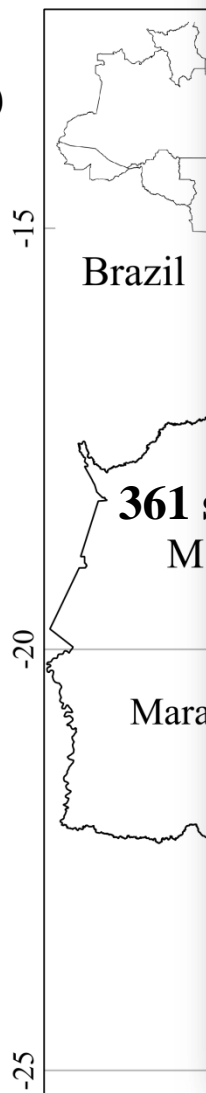
Lixisols

Acrisols

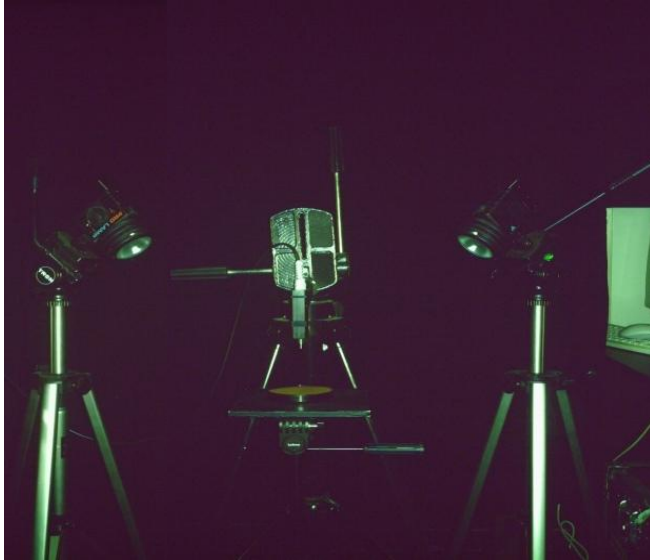
Alisols

Planosols

Arenosols



Reflectance Spectroscopy

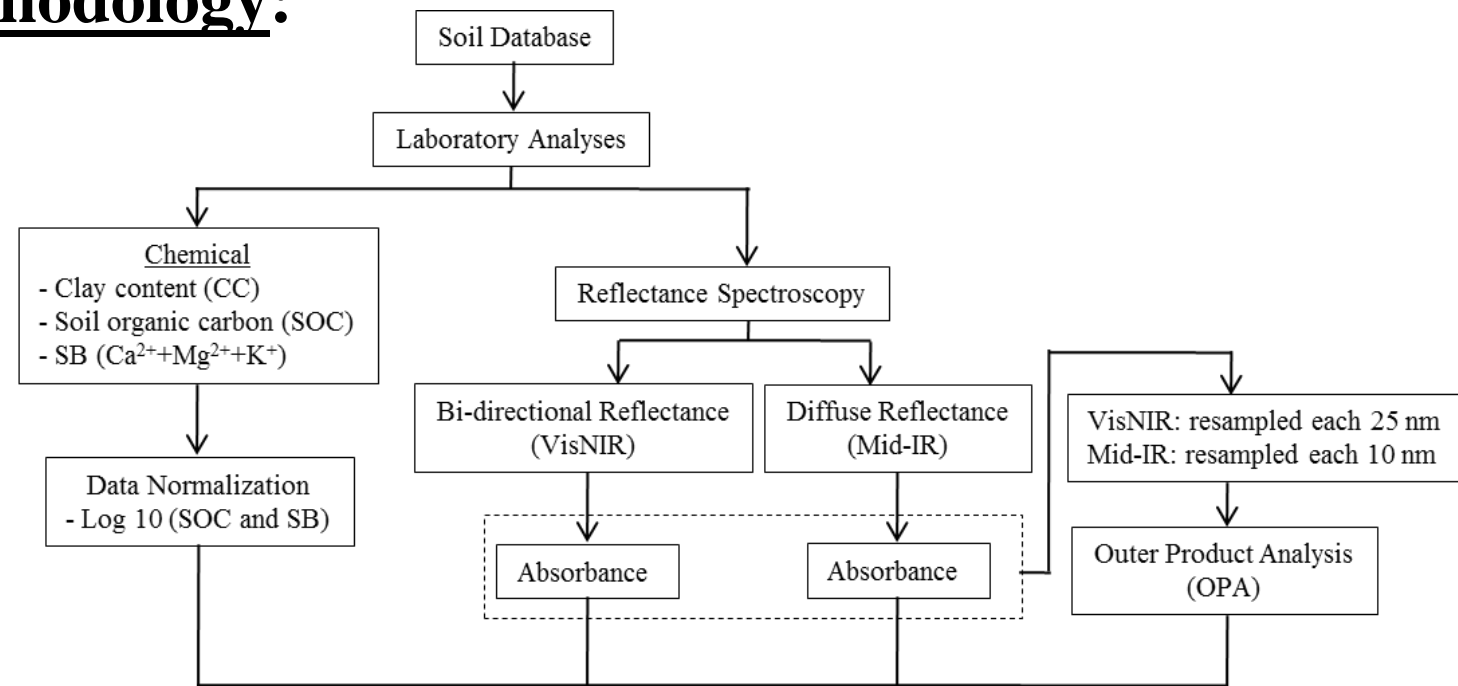


- Mid-IR (4000 to 400 cm^{-1}): soil < 200 μm
- Equipment: Thermo Nicolet 6700 FTIR
 - Accessory: Smart Diffuse Reflectance
 - Acquiring: resolution of 1.2 nm
average of 64 scans/min
 - Calibration: diffuse gold plate
every 1 sample

- VisNIR (350 to 2500 nm): soil < 2 mm
- Equipment: FieldSpec Pro
 - Acquiring: resolution of 1 nm
average of 100 scans
 - Calibration: barium sulfate plate
every 20 samples



Methodology:



RPD classification: Chang et al. (2001)

RPIQ: Bellon-Maurel et al. (2010)

RPD > 2 : Excellent
1.4 < RPD < 2 : Reasonable
RPD < 1.4 : non-reliable
RPD = Standard Deviation / RMSE
RPIQ = Inter Quartil / RMSE

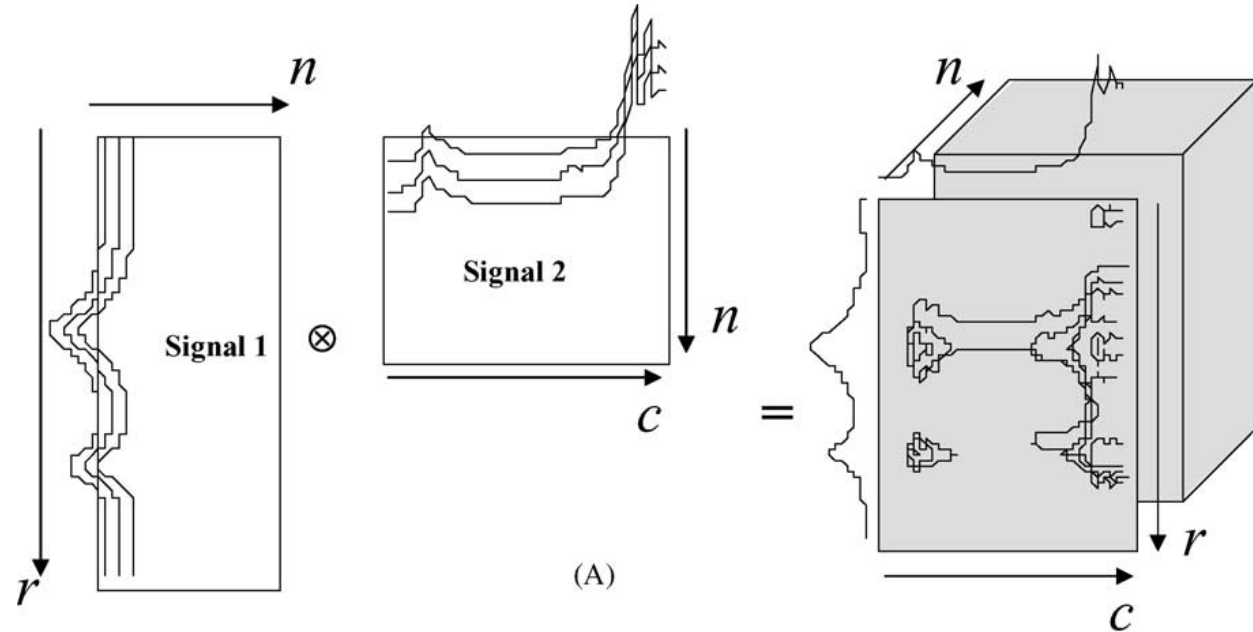
3 treatments: VisNIR, Mid-IR, OPA
4 variables: R², RMSE, RPD, RPIQ
2 blocks: calibration and test
3 repetitions each block

Mean Comparison:
ANOVA
and
Tukey's test

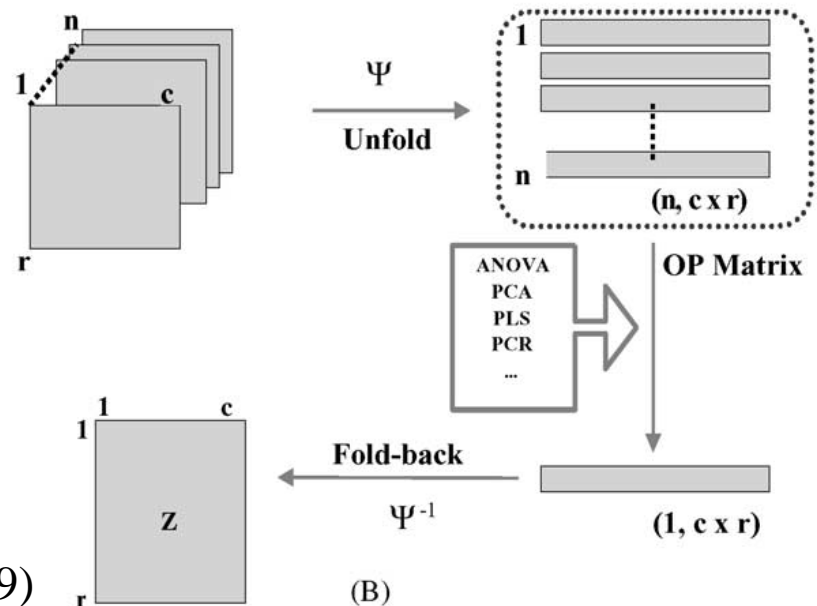
Comparison among predictions:
spectral range (individual e combined)
R², RMSE, RPD, RPIQ

The most appropriate spectral range
to predict specific property

Methodology: Outer Product Analysis (OPA): ‘data fusion’

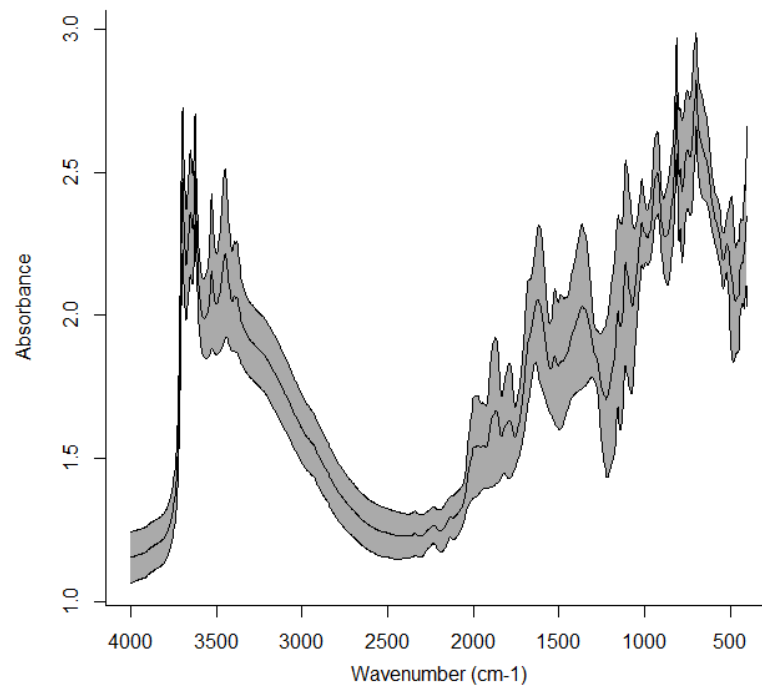
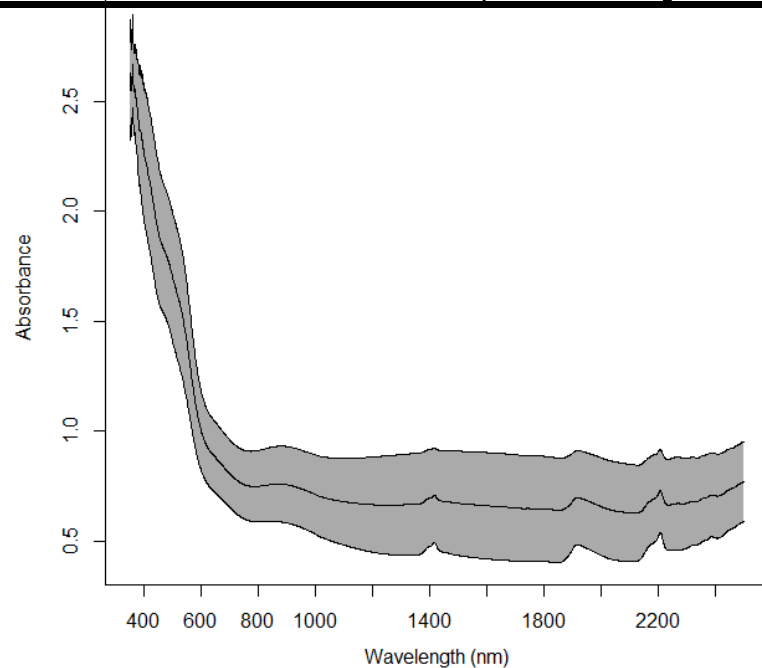


- To emphasise co-evolutions of different spectral regions in the same domain;



Adapted from Jaillais et al. (2009)

Soil spectral behaviour (Absorption)



488 and 903 nm:

- Fe oxide and hydroxide (hematite and goethite)

1414 nm:

- Clay minerals (1:1 / 2:1) (kaolinite, montmorillonite, illite)

- Hydroxyl (water molecules)

1917 nm: - Hydroxyl (water molecules)

2205 nm:

- Clay minerals (1:1 / 2:1) (kaolinite, montmorillonite, illite)

2251 nm: - Al hydroxide (gibbsite)

2314 nm: - Carbonates and organic compound (methyl)

2355 and 2448 nm: 2:1 clay mineral (illite)

2382 nm: Carbohydrates

3605 to 3394 cm⁻¹:

- Clay minerals (1:1 / 2:1) (kaolinite, montmorillonite, illite)

- Al hydroxide (gibbsite)

2233 to 1975 cm⁻¹:

Organic compounds (alkyne groups)

Quartz

1867 to 1362 cm⁻¹:

- Quartz

- Clay minerals (1:1 / 2:1)

(kaolinite, montmorillonite, illite, vermiculite)

- Fe oxide and hydroxide (hematite and goethite)

- Organic compounds

(amide, aromatic, aliphatic, phenolic)

1157 to 926 cm⁻¹:

- Organic compounds (aliphatic, polysaccharide)

- Quartz

- Fe oxide (hematite)

- Al hydroxide (gibbsite)

- Clay minerals (1:1 / 2:1)

814 to 436 cm⁻¹:

- Quartz

- Fe oxide and hydroxide (hematite and goethite)

- Al hydroxide (gibbsite)

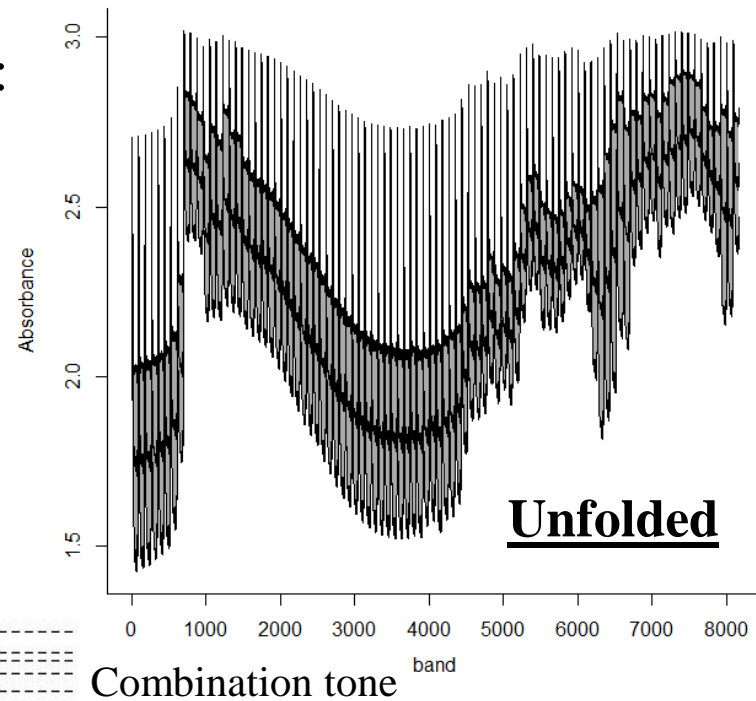
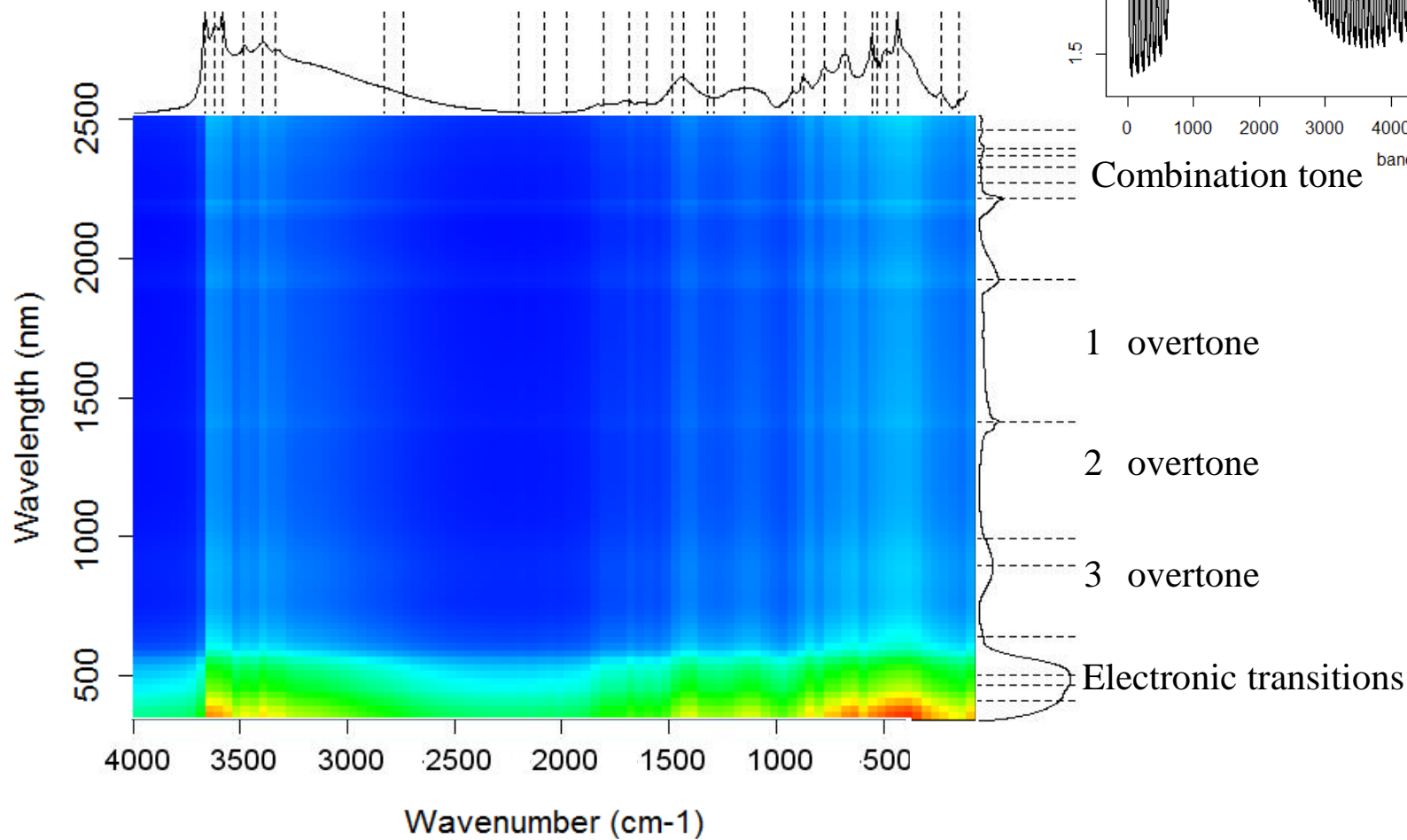
Co-evolution between spectral ranges:

Fundamental vibrations (stretching and bending)

Overtone and combination tones

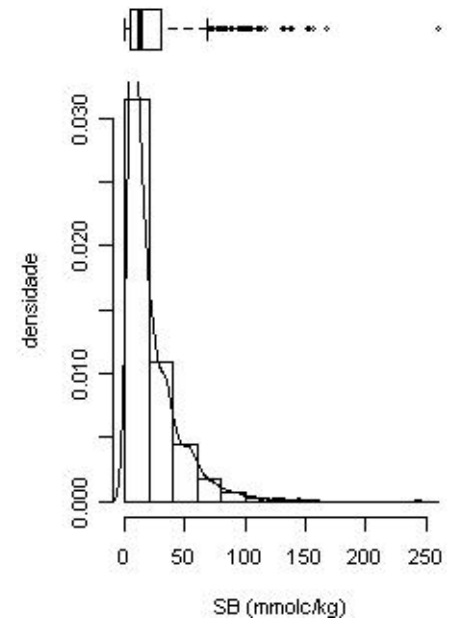
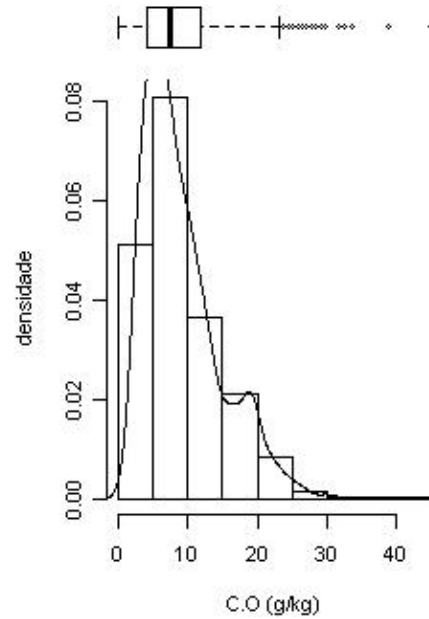
Folded: matrix representation

X-H stretching triple bond double bond fingerprint

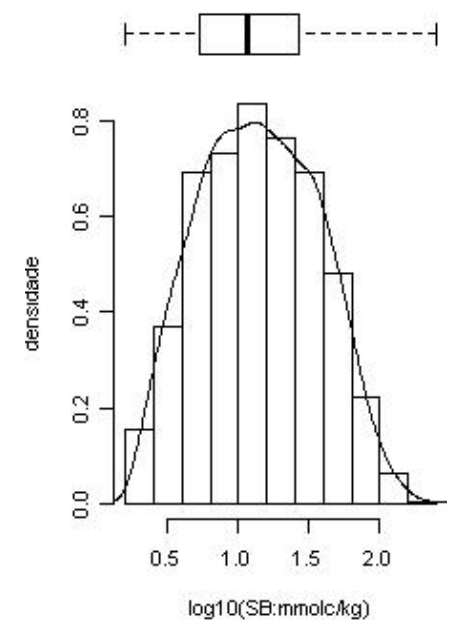
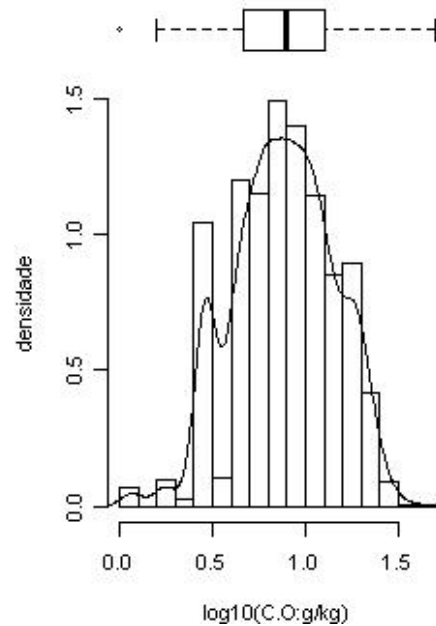


Soil property normalization

Before

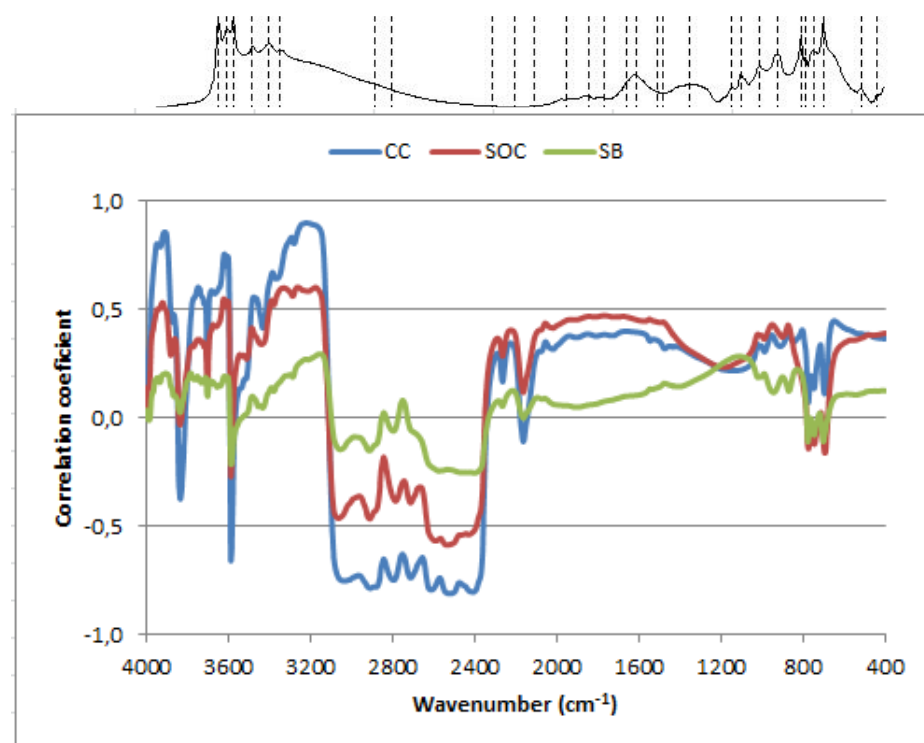
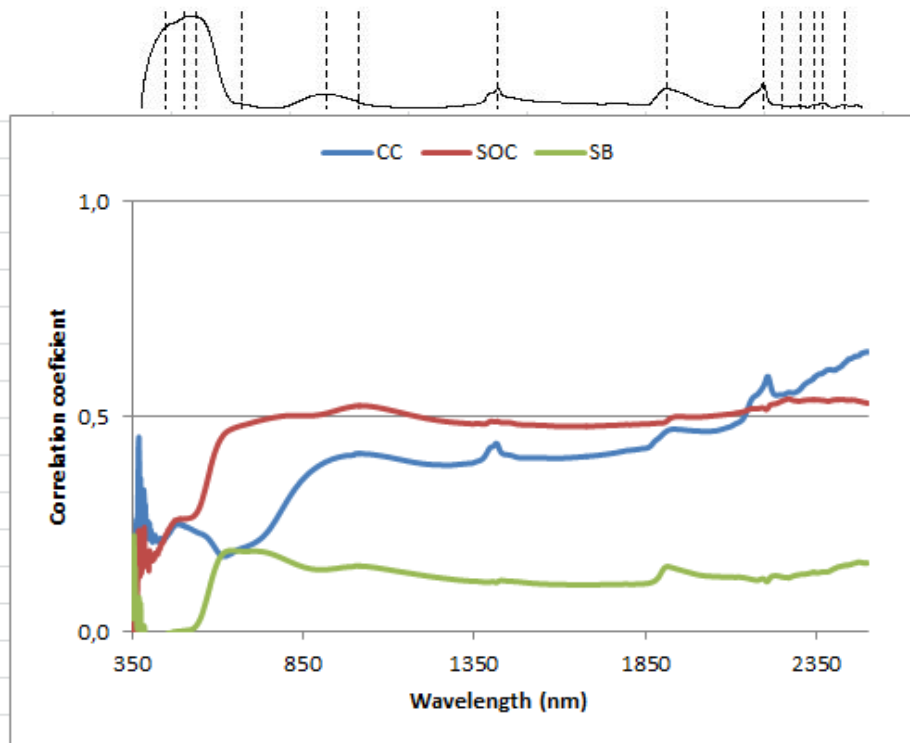


After



Correlation: Interactions - attributes vs spectral behavior

- MIR generally higher



Prediction performances: Mean comparison

CC varied from 10 g kg⁻¹ to 930 g kg⁻¹

SOC from 1.2 g kg⁻¹ to 41 g kg⁻¹

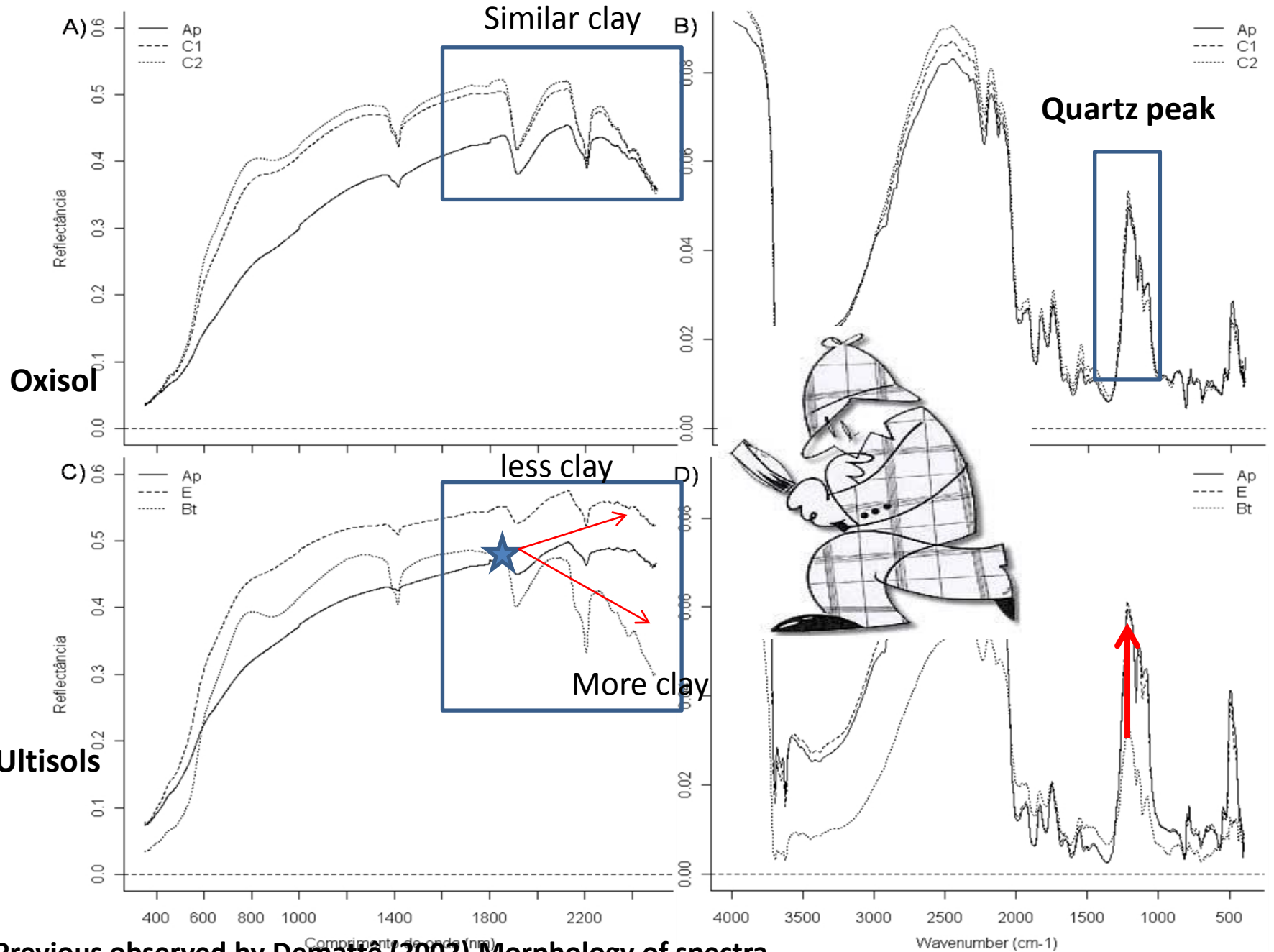
SB from 2.1 mmol_c kg⁻¹ to 290.5 mmol_c kg⁻¹.

Clay content (CC)								
Range	Features	DP	1Q	3Q	R ²	RMSE	RPD	RPIQ
OPA	8178	250.06	220.00	710.00	0.91a	75.70a	3.30a	6.43a
Mid-IR	934	251.80	220.00	710.00	0.90a	78.70a	3.20a	6.23a
VisNIR	2151	251.28	220.00	720.00	0.84a	102.00b	2.46b	4.90b
Soil organic carbon (SOC): Log10 (normalization)								
Range	Features	DP	1Q	3Q	R ²	RMSE	RPD	RPIQ
OPA	8178	0.27 (1.86)	0.67 (4.68)	1.06 (11.48)	0.70a	0.15a (1.41)	1.80a	2.60a
Mid-IR	934	0.27 (1.86)	0.67 (4.68)	1.08 (12.02)	0.69b	0.15a (1.41)	1.80a	2.73a
VisNIR	2151	0.27 (1.86)	0.67 (4.68)	1.06 (11.48)	0.64c	0.16b (1.44)	1.69b	2.44b
Sum of bases (SB): Log10 (normalization)								
Range	Features	DP	1Q	3Q	R ²	RMSE	RPD	RPIQ
OPA	8178	0.41 (2.57)	0.83 (6.76)	1.48 (30.20)	0.54b	0.28b (1.90)	1.46b	2.32b
Mid-IR	934	0.41 (2.57)	0.83 (6.76)	1.48 (30.20)	0.60a	0.26a (1.82)	1.58a	2.50a
VisNIR	2151	0.42 (2.63)	0.78 (6.02)	1.47 (29.51)	0.39c	0.33c (2.14)	1.27c	2.09c

MIR validation set 395 samples

Atributte	Normalização	Algoritmo	R ²	RMSE	RPD	RPIQ
P	Logaritmo / base 10	SVM (Linear)	0,36	0,35	1,26	1,71
K	Logaritmo / base 10	SVM (Radial)	0,21	0,45	1,13	1,33
Ca	Logaritmo / base 10	SVM (Linear)	0,71	0,25	1,84	2,80
Mg	Logaritmo / base 10	SVM (Radial)	0,54	0,28	1,46	1,93
Al	Raiz quadrada	SVM (Linear)	0,81	0,75	2,28	3,77
H+Al	Raiz quadrada	SVM (Linear)	0,80	0,81	2,23	2,88
V%	Raiz quadrada	SVM (Linear)	0,76	0,99	2,05	3,24
m%	Raiz quadrada	SVM (Radial)	0,66	1,93	1,72	3,56
Ativ. Arg.	Raiz quadrada	SVM (Linear)	0,66	2,14	1,71	1,79
Cu	Raiz quadrada	SVM (Radial)	0,53	0,69	1,46	2,32
Fe	Raiz quadrada	SVM (Radial)	0,29	1,84	1,20	1,39

IN practice for soil classification



Conclusions:

- Predictions by OPA were better for CC and SOC but the fusion did not bring a considerable increase in the predictive efficiency (despite co-evolutions and a large number of spectral features)
- OPA may not be the best way to combine spectra of the same type
- Other types of data fusion need to be tested
- Mid-IR spectra are still the best option to quantitative assessment of soil properties even for tropical soils
- Both, Mid-IR and Vis-Nir can be used for assistance on soil classification approachbo

Acknowledgments

- University of São Paulo (USP), “Luiz de Queiroz” College of Agriculture (ESALQ), Department of Soil Science (LSO)
- Australian Commonwealth Scientific and Industrial Research Organization (CSIRO)
- National Council for Scientific and Technological Development (CNPq)
- Coordination for the Improvement of Higher Education Personnel (CAPES)

