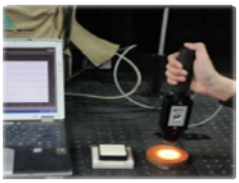



Improving the estimates of soil organic carbon using proximally sensed vis–NIR spectra

Wenjun Ji | Post doc
Department of Bioresource Engineering

24 April 2015

PhD supervisor:
Prof. Zhou Shi
Dr. Rapahel Viscarra Rossel

Post doc supervisor:
Prof. Viacheslav Adamchuk
Prof. Asim Biswas

McGill

Outline

Research background and Review

Proximally sensed spectra VS. Laboratory-based spectra

① Non-linear data mining algorithms

② Removing the environmental effects from the field spectra

③ Using existing Chinese soil spectral library to predict soil carbon rapidly

McGill

Background

McGill

Paddy terraces

McGill

Background

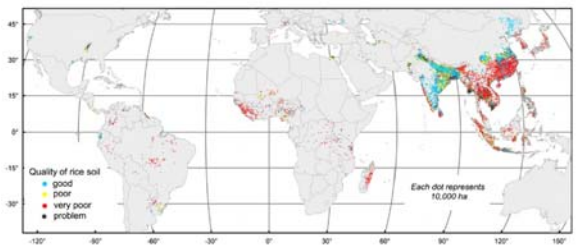


Figure 1-1 The spatial distribution of paddy soils in the world

(Haefele et al., 2014)

McGill

Background

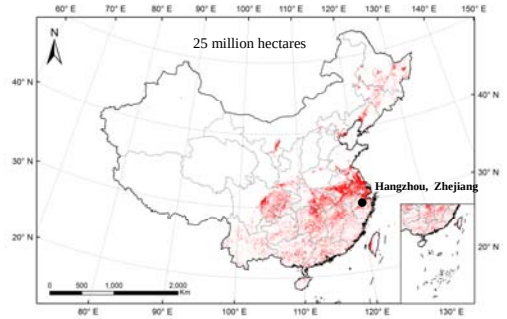
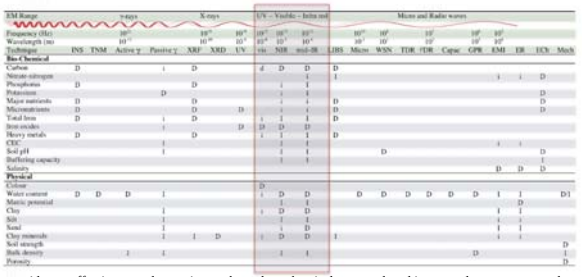


Figure 1-2 The spatial distribution of paddy soils in China

McGill

Background

vis-Near Infrared Spectroscopy



rapid, cost effective, non-destructive, no hazardous chemicals are used, and importantly,can measure a lot of soil properties using a single spectrum.

Viscarra Rossel et al., 2011 Advances in Agronomy

Background

Laboratory-based vis-NIR measurement	Proximally sensed vis-NIR measurement
Sample collection, Transportation, Drying, Grinding, and Sieving	In situ measurement Rapid !
Controlled indoor condition	Environmental effects（such as ambient light, soil moisture content, structure, temperature, dust, contamination by stones and excessive residues）

review

Proximally sensed vis-NIR spectroscopic measurement

- "Static in situ" — accomplished by holding a spectrometer stationary on a soil face.
  - bare optical fiber
    Kooistra et al.（2003）
    Stevens et al.（2008）
    Barrett et al.（2002）
  - contact reflectance probe
    Waiser et al.（2007）
    Viscarra Rossel et al.（2009）
    Ji et al.（2014）
- "on-the-go"
  - modified soil probe
    Kusumo et al.（2010）
    Ben-Dor et al.（2008）

review

Proximally sensed vis-NIR spectroscopic measurement

- "Static in situ" — accomplished by holding a spectrometer stationary on a soil face.
- "on-the-go" — typically involves a spectrometer either enclosed within or connected to (via fiber optics) an implement that is inserted into the soil and pulled behind a tractor.

Christy（2008）
Bricklemyer&Brown（2010）

Mouazen et al.(2005)
Mouazen et al.(2007)

review

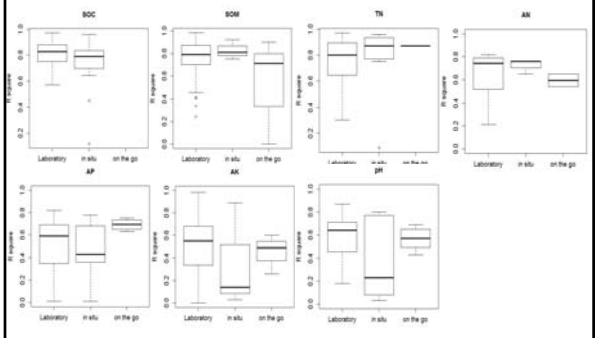


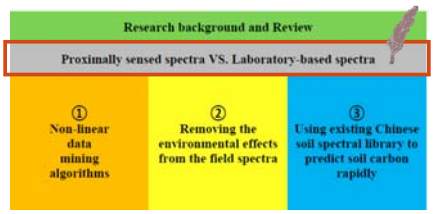
Fig. 1-1. Comparison of prediction accuracy of soil properties using laboratory, field in situ and on-the-go measured vis-NIR spectroscopy

problem

Laboratory-based vis-NIR measurement	Proximally sensed vis-NIR measurement
Sample collection, Transportation, Drying, Grinding, and Sieving	In situ measurement Rapid !
Controlled indoor condition	Environmental effects（such as ambient light, soil moisture content, structure, temperature, dust, contamination by stones and excessive residues） Accurate ?

Aim

Improving the estimates of soil organic carbon using proximally sensed vis–NIR spectra



Experimental design

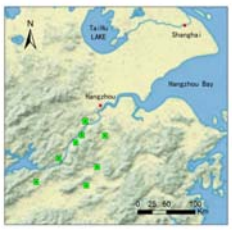


Fig. 2-1 The geographic distribution of the study fields

China National Rice Research Institute
In each field: 8-16 sensing locations
A total of 104 sensing locations.

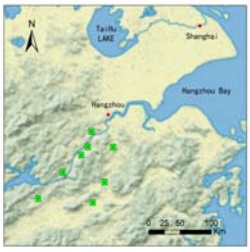


Fig. 2-1 The geographic distribution of the study fields

Static in situ measurement of Paddy Soil with vis-NIR Spectroscopy

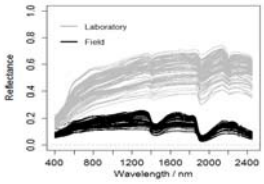
1. Moisture measurement
2.Soil sampling
3. Proximally sensed vis-NIR measurement

Drying Grinding and Sieving to 2mm

OC: dry combustion at 1100uC with a multi N/C 3100 (Analytik Jena AG, Germany).

5. Traditional chemical analysis
4. Laboratory-based vis-NIR measurement

3. Proximally sensed vis-NIR measurement
4. Laboratory-based vis-NIR measurement



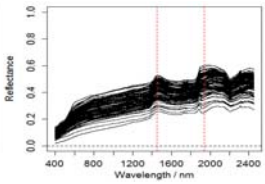


Fig. 2-6 (a) the field and laboratory spectra and (b) their difference spectra of 104 paddy soil samples

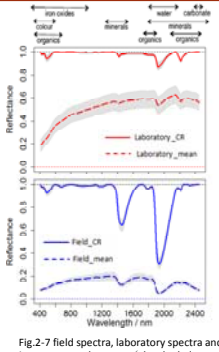


Fig.2-7 field spectra, laboratory spectra and their continuum-removal spectra（the shaded areas represent mean spectra±SD）

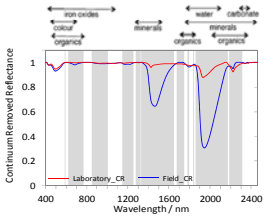


Fig. 2-8 Wavelength specific t-tests between continuum removed laboratory and field spectra.
Note: The shaded regions show where significant differences occur between the spectra at α=0.01 significance level.

How to improve the estimates of organic carbon using proximally sensed vis–NIR spectra?

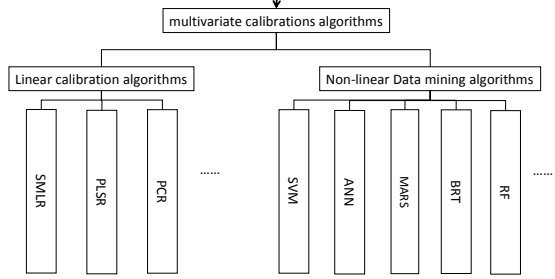
Research background and Review

Proximally sensed spectra VS. Laboratory-based spectra

①	②	③
Non-linear data mining algorithms	Removing the environmental effects from the field spectra	Using existing Chinese soil spectral library to predict soil carbon rapidly

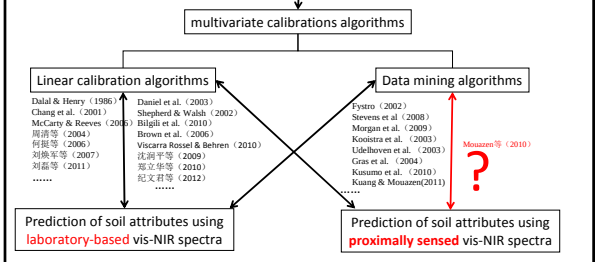
PART 1: Non-linear data mining algorithm

1. Near Infrared (NIR) spectra are dominated by weak overtones and combinations of fundamental vibration which are usually broad and weak and some of them are difficult to distinguish with the naked eye;
2. Their location is also often slightly shifted from the exact expected location because real molecules do not behave totally harmonically (Bishop et al., 1994);



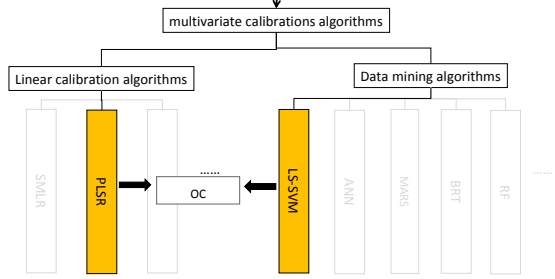
PART 1: Non-linear data mining algorithm

1. Near Infrared (NIR) spectra are dominated by weak overtones and combinations of fundamental vibration which are usually broad and weak and some of them are difficult to distinguish with the naked eye;
2. Their location is also often slightly shifted from the exact expected location because real molecules do not behave totally harmonically (Bishop et al., 1994);



PART 1: Non-linear data mining algorithm

1. Near Infrared (NIR) spectra are dominated by weak overtones and combinations of fundamental vibration which are usually broad and weak and some of them are difficult to distinguish with the naked eye;
2. Their location is also often slightly shifted from the exact expected location because real molecules do not behave totally harmonically (Bishop et al., 1994);



PLSR	LS-SVM
Wold *et al.* (1983)	Suykens *et al.* (2002)

PLSR aims to link the centred response varable vector, **y**, to the matrix of centred predictors, **X**, through *k* latent variables (factors) by:

$$\mathbf{X} = \mathbf{t}_1\mathbf{p}_1' + \ldots + \mathbf{t}_k\mathbf{p}_k' + \mathbf{E}_k$$

$$\mathbf{y} = \mathbf{t}_1 q_1 + \ldots + \mathbf{t}_k q_k + \mathbf{f}_k$$

After the model parameters are estimated, they can be combined into the final prediction model as

$$\hat{\mathbf{y}} = \boldsymbol{b}_0 + \boldsymbol{x}_i\hat{\boldsymbol{b}}_i$$

Where $\boldsymbol{b}_0$ is the intercept and $\hat{\boldsymbol{b}}_i$ are regression vectors.

LS-SVM is an optimized algorithm based on standard SVM.

It is an is a kernel-based learning algorithm. The kernel-based learning methods use an implicit mapping of the input data in a high dimensional feature space, a special type of hyperplane defined by a kernel function, in which a regression model is built.

The LS-SVM uses nonlinear regression function:

$$y(x) = \sum_{i=1}^{n} \alpha_i K(x, x_i) + b_0$$

Where $K(x, x_i)$ is defined by the kernel function. We used radial basis function kernel (RBF), which is the typical general-purpose kernel:

$$K(x, x_i) = e^{-(\|x - x_i\|^2)/2\sigma^2}$$

PART 1: Non-linear data mining algorithm

	Unit	Mean	SD	Medium	Max	Min
OC	g/kg	16.93	8.52	14.57	36.29	4.12

Assessment of prediction accuracies : (Chang *et al.*, 2001)

RPD >2.0 : good,
RPD of 1.4–2.0 : moderate
RPD <1.4 : unacceptable.

Table 3-3 prediction accuracy of soil organic carbon (g/kg)

Algorithms	Measurement Conditions	calibration (n=78)		validation (n=26)		
		R^2	RMSE	R^2	RMSE	RPD
PLSR	Laboratory-based	0.865	3.121	0.809	3.955	2.22
	Proximally sensed	0.726	4.448	0.744	4.598	1.91
LS-SVM	Proximally sensed	0.999	0.180	0.799	4.230	2.08

(Ji et al., 2014)

Aim

Improving the estimates of soil organic carbon using proximally sensed vis–NIR spectra

Research background and Review		
Proximally sensed spectra VS. Laboratory-based spectra		
① Non-linear data mining algorithms	② **Removing the environmental effects from the field spectra**	③ Using existing Chinese soil spectral library to predict soil carbon rapidly

How to deal with the effects of environment on proximally sensed vis-NIR spectroscopy??

(i) improve the leverage of multivariate calibrations by '**spiking**';

(ii) **Spectral classification** according to the different amounts of water or a related attribute, and developing calibrations separately for each class (Mouazen et al., 2006; Nocita et al., 2013);

(iii) **External parameter orthogonalisation (EPO)**- remove the effects of 'unwanted' spectral parameters from the spectra;

(iv) improve the similarity between field and laboratory spectra using **spectral transfer algorithms**.

（iii) EPO, External parameter orthogonalisation

EPO algorithm projects all the soil spectra orthogonal to the space of unwanted variation (i.e. moisture), and thus the variations of soil moisture can be effectively removed.

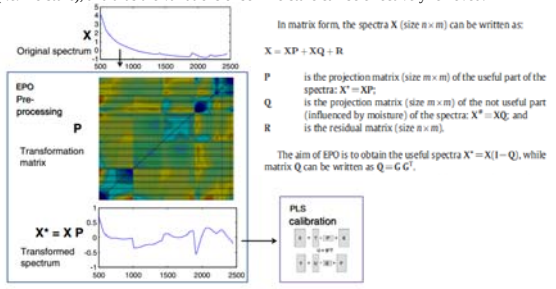


Fig.4-1 An overview of the external parameter orthogonalization (EPO) algorithm

(Rogers et al. 2003; ;Minasny et al., 2012)

（iv）Spectral transfer methods　Instrumental standardization （Wang et al.，1991）

✓make the spectra recorded in one instrument similar to that recorded in another instrument. ;

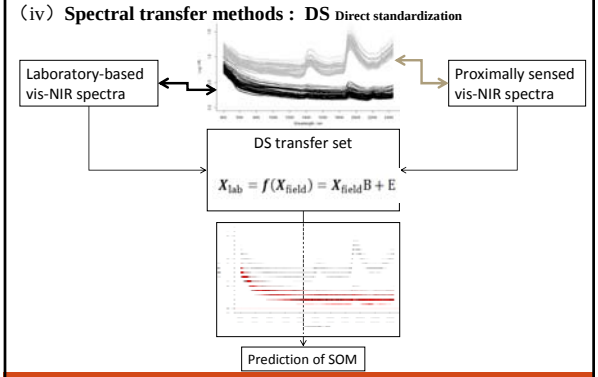
✓make the spectra recorded in the field environment similar to that recorded in the laboratory condition;

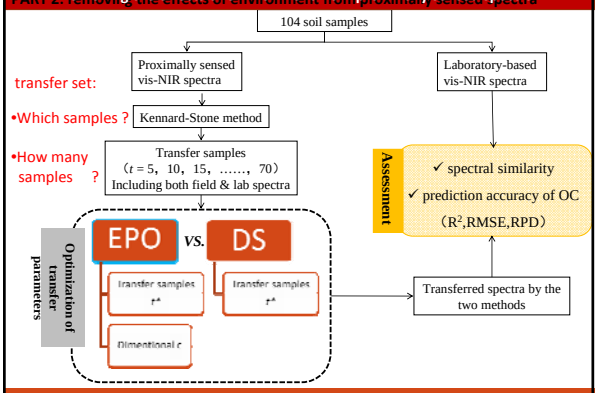
European Journal of Soil Science, 2015　doi: 10.1111/ejss.12239

Accounting for the effects of water and the environment on proximally sensed vis–NIR soil spectra and their calibrations

W. Ji[a,b], R. A. Viscarra Rossel[b] & Z. Shi[a]
[a]Institute of Applied Remote Sensing and Information Technology, College of Environmental and Resource Sciences, Zhejiang University, 866 Yuhangtang Road, Hangzhou 310058, China, and [b]CSIRO Bruce E. Butler Laboratory, Land and Water Flagship, GPO Box 1666, Canberra, Australian Capital Territory 2601, Australia

（iv）Spectral transfer methods： DS Direct standardization





N=50

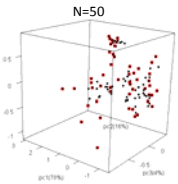


Fig. Principal component scores plot of the 50 transfer samples (black discs) selected from 104 samples (grey discs)

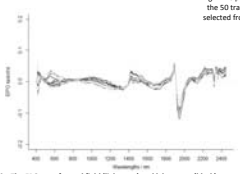


Fig. The EPO transformed field (light grey) and laboratory (black) spectra

EPO

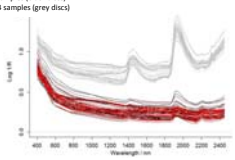


Fig. The field spectra (light grey), laboratory spectra (black) and DS-transferred field spectra (red)

DS

Table 4-1. Statistics of soil organic carbon content of 104 paddy soil samples

	dataset	n	mean	St.dev	medium	max	min	Skew
OC g/kg	all	104	16.93	8.52	14.57	36.29	4.12	412.2
	calibration	70	17.82	9.07	14.96	36.29	4.13	394.14
	validation	34	15.09	7.05	14.23	33.62	4.12	273.04

Table 4-4. PLSR prediction accuracies of SOC content using EPO-, DS-and PDS-transferred field spectra

Method	Calibration Dataset (N=70)	t^*	Validation Dataset (N=34)	R^2	RMSE /$\log_{10}$ (OC %)	RPD
Original	Lab70	/	Lab34	0.86	0.099	2.31
	Field70	/	Field34	0.78	0.119	1.91
EPO	Field 70_EPO	50	Field 34_EPO	0.80	0.105	2.18
DS	Field 70_DS	50	Field 34_DS	0.83	0.102	2.24

(iv) Spectral transfer methods : PDS piecewise direct standardization

In DS, each wavelength *i* of the laboratory spectra is related to all wavelengths of the field spectra simultaneously.

In PDS, each wavelength *i* of the laboratory spectra is modelled by a small wavelength window (ws=2*i* +1) around the same wavelength *i* of field spectra.

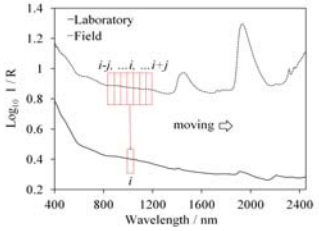


Figure 1 Overview of the piecewise direct standardization (PDS) algorithm.

(iv) Spectral transfer methods : PDS

In PDS, each wavelength *i* of the laboratory spectra is modelled by a small wavelength window (ws=2*i* +1) around the same wavelength *i* of field spectra.

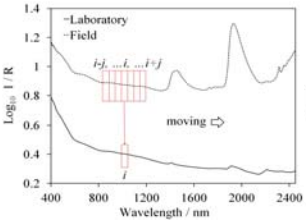


Figure 1 Overview of the piecewise direct standardization (PDS) algorithm.

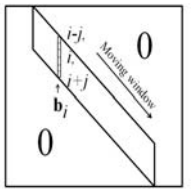


Figure Structure of the diagonal transfer matrix **B** for the piecewise direct standardization (PDS) algorithm

(Ji et al., 2015b, EJSS)

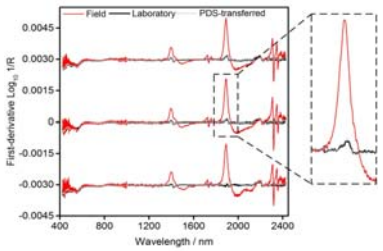


Figure 4 First-derivative absorbance spectra of three samples selected at random from the 42 validation samples: field spectra, laboratory spectra and the field spectra standardized with the piecewise direct standardization (PDS) algorithm

(Ji et al., 2015b, EJSS)

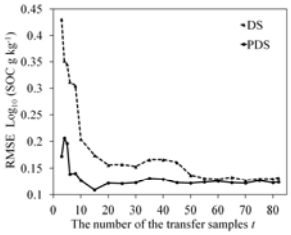


Figure 5 Prediction accuracies obtained when different numbers of transfer samples were used in PDS and DS.

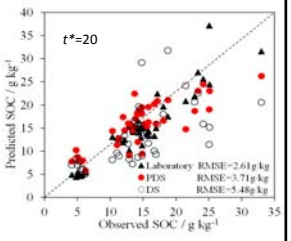


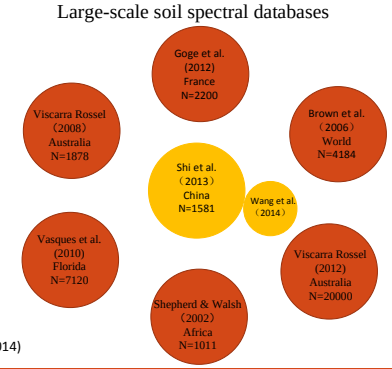
Figure 6 Scatter plot of the predicted values and observed values of SOC.

Aim

Improving the estimates of soil organic carbon using proximally sensed vis–NIR spectra

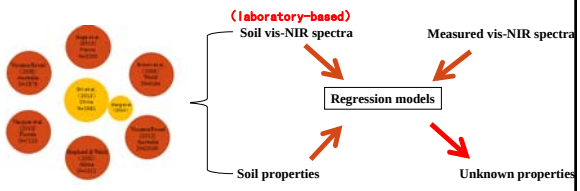
Research background and Review		
Proximally sensed spectra VS. Laboratory-based spectra		
① Non-linear data mining algorithms	② Removing the environmental effects from the field spectra	③ Using existing Chinese soil spectral library to predict soil carbon rapidly

Large-scale soil spectral databases



(Shi et al., 2014)

Large-scale soil spectral databases



It is of great significance to remove the effects of environmental factors from spectra recorded under field conditions, so that spectroscopic calibrations derived in laboratory studies can be used with field spectra to predict soil properties.

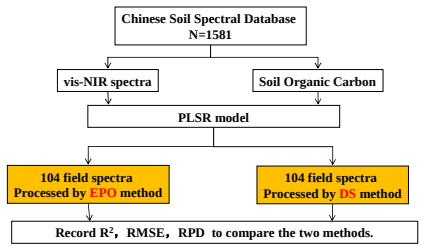
Chinese Soil Spectral Database (CSSD）

Basic information

- The CSSD comprised 6000+ soil samples collected from 22 provinces in China, representing 20 orders of the China Soil Taxonomy;
- Soil samples were taken from the topsoil (0–20 cm).;
- Soil samples were air-dried and sieved (< 2 mm);
- Soil samples were measured the diffuse reflectance spectra in the 350–2500 nm range with an ASD Fieldspec ProFR vis–NIR spectrometer with a high intensity contact probe;
- The spectra were measured under laboratory conditions;
- The104 samples that we describe in this study were not included in the CSSD.

Table 5-2 Statistics of soil organic carbon (SOC) of 104 paddy soil samples and 1581 samples from the Chinese soil spectroscopic database (CSSD).

Category	*N*	Mean	SD	Min.	Median	Max.	Skewness
CSSD	1581	13.49	6.68	0.97	13.15	43.41	203.31
Paddy soil	104	16.93	8.52	4.12	14.57	36.29	412.2



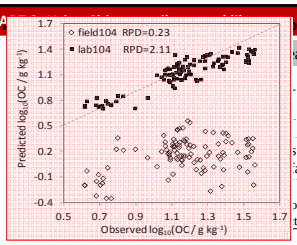
Spectral pretreatment

- kepp 420-2425 nm
- Saviziky-Golay smoothing（2+11）
- 1st derivative变换
- $\log_{10}$(1/Reflectance)
- Mean center
- SNV

Leave-one-out cross validation
Number of PLSR factors=15

Table 5-3 Validation statistics for predictions of soil organic carbon (SOC) with spectra from the Chinese soil spectral database (CSSD).

Methods	Calibration dataset	t*	Validation dataset	R^2	RMSE / $\log_{10}$ (OC g/kg)	RPD
Original	CSSD	/	Lab 104	0.813	0.114	2.11
		/	Field 104	0.139	1.042	0.23
EPO	EPO transferred CSSD	50	EPO transferred Field 104	0.571	0.161	1.50
DS	CSSD	50	DS transferred Field 104	0.800	0.117	2.06



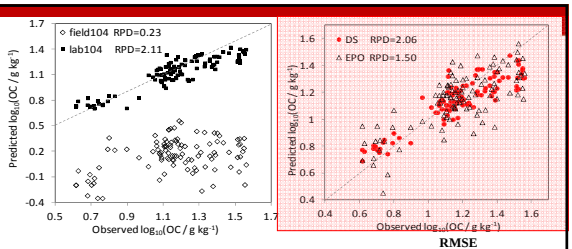
atment
- $\log_{10}$(1/Reflectance)
- Mean center
- SNV

s validation
actors=15

of soil organic carbon (SOC) with spectra
tral database (CSSD).

Methods	Calibration dataset	t*	Validation dataset	R^2	RMSE / $\log_{10}$ (OC g/kg)	RPD
Original	CSSD	/	Lab 104	0.813	0.114	2.11
		/	Field 104	0.139	1.042	0.23
EPO	EPO transferred CSSD	50	EPO transferred Field 104	0.571	0.161	1.50
DS	CSSD	50	DS transferred Field 104	0.800	0.117	2.06

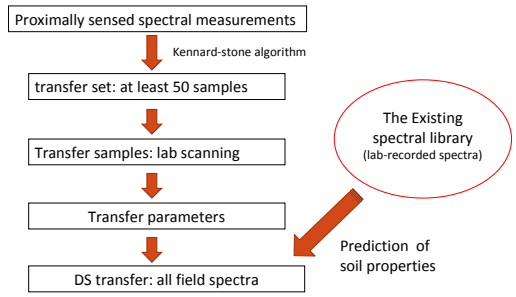
PART 3: Using Chinese soil spectral library to predict soil carbon rapidly



Methods	Calibration dataset	t*	Validation dataset	R^2	RMSE / $\log_{10}$ (OC g/kg)	RPD
Original	CSSD	/	Lab 104	0.813	0.114	2.11
		/	Field 104	0.139	1.042	0.23
EPO	EPO transferred CSSD	50	EPO transferred Field 104	0.571	0.161	1.50
DS	CSSD	50	DS transferred Field 104	0.800	0.117	2.06

PART 3: Using Chinese soil spectral library to predict soil carbon rapidly

Procedures for field-based spectroscopic predictions:



Summary

① Non-linear data mining algorithms

② Removing the environmental effects from the field spectra

③ Using existing Chinese soil spectral library to predict soil carbon rapidly

Improving the estimates of soil organic carbon using proximally sensed vis–NIR spectra

Thank you!

WENJUN JI | POST DOC

DEPARTMENT OF BIORESOURCE ENGINEERING

PART 3: Using Chinese soil spectral library to predict soil carbon rapidly

Table 4. Comparison among the performances of external parameter orthogonalization (EPO), direct standardization (DS), piecewise direct standardization (PDS) and spiking.

Requirements		EPO	DS	PDS	Spiking
If transfer samples are needed		Y	Y	Y	Y
Number of transfer samples needed	Ji *et al.* (2015b)	–	50 (82, 42)	20 (82, 42)	–
	Viscarra Rossel *et al.* (2009)	–	–	–	74 (892, 39)
	Minasny *et al.* (2011)	60 (271, 20)	–	–	–
	Ge *et al.* (2014)	177 (2017, 58)	–	–	–
	Ji *et al.* (2015a)	50 (1581, 54)	50 (1581, 54)	–	50 (1581, 54)
Spectral pre-treatment		N	N	Y or N	N
Re-calibration		Y	N	Y or N	Y

Note: the numbers in parentheses represent the number of samples from the calibration and validation sets, respectively.

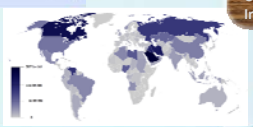
Quantification of Bitumen in Remediated Tailing Soils Using Reflectance NIR Spectroscopy with Partial Least Squares Analysis

Serella Gan
Ph. D student, supervised by Dr. Ashraf Ismail, Food Science & Agricultural Chemistry Department

Table of contents

Background – map of world oil reserves & consumption

Map of world oil consumption



Map of world oil reserves, 2013

OPEC, 2013:
US & China:
30 million barrels
Venezuela (20%),
Saudi Arabia (18%),
Canada (13%),
Iran (9%)

Background – oil sands & tailing soils

- Heavy, viscous, not free-flowing
- "Oil sand", mixed with sand and clay minerals
- Each grain of sand is surrounded by a layer of water and a film of bitumen
- Steam extraction:
  - Bitumen slurry ---upgrading;
  - Tailings (sand, water, bitumen residue) --- clean up (remediation)

Background – tailings ponds

- 1.5, 3.2 (2019), 4 (million barrels)
- 170 km^2 (2012), 1.5 times the size of Vancouver, still growing…
- Problems: land disturbed; large water consumption; leakage…
- Energy Resources Conservation Board (ERCB) Directive 74 (2009): clean up soil, water for suitable vegetation

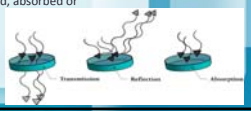
Alberta Government Said "STOP!"

Background – remediation

- Gradek Energy: Reusable Hydrocarbon Sorbent (RHS) to remove bitumen residue from soil.
- Fast and on-line hydrocarbon content monitoring method is required

Near-infrared (NIR) spectroscopy

- NIR spectroscopy coupled with multivariate calibration has become increasingly important for process analysis in many fields.
- Non-invasive, little/no sample preparation, rapid
- Principle: light wavelength = transition energy of the vibrated bond, light at that wavelength is absorbed
- Interactions between light and matter are wavelength-dependent and amount of light absorbed is proportional to concentration. Therefore, it can be used for quantitative chemical analysis.
- The light radiated onto material may be reflected, absorbed or transmitted.



Current method to quantify bitumen

- Most common method in use today:

Chloroform extraction (Soxhlet) → solvent evaporation → chloroform re-added to dissolve bitumen → determined by FTIR spectroscopy (2930 cm^{-1})

- Drawbacks:

i. Not amenable to on-line or even at-line analysis
ii. Long waiting periods for results
iii. High cost per sample

Due to these drawbacks, a new low-cost on-line method for assessing bitumen in soil, is greatly needed

Reflectance NIR spectroscopy of hydrocarbons

- Hydrogenic bonds (C-H, 93% of bitumen) are NIR active (4000 – 12000 cm^{-1}, 700 – 2500 nm)
- No sample pretreatment required
- Can directly measure samples
- Chemometrics is required: Calibration model is built by modeling the NIR absorption against reference data, which is determined by traditional chemical analysis
- Model can be used to predict unknown samples without further chemical analysis

NIR or MIR ?

NIR (12,000 – 4000 cm^{-1})

- Lower intensity (direct measurement)
- Vibrations involving hydrogenic bonds are NIR-active
- Can use thick samples or long optical fibers (**on-line or at-line** applications)
- Overlapping peaks due to combination and overtone modes, complex chemometric methods are required)

MIR (4000 – 400 cm^{-1})

- Sample pretreatment may be required (high signal intensity)
- Almost all vibrations are IR-active
- Uses short pathlengths or short optical fibers (**at-line** applications)
- Spectra can be interpreted directly in some cases

Objective

o Establish rapid, on-line method for hydrocarbon analysis in remediated tailing soils using reflectance NIR spectroscopy coupled with Partial Least Squares (PLS) calibration model

Methodology

Methodology

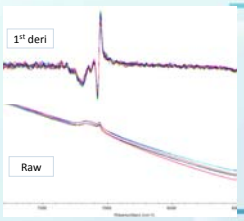
- Soils (n=32) were dried, ground and passed through 2 mm sieve
- Each sample was separated into two subsamples
- One subsample was submitted for chemical analysis (total combustion)
- One subsample was scanned using Tango (Bruker, reflectance, 4000 – 11500 cm^{-1}, 16 cm^{-1} resolution, 64 scans). Each sample was scanned in duplicate (shake, reload)
- Software: DataAnalysis

Spectral pretreatment – 1st derivative

- 1st derivative (11000-4000 cm^{-1}):

Remove baseline shifts, resolve overlapping peaks

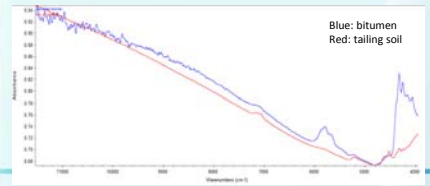
- Disadvantages: noise enhanced, difficult spectral interpretation
- Higher-order derivatives are not common in practice



Additive effect: simple baseline shift

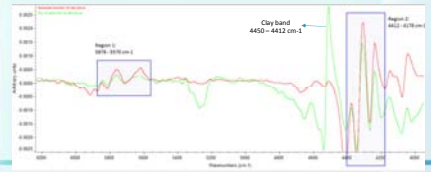
Result – spectral interpretation

NIR spectra – pure bitumen & dried tailing soil



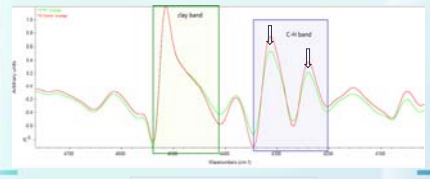
Blue: bitumen
Red: tailing soil

NIR spectra (1st derivative) – pure bitumen & dried tailing soil



Red: pure bitumen
Green: tailing soil

NIR spectra (1st derivative) of tailing soil before and after process showing change in hydrocarbon:clay ratio



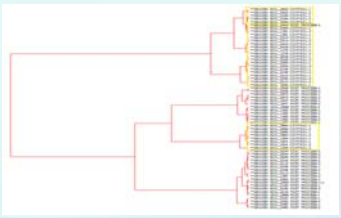
Red: before
Green: after

Results – soil classification

Soil classification using Hierarchical Cluster Analysis and Principal Component Analysis

- Cluster soils into two groups: before and after remediation.
- Based on chemical variation (hydrocarbon).
- Samples: 32 soil samples (64 spectra) were collected from different batches before and after remediation process
- Spectral pre-treatments (1st derivative) was performed prior to HCA and PCA to minimize the effects of physical variations that can mask the chemical variations.

Soil classification – HCA (broad region)



- Based on broad spectral region
  Two types of soil mixed

Yellow: control

Soil classification – HCA (optimized regions)

- Cluster two kinds of soils: control & post processed
- Based on optimized regions

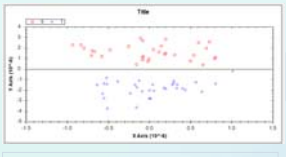
Yellow: control
Blue: post processed

Sample heterogeneity

13/32 (40%) sets grouped together, rest mixed up

Green: grouped well
Purple: mixed

Soil classification – PCA scores plot (PC2 vs. PC3)

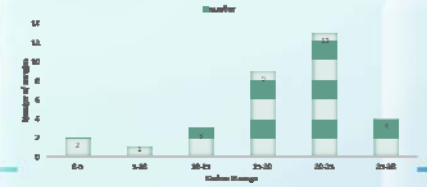


PC 2 separates soils well

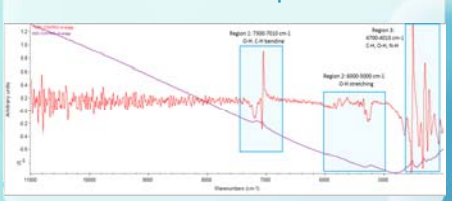
Red: control; Blue: post processed

Results – calibration model

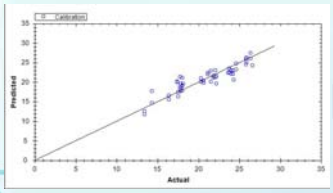
Total carbon content in dried tailing soils



Soil and the 1st derivative NIR spectra

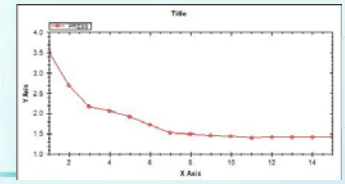


Hydrocarbon content NIR calibration based on total combustion values



N_{cal} = 52
R^2 = 0.91

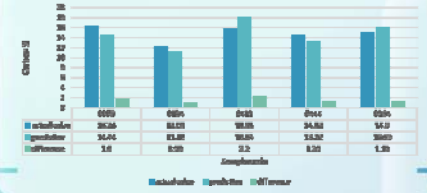
Hydrocarbon PLS - PRESS



Factors: 7
RMSECV = 1.53

Coefficient of variation: 5-11%

Prediction of hydrocarbon content of unknowns



Conclusion

- A PLS calibration model for the prediction of hydrocarbon content of tailings samples was developed, with r^2 = 0.91, 1.51% RMSECV, in 13-26% hydrocarbon content range
- Principal component analysis in the selected region successfully clustered control and post processed groups based on the chemical difference reflected in the spectra.
- These preliminary results indicate the potential utility of reflectance NIR spectroscopy as a fast, nondestructive and real-time monitoring method for tailings remediation processes.
- Several factors can influence the accuracy of the NIR method, such as sampling, instrument, experiment, and modeling. The effects of these factors will be carefully studied and minimized (e.g. through appropriate sample presentation, math pre-treatments, etc.).

Thank you