
Food and Agriculture Organization of the United Nations
GLOSOLAN
Soil spectroscopy training workshops
Online webinars
GLOBAL SOIL PARTNERSHIP

Can we take vis-NIR spectroscopy to field to leverage digital soil mapping?

uoguelph.ca/ses

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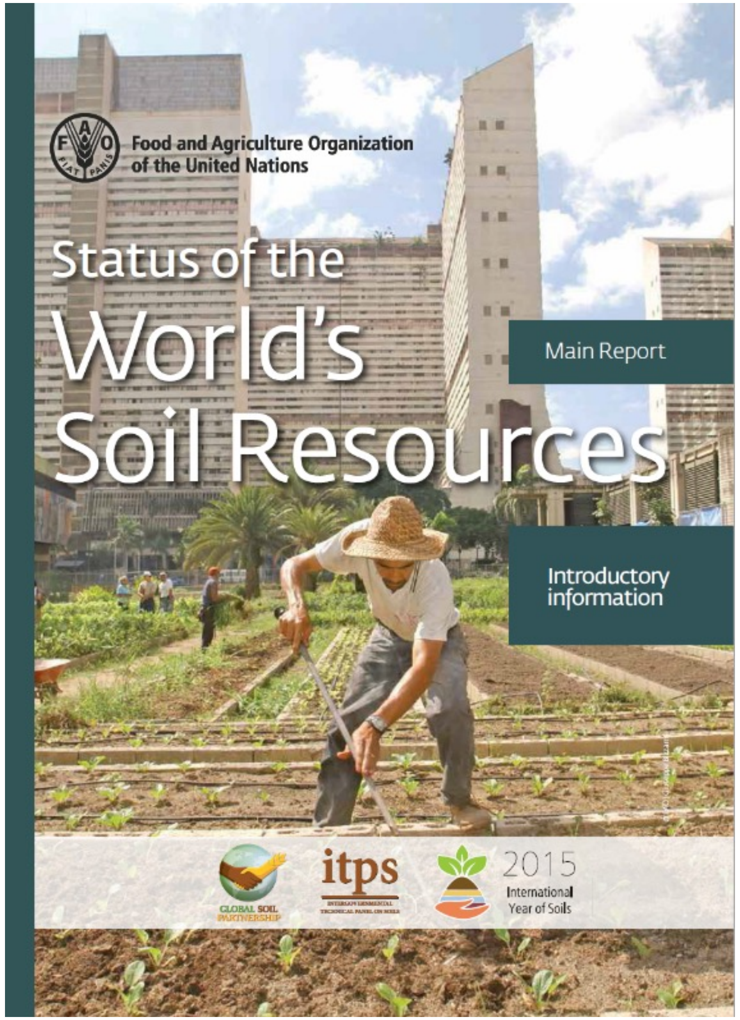
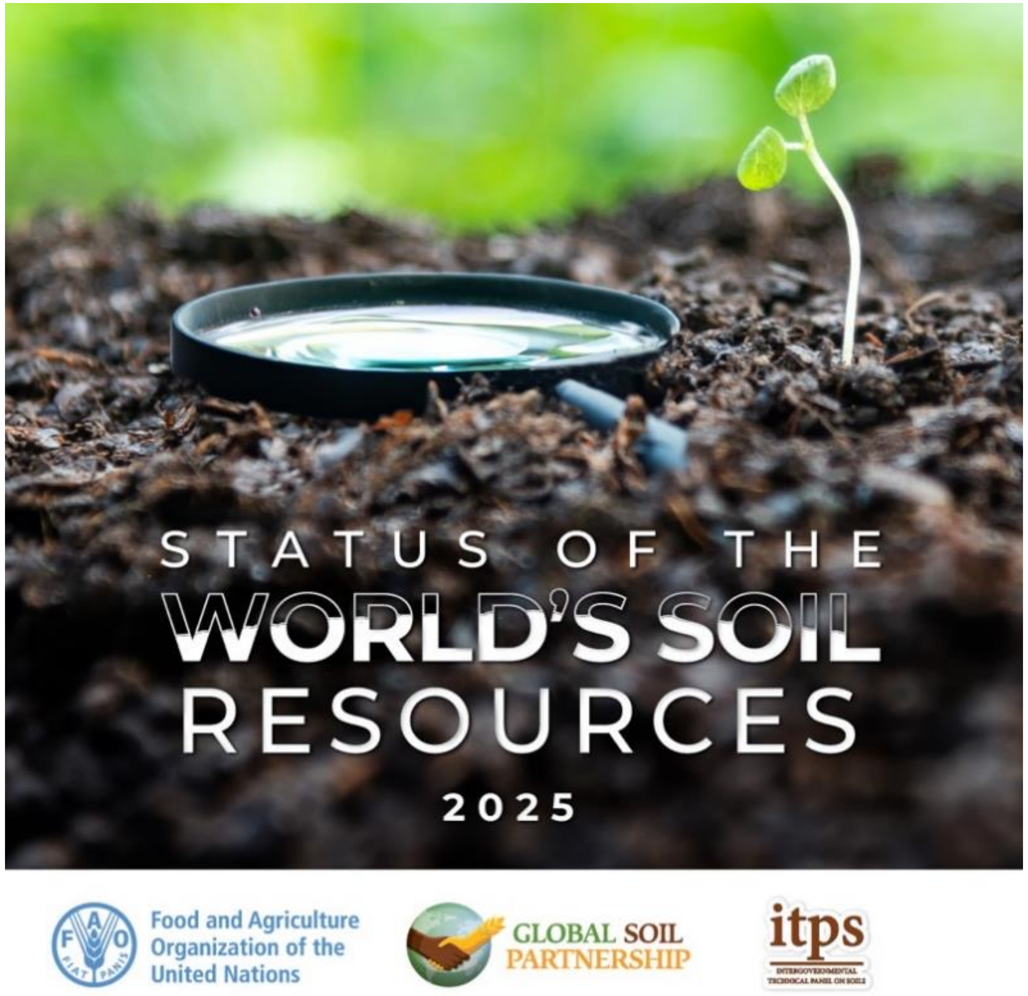
Soil

Soil is a strategic resource to ensure food security
Where food Begins
95%
of our food comes from soils

SUSTAINABLE DEVELOPMENT GOALS
NO POVERTY 1
ZERO HUNGER 2
GOOD HEALTH AND WELL-BEING 3
QUALITY EDUCATION 4
GENDER EQUALITY 5
CLEAN WATER AND SANITATION 6
AFFORDABLE AND CLEAN ENERGY 7
DECENT WORK AND ECONOMIC GROWTH 8
INDUSTRY, INNOVATION AND INFRASTRUCTURE 9
REDUCED INEQUALITIES 10
SUSTAINABLE CITIES AND COMMUNITIES 11
RESPONSIBLE CONSUMPTION AND PRODUCTION 12
CLIMATE ACTION 13
LIFE BELOW WATER 14
LIFE ON LAND 15
PEACE, JUSTICE AND STRONG INSTITUTIONS 16
PARTNERSHIPS FOR THE GOALS 17

Status of Soil





“If you can’t measure it,
you can’t manage it”

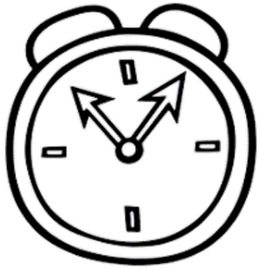
Better Management
through
Better Measurement

Traditional Soil Measurement

- Harsh chemical

- Proximal soil sensing (PSS) offers an alternative approach
  - Use of spectroscopy to determine several properties simultaneously

- Time



Spectroscopy

- Type of PSS that evaluates electromagnetic radiation against an object
  - Visible (vis) 342-1023 nm
  - Near Infrared (NIR) 1070-2220 nm

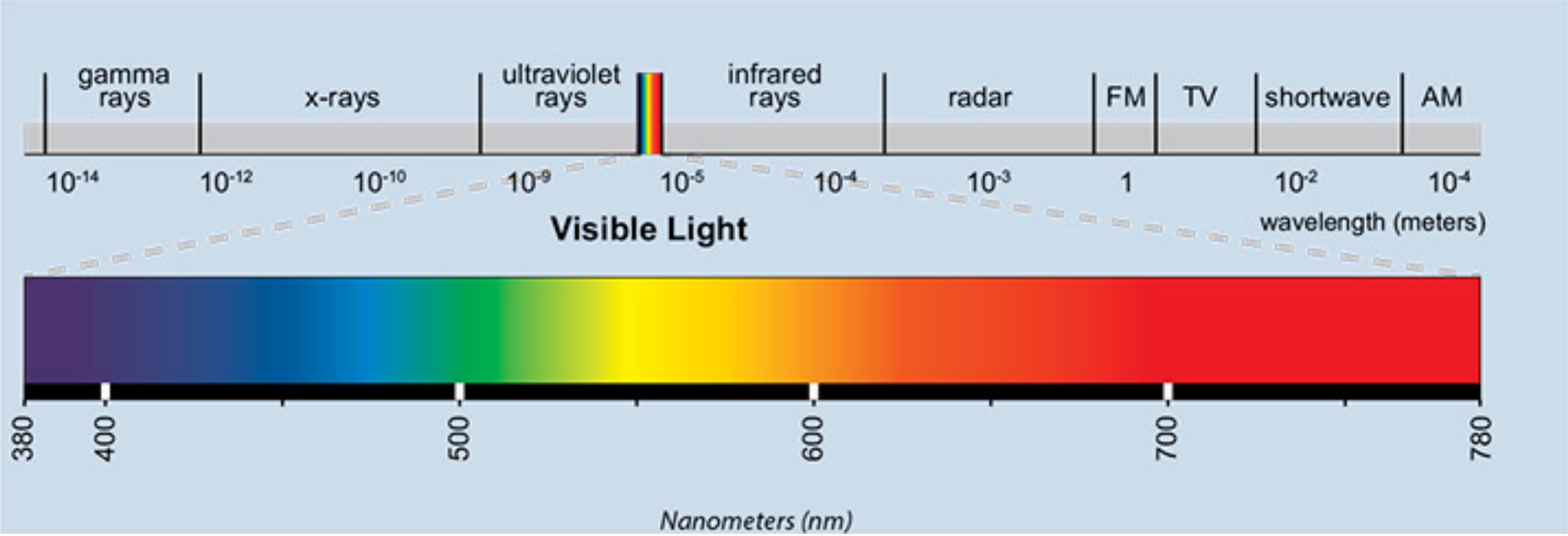
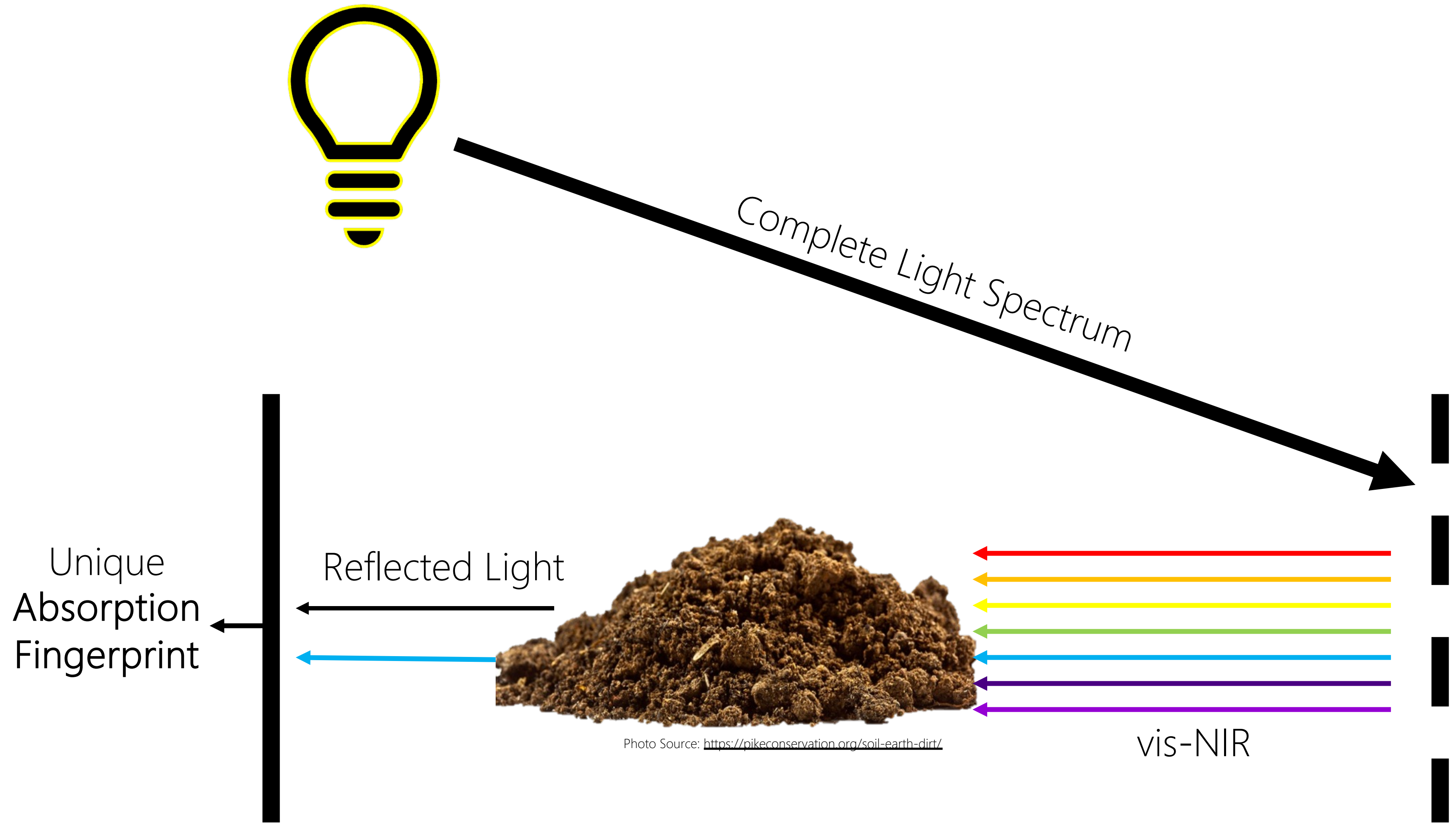
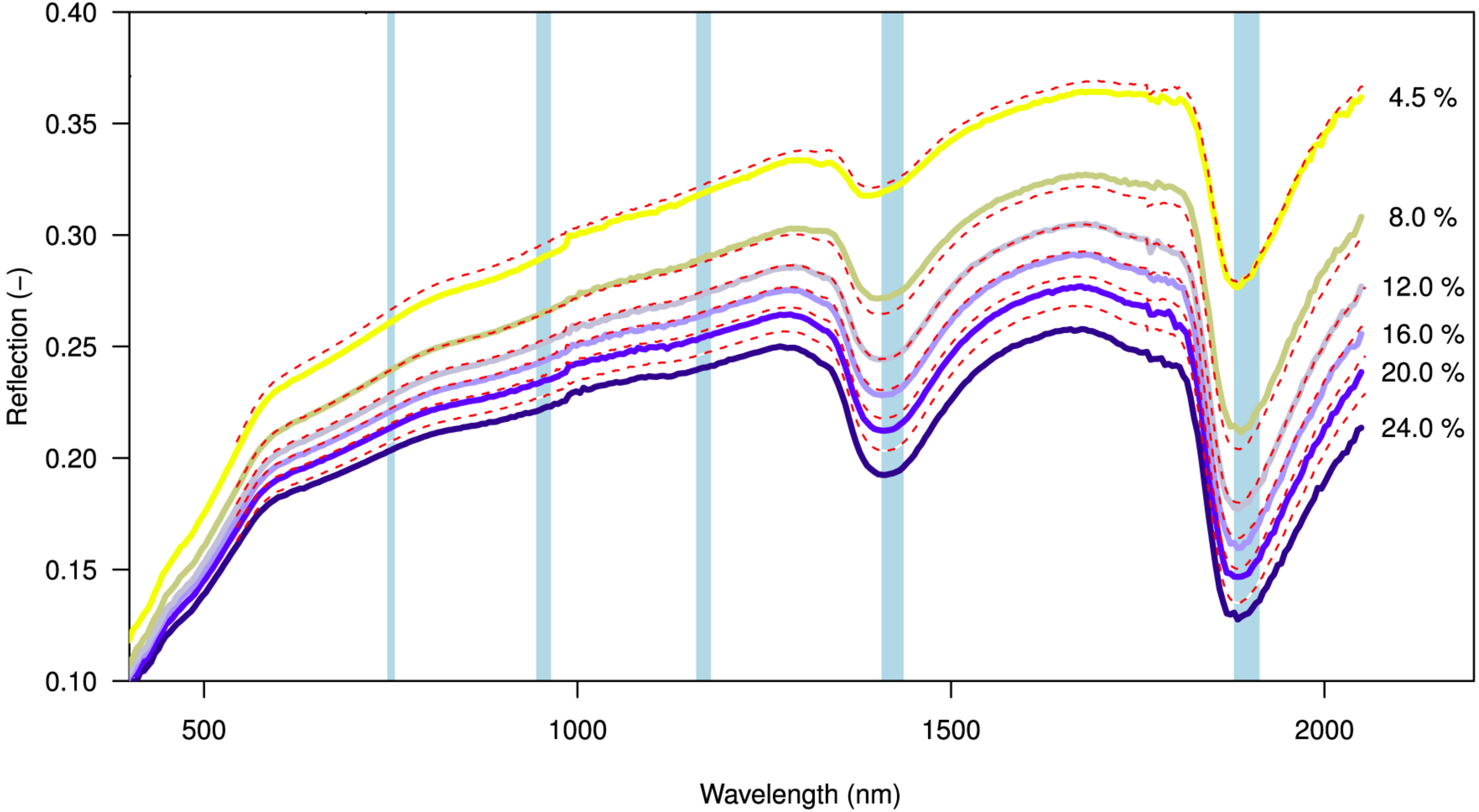


Photo Source: https://eyelighting.com/lighting-technology-education/general-lighting-basics/light-spectrum

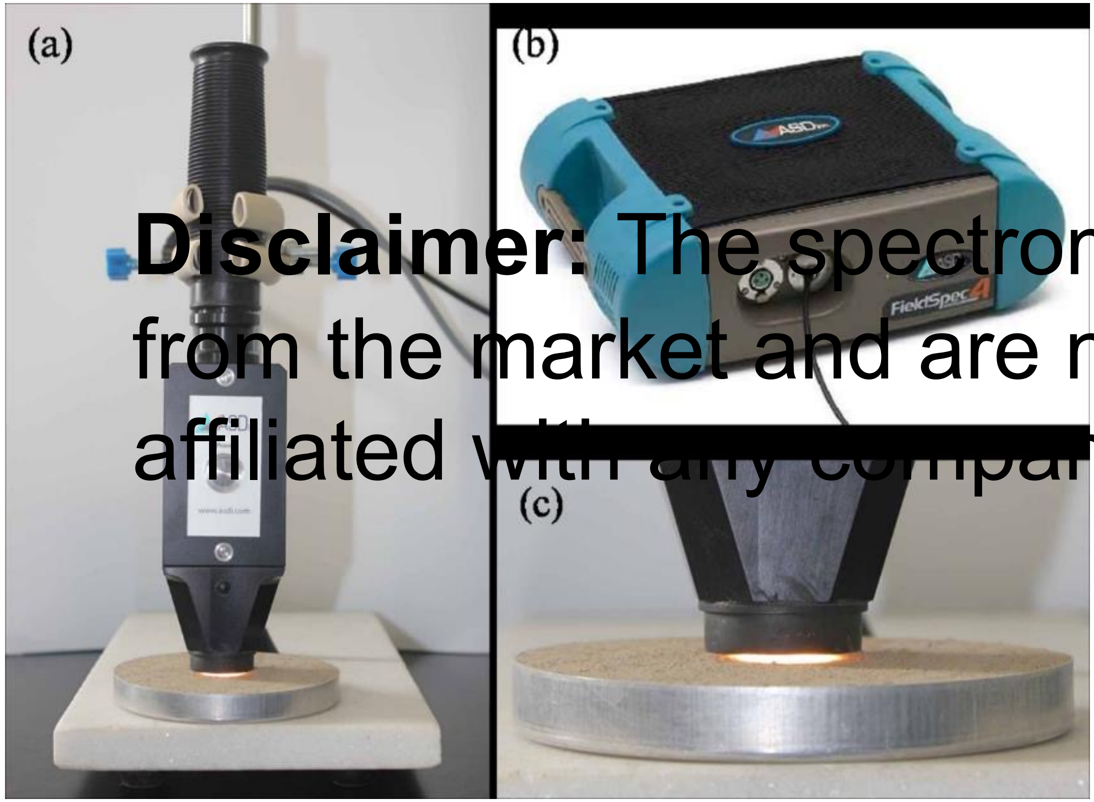
Soil Spectroscopy

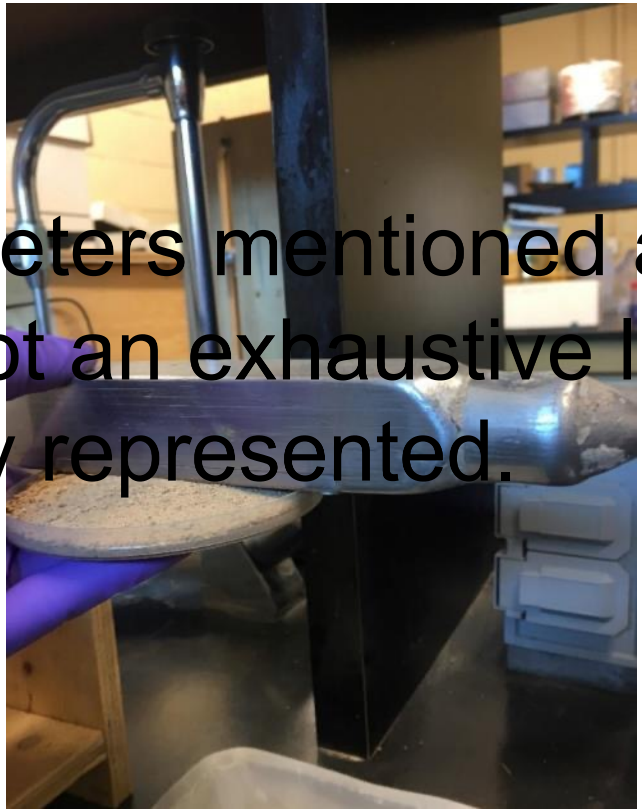


Soil Spectra



Soil Spectrometer(s)





Disclaimer: The spectrometers mentioned are examples from the market and are not an exhaustive list. I am not affiliated with any company represented.

ASD FieldSpec 4 Pro

https://www.malvernpanalytical.com/

Veris Technologies, Inc. (Salina, Kansas)

http://www.veristech.com

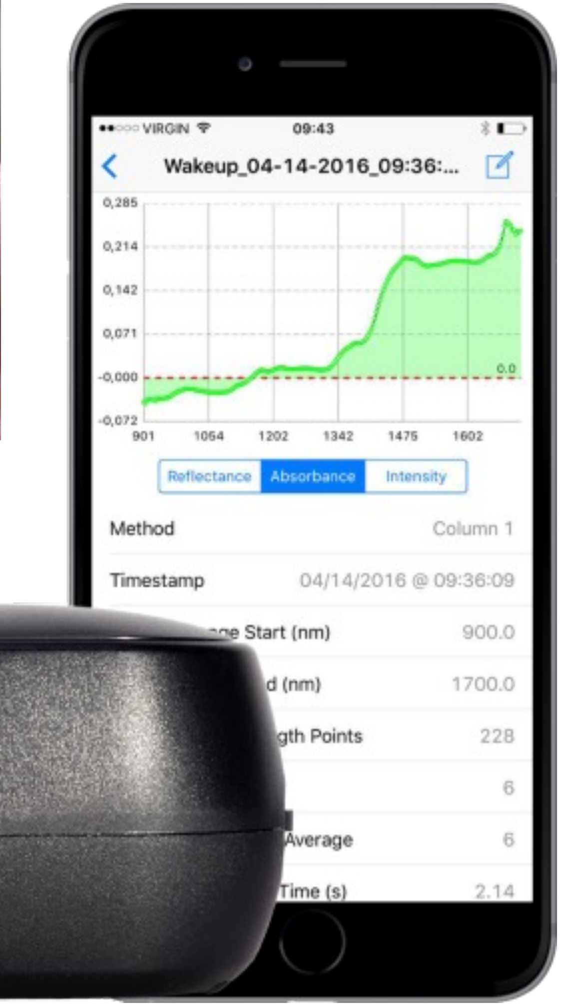
Spectral Evolution, Inc. (Haverhill, MA)

https://spectralevolution.com/

Soil Spectrometer(s)

Soil Spectrometer(s)

sagitto
HITTING THE TARGET

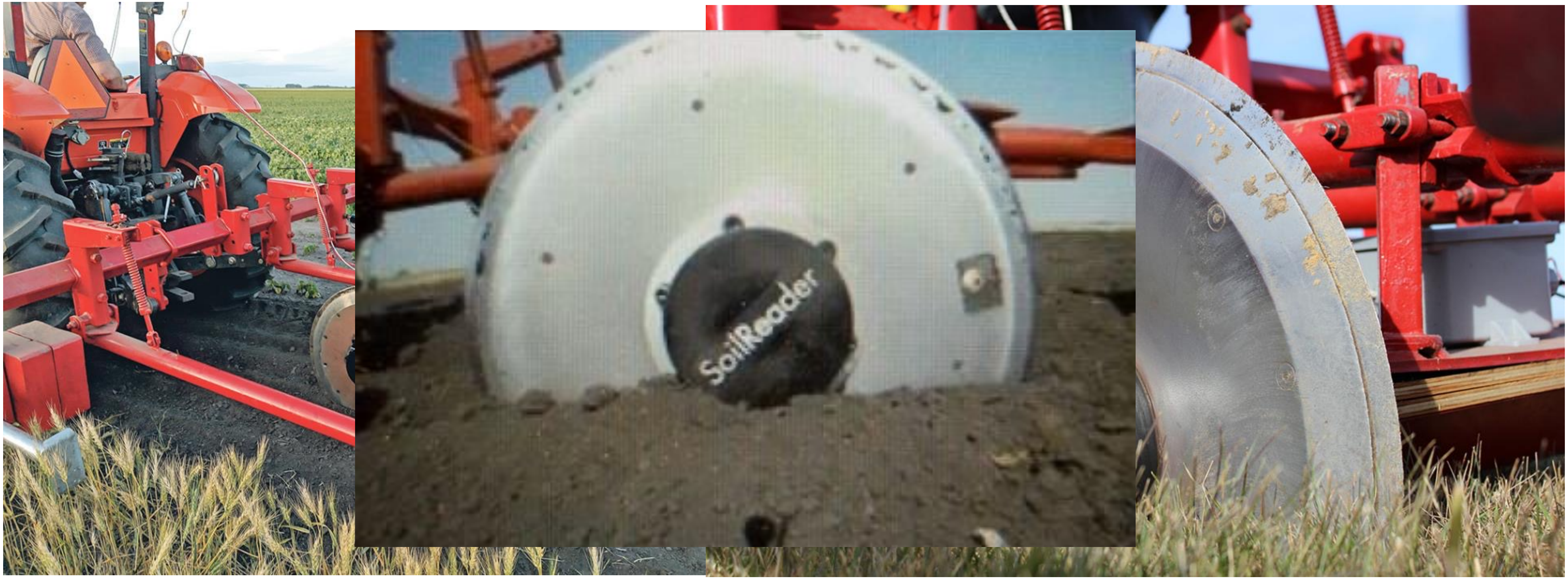


Soil Spectrometer(s)

Veris Technologies, Inc. (Salina, Kansas)

http://www.veristech.com

Soil Spectrometer(s)



SoilReader, Inc. (Winnipeg, Manitoba)

https://soilreader.com/

Status, Challenges and Opportunities

- Spectroscopy
  - Measures multiple soil properties simultaneously
  - Cheaper, simpler, less labour, environmentally safe, portable, scalable
- Laboratory vs field measurements
  - Lab measurements-
    - Highly promising
    - Ex-situ, ground & processed samples, controlled conditions
  - Field measurements-
    - On-site measurement and decision making, transportation and preparation
    - Environmental and physical conditions, variability, instrument performances

Today's Focus

Can we take vis-NIR spectroscopy to field to leverage digital soil mapping?

Lab Measurements
- Processed samples

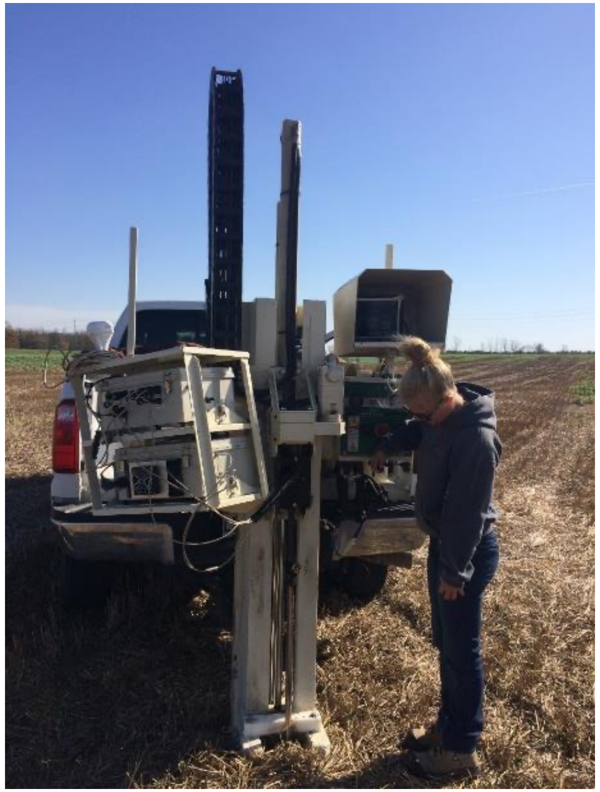
Lab measurements
- Unprocessed samples

Field measurements
- In-situ, unprocessed samples

Digital Soil Mapping

Today's Focus

Can we take vis-NIR spectroscopy to field to leverage digital soil mapping?



Can we predict soil properties from processed samples using vis-NIR spectroscopy?

Lab Measurements

- Processed samples

Lab measurements

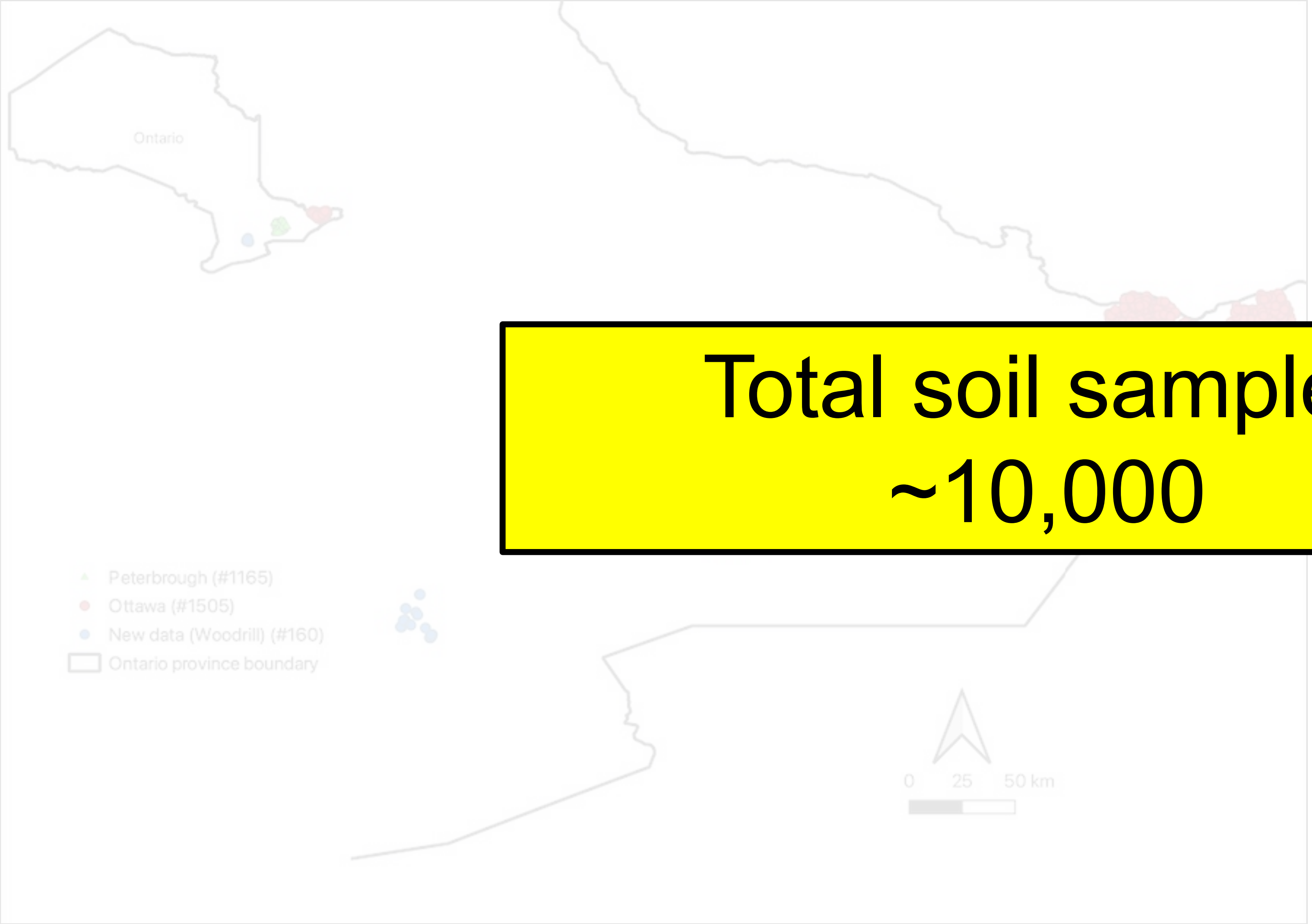
- Unprocessed samples

Field measurements

- In-situ, unprocessed samples

Digital Soil Mapping

Soil Samples



Total soil samples ~10,000

- Ottawa Soil Survey (1505)
- ...borough soil ...y (1165)
- Woodrill Project (160)

Descriptive Statistics

Soil Property	Mean	Median	Min	Max	s	n
OM %	5.3	1.8	0.0	85.2	12.5	9452
pH_H_2O	6.9	7.2	3.3	9.1	0.9	9459
TN %	0.2	0.1	0.0	3.3	0.4	8789
AvailP ug/g	38.3	5.7	0.3	1506.0	1.3	8825
K mg/L $_d$soil	200.5	80.9	1.9	6688.0	465.2	8888
Ca mg/L $_d$soil	4235.1	2940.0	18.2	157040.0	9944.5	9158
Mg mg/L $_d$soil	316.2	187.0	8.2	4240.0	333.9	8722

Scanning Soil Samples

Data Processing

Spectra cleaning

- Trim edges (350-399 nm and 2451 and 25900 nm)
- log1/R (to reduce linearization)

Spectra pre-processing

- Pre-processing algorithms

Modeling

- Data splitting (calibration, cross validation, external validation)
- Modelling
- Uncertainty estimation

Data Processing

Preprocessing Algorithms	Modelling Algorithms
1st Derivative	Partial Least Square Regression (PLSR)
1st Derivative + Gap	Random Forest
2nd Derivative	Cubist
2nd Derivative + Gap	
Savitzky Golay + Gap	
Gap Derivative	
Savitzky Golay	
Savitzky Golay + 1st Derivative	
Savitzky Golay + 2nd Derivative	
Savitzky Golay + SNV	
Savitzky Golay + SNV + Detrend	
SNV	
SNV + Detrend	

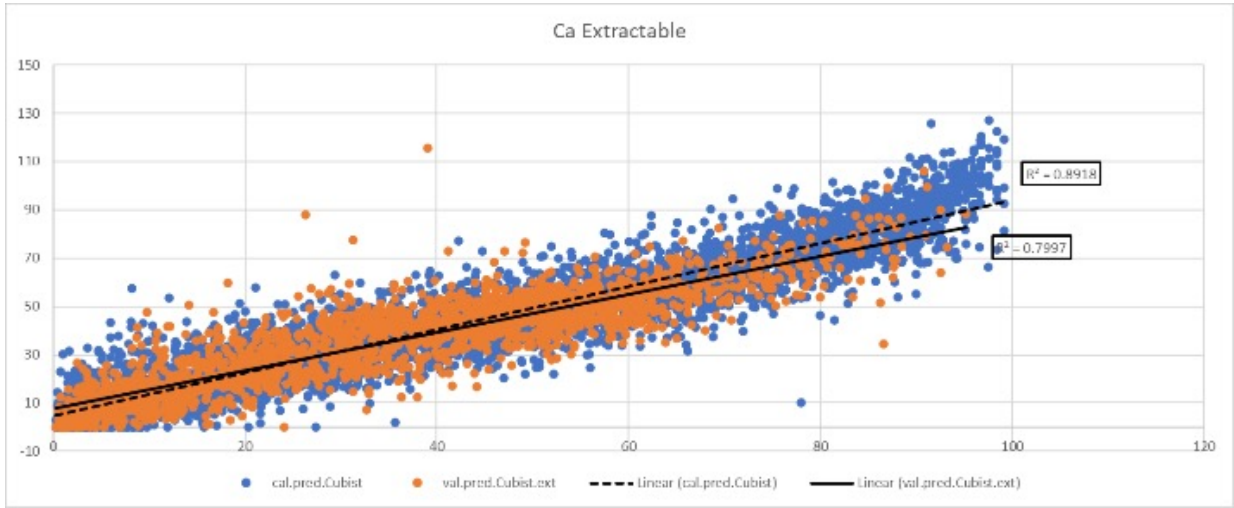
Modelling Performance (SOM)

	R^2	CCC	MSE	RMSE	bias	MSE_c	$RMSE_c$	RPD	RPIQ
cal.PLSR	0.81	**0.89**	33.78	5.81	0.00	33.78	5.81	2.27	0.62
val.PLSR	0.84	**0.91**	24.82	4.98	-0.46	24.61	4.96	2.54	0.72
val.PLSR.ext	0.81	**0.88**	21.12	4.60	-0.61	20.75	4.56	2.30	0.72
cal.Cubist	0.94	**0.97**	10.01	3.16	-0.10	10.00	3.16	4.18	1.15
val.Cubist	0.92	**0.96**	13.04	3.61	-0.30	12.95	3.60	3.50	0.99
val.Cubist.ext	0.93	**0.96**	7.92	2.81	-0.38	7.78	2.79	3.75	1.17
cal.RF	0.97	**0.98**	4.93	2.22	0.00	4.93	2.22	5.95	1.63
val.RF	0.89	**0.94**	17.43	4.17	-0.21	17.38	4.17	3.03	0.85
val.RF.ext	0.90	**0.94**	10.84	3.29	-0.16	10.81	3.29	3.21	1.00

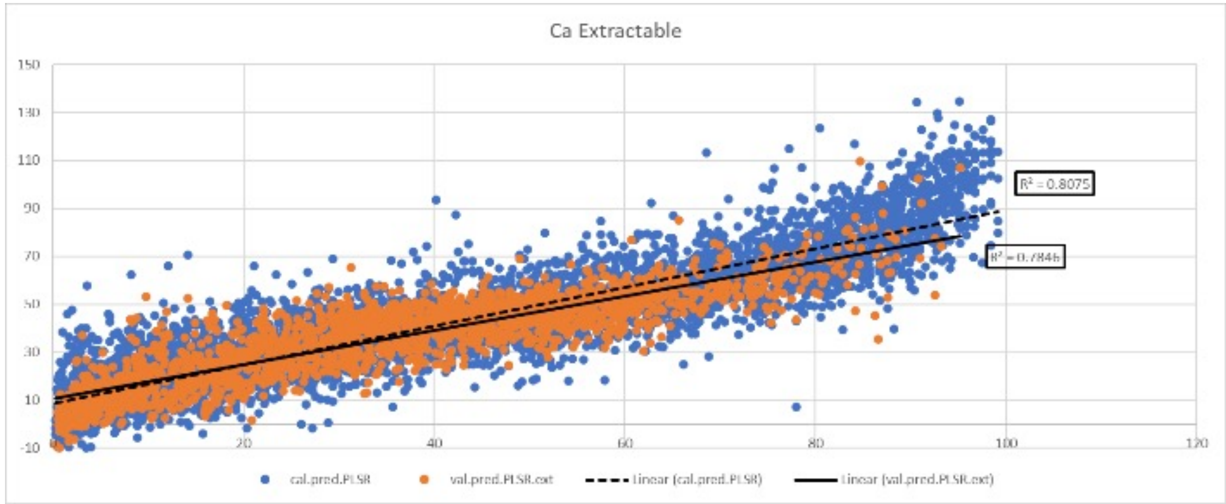
**cal.xxx- Calibration; val.xxx- validation; Val.xxx.ext- external validation

Ca-Extractable

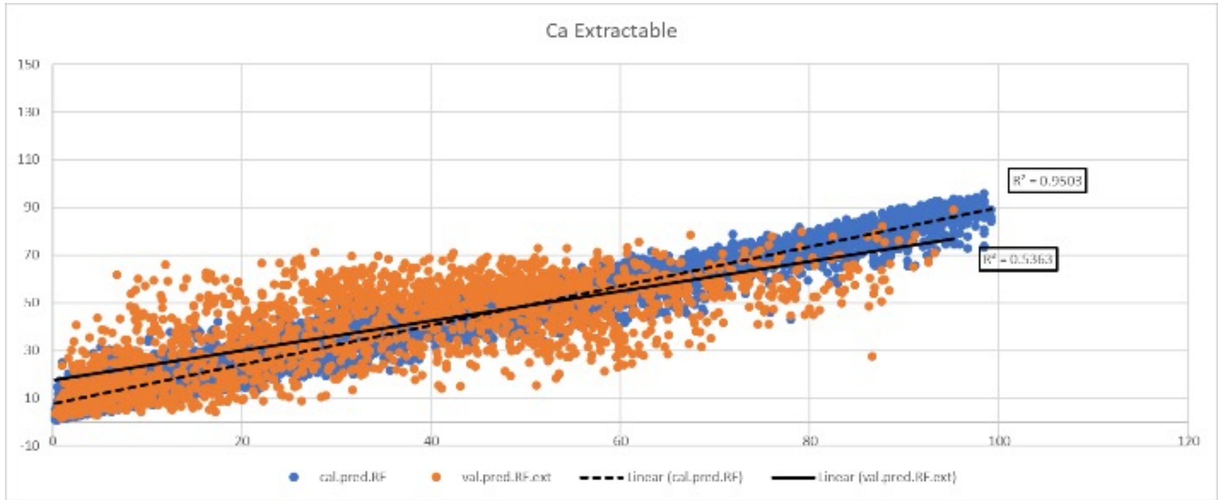
Cubist



PLSR

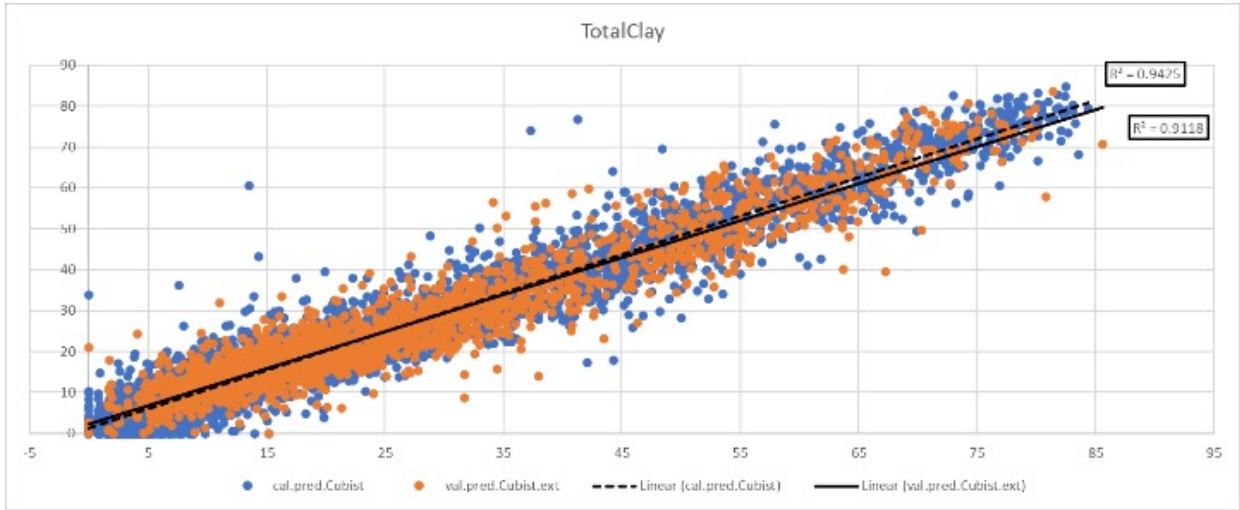


RF

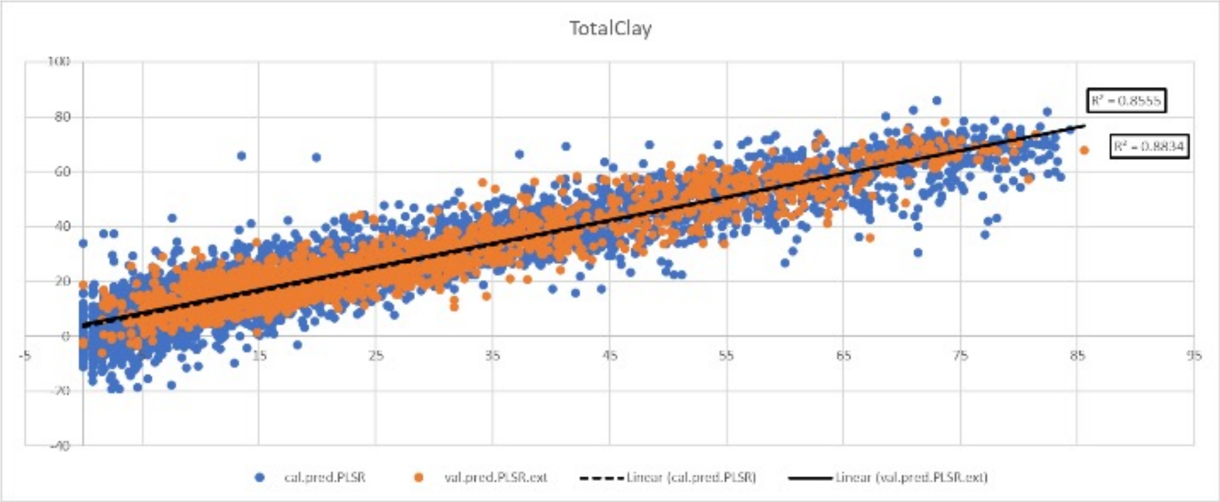


Clay

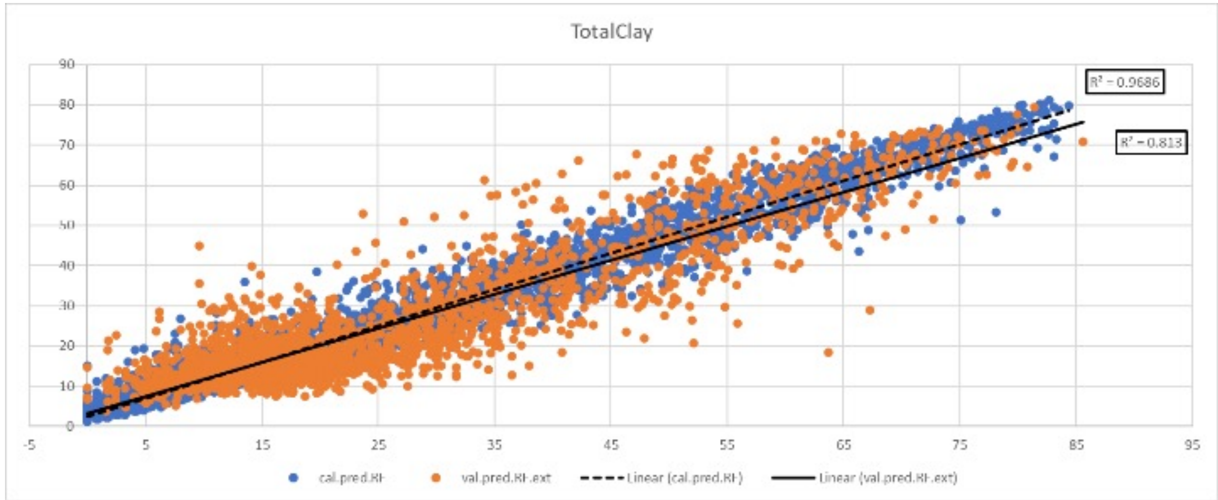
Cubist



PLSR



RF



Soil Properties Combined- Soil Quality Index

Indicators	Weights	Scoring function
OM %	0.35	More is better
pH_H_2O	0.20	Optimum
TN %	0.15	More is better
P ug/g	0.10	More is better
K mg/L soil dry	0.10	More is better
Ca mg/L soil dry	0.05	More is better
Mg mg/L soil dry	0.05	More is better

$$SQI = \sum_{i=1}^{i=n} Wi \times Si$$

SQI

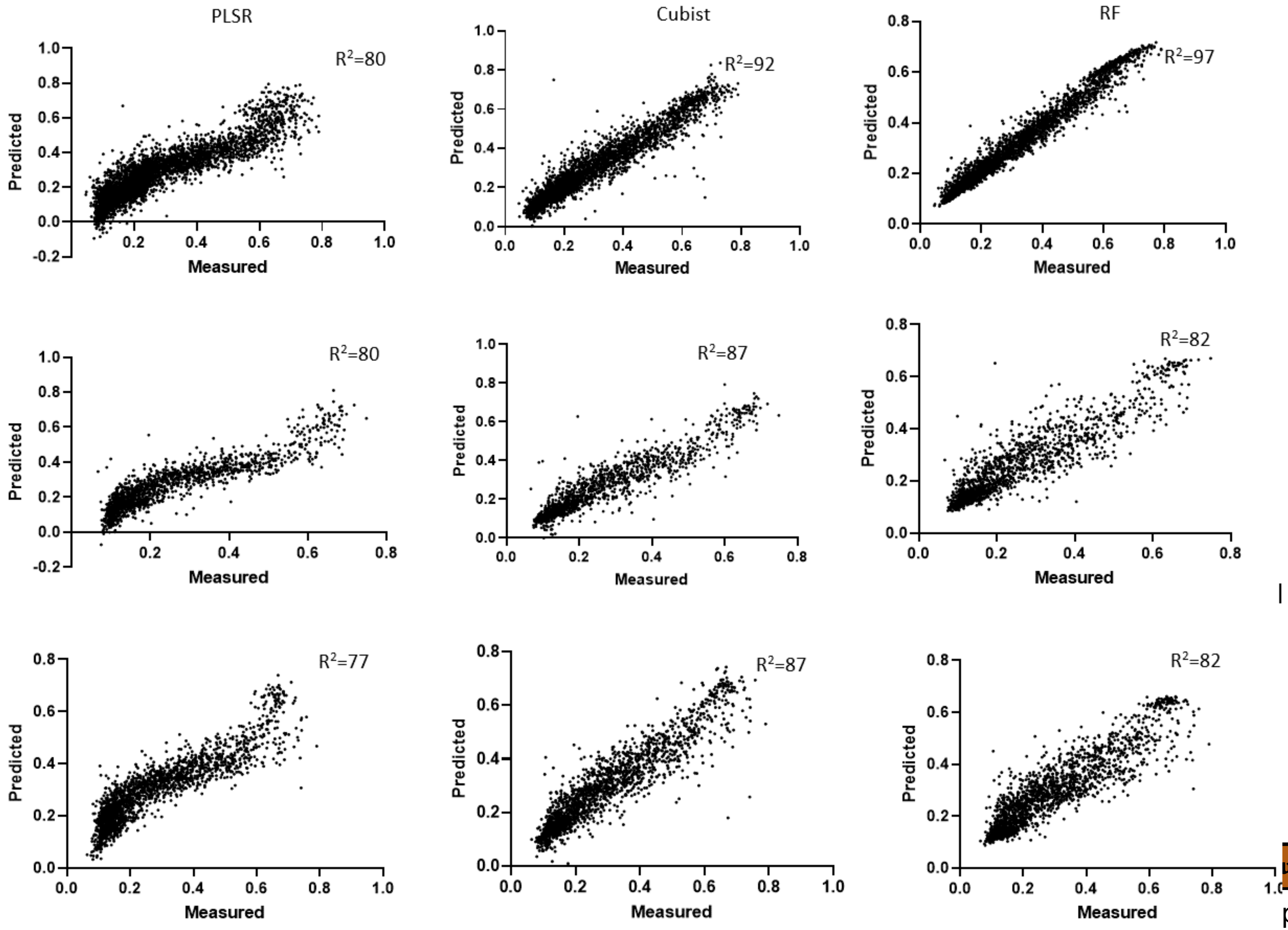
	Mean	Median	Min	Max	s	n
Measured SQI	0.271	0.221	0.047	0.790	0.160	8093
Predicted SQI	0.355	0.340	0.069	0.763	0.166	8093
Direct prediction of SQI	0.270	0.227	0.000	0.836	0.152	8093

Soil Properties Combined- Soil Quality Index

Calibration

Cross Validation

External Validation



Can we predict soil properties from un-processed samples using vis-NIR spectroscopy?

Lab Measurements
- Processed samples

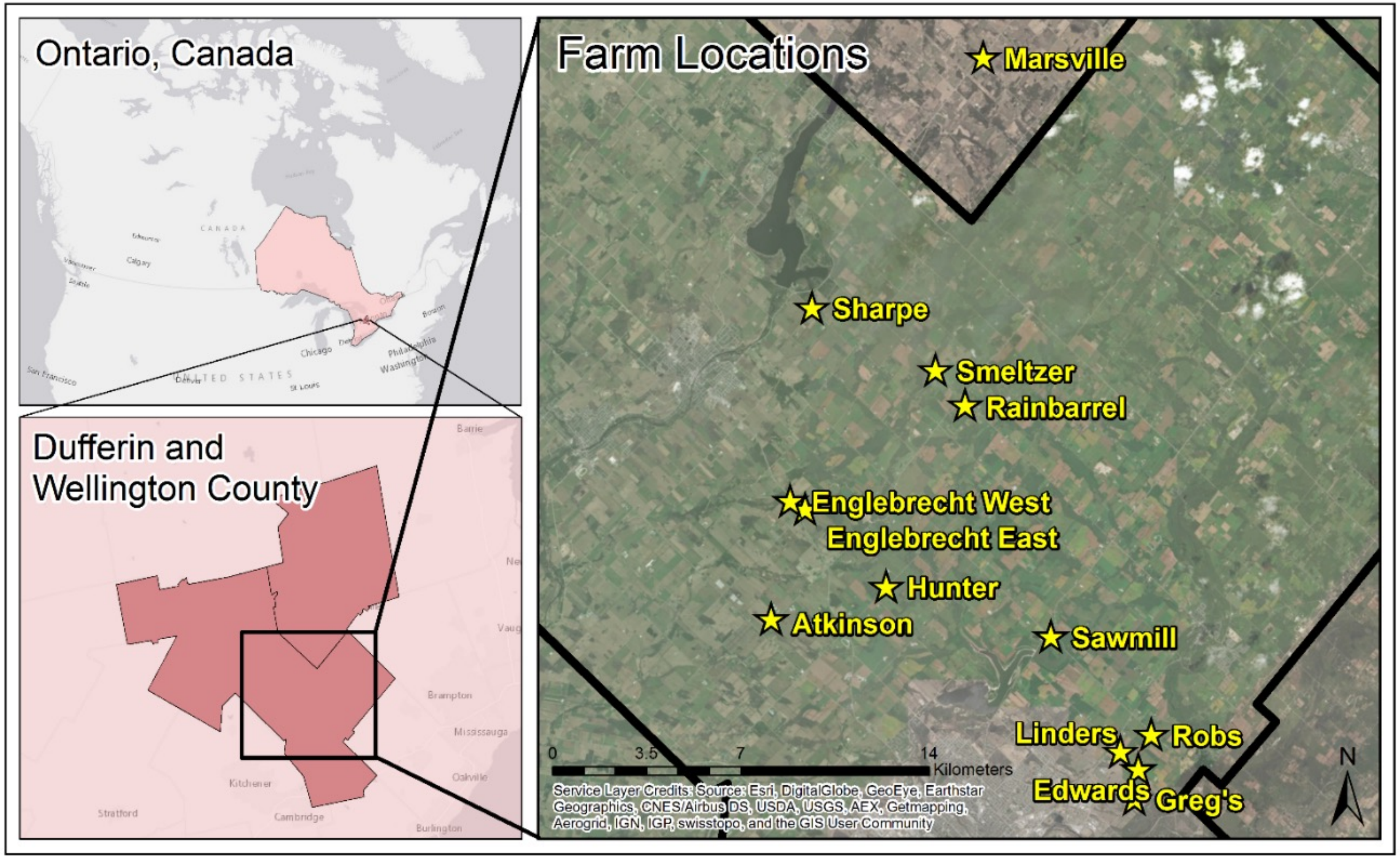
Lab measurements
- Unprocessed samples

Field measurements
- In-situ, unprocessed samples

Digital Soil Mapping

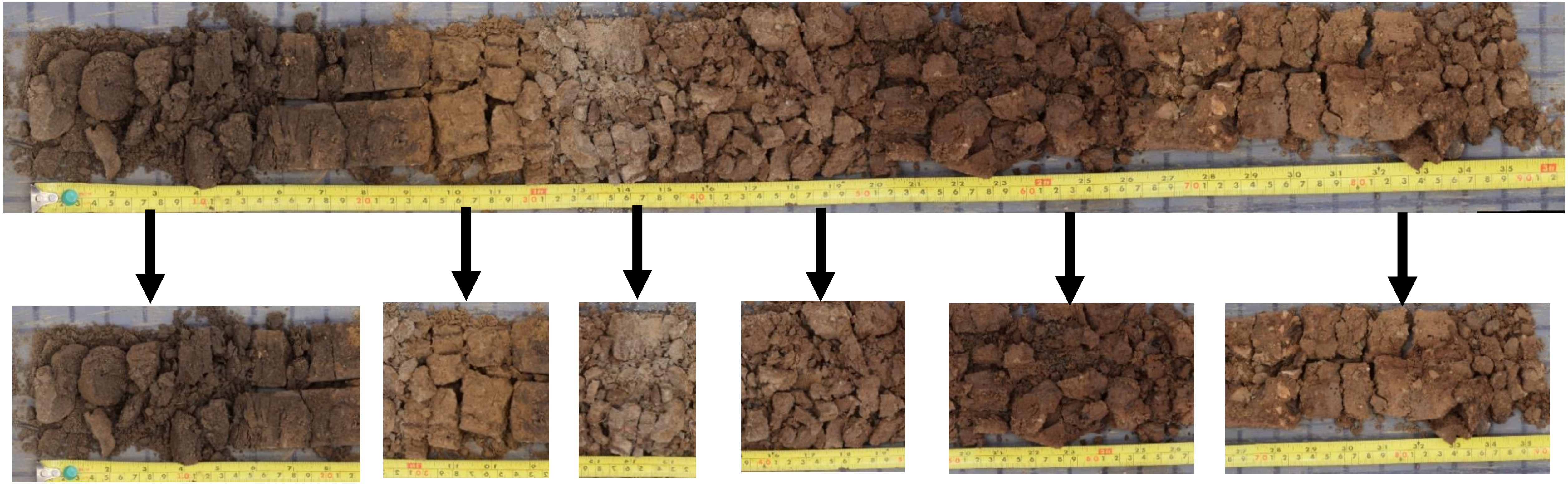
Case Study 2

- 205 soil cores were collected from 13 farms



Soil samples

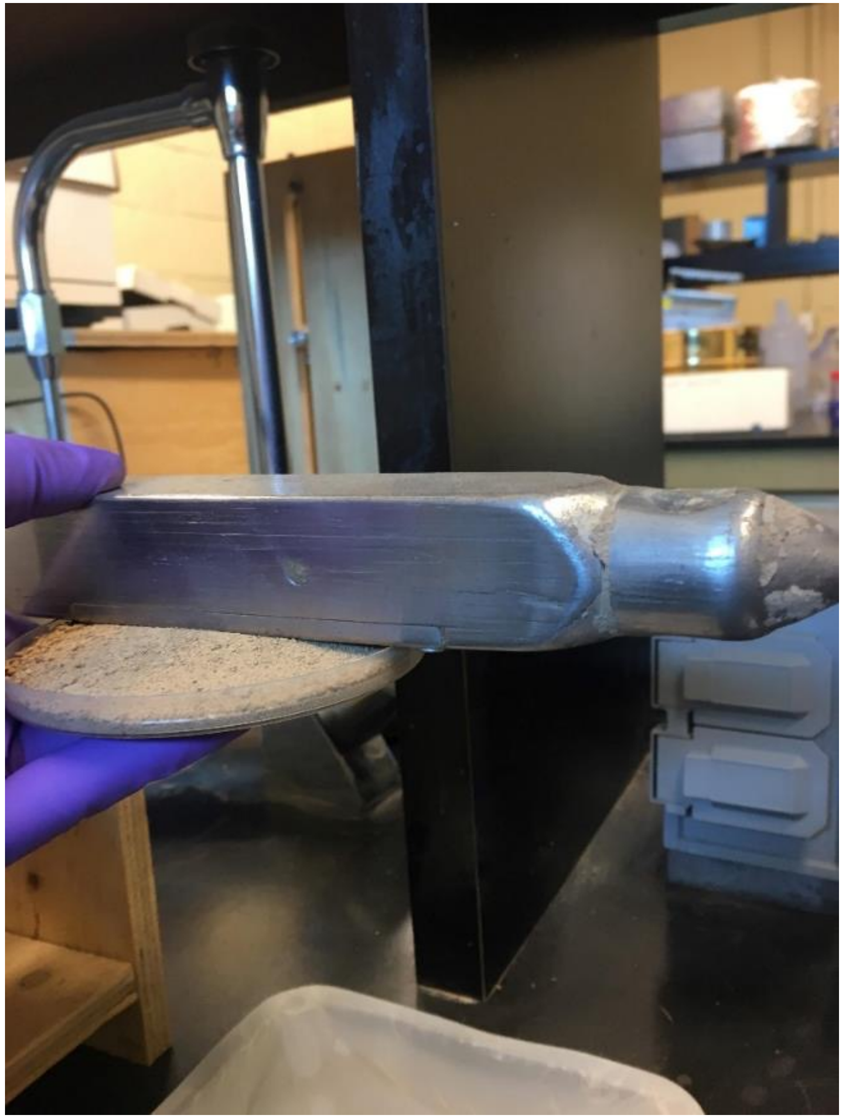
- Profile Description completed by Woodrill Ltd.



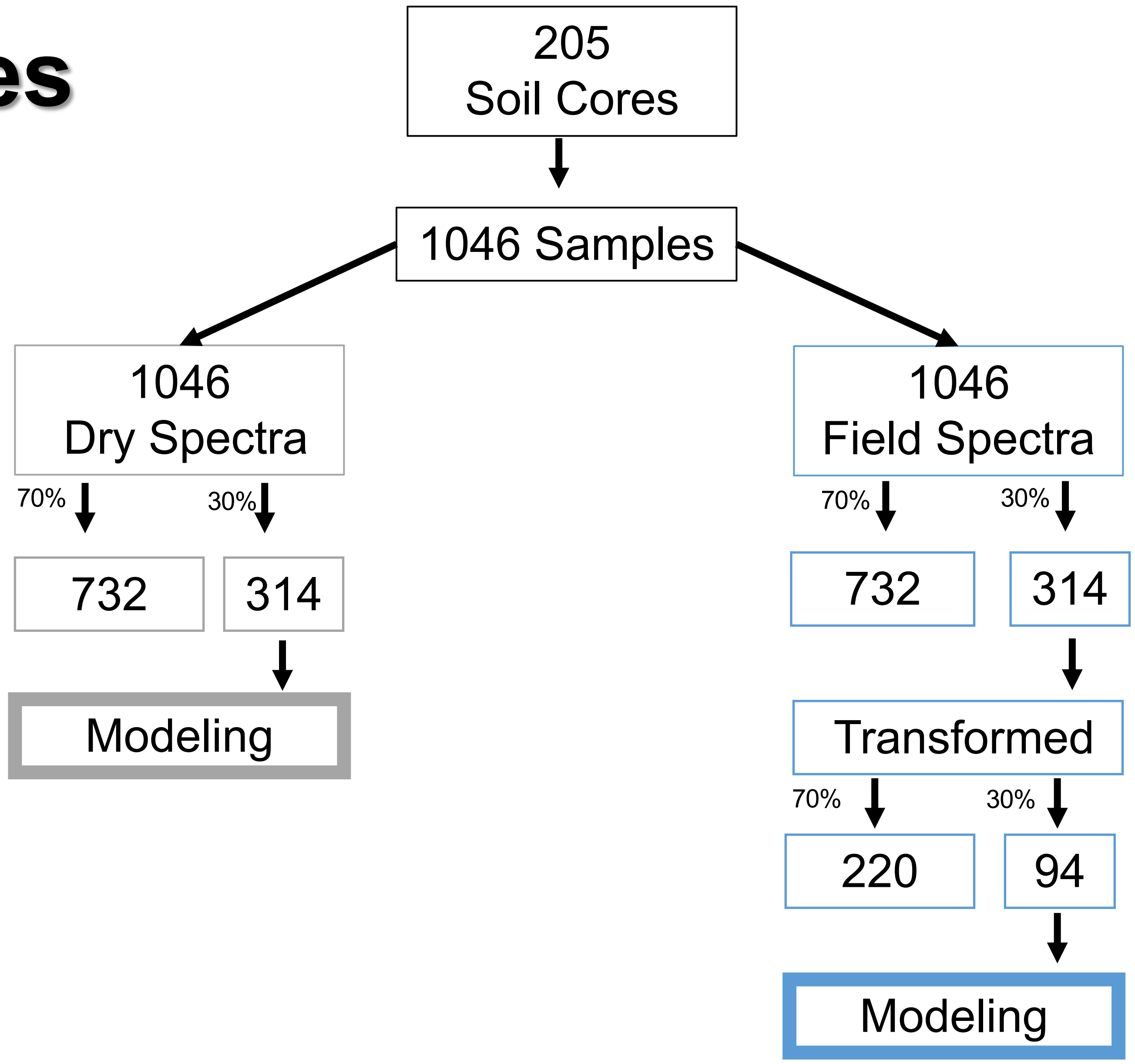
- Samples split by horizon – 1046 samples total

Soil samples

- 1046 samples total
- Each sample was split in half
  - ½ air dried and ground (processed)
  - ½ left at field condition (unprocessed)
- pH, EC, OM – on all samples
- Texture – on a subset
- 2 sets of spectra in lab
  - Dry (processed- Air dried, sieve, ground)
  - Field (unprocessed- Field moist)



Soil Samples



Prediction of Soil Properties

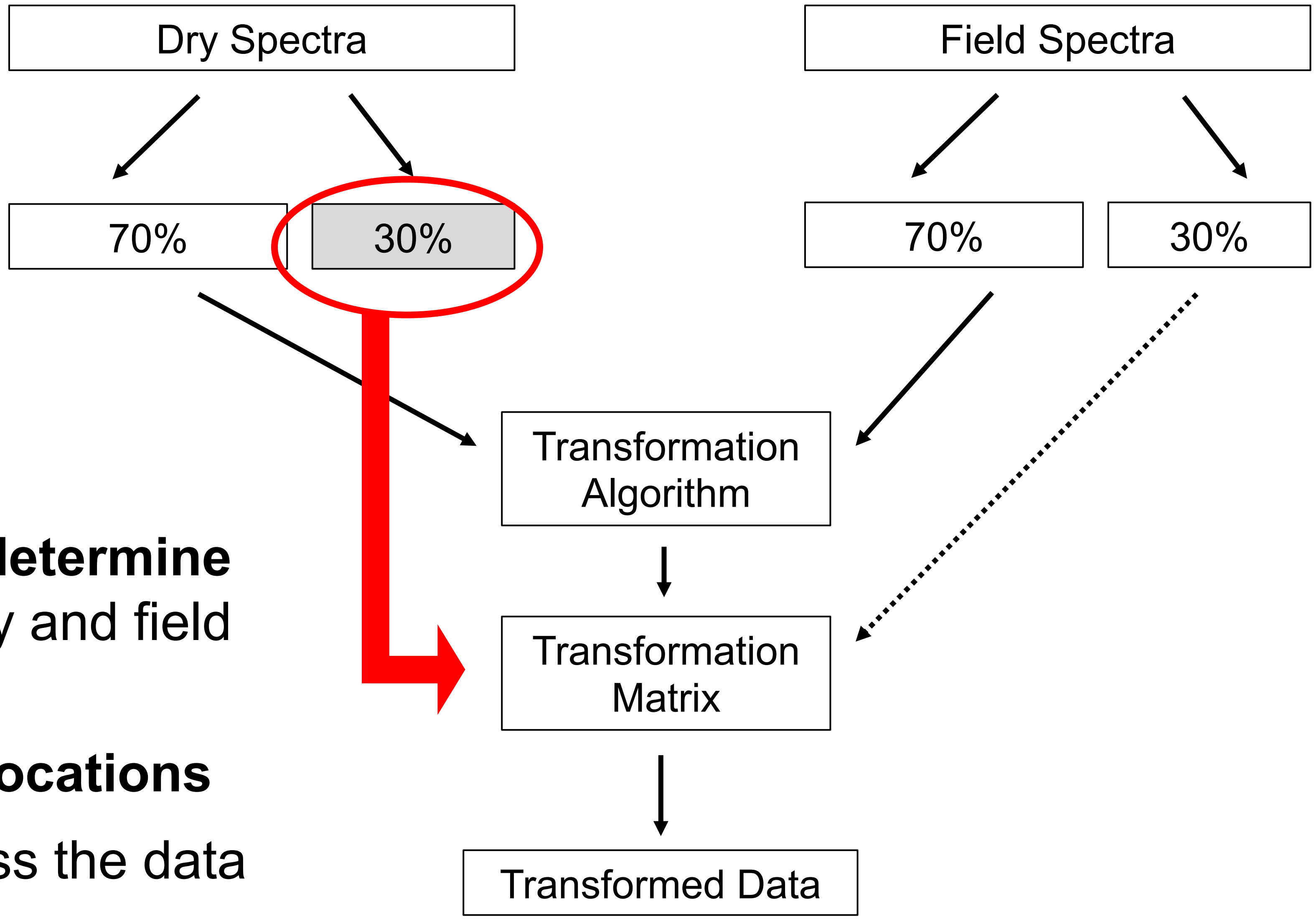
	1st Derivative + Gap				2nd Derivative + Gap				SNV			
	PLSR	Cubist	RF	ELM	PLSR	Cubist	RF	ELM	PLSR	Cubist	RF	ELM
	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$
EC	-0.02	0.00	-0.02	-0.02	-0.01	-0.03	-0.03	**0.22**	-0.01	-0.01	0.04	-0.04
OM	0.76	**0.83**	**0.83**	**0.83**	0.82	0.82	0.81	0.67	0.58	0.69	0.66	0.66
pH	0.57	0.62	**0.63**	0.52	0.48	0.54	0.53	0.48	0.49	0.61	0.48	0.35
%Sand	0.48	0.47	**0.70**	0.53	0.29	0.40	0.46	0.45	0.54	0.43	0.47	0.39
%Silt	0.46	0.53	**0.70**	0.60	0.40	0.39	0.42	0.25	0.59	0.55	0.44	0.26
%Clay	0.13	0.26	0.20	0.19	0.23	0.20	0.25	0.25	**0.36**	0.23	0.22	0.16
%VCS	0.18	-0.02	0.17	0.04	0.11	0.00	0.02	-0.01	0.29	0.16	**0.55**	0.09
%CS	**0.68**	0.08	0.15	0.46	0.30	0.58	0.22	0.02	0.07	0.00	0.09	0.04
%Med	0.50	0.24	**0.53**	0.39	0.31	0.28	0.32	0.09	**0.53**	0.26	0.51	0.39
%fs	-0.01	**0.49**	-0.02	-0.02	0.01	0.03	0.14	-0.01	0.08	0.01	0.03	0.03

- **Best** Predicted → **OM, %sand and %silt**
- **Worst** Predicted → **EC and %clay**
- **Best** preprocessing and Modeling →**1st Derivative + Gap** and **RF**

Field Moist Samples- Data Transformation

- 3 replications spectral data collected on **field** samples
- 2 transformation methods were compared
  - External Parameter Orthogonalization (**EPO**)
  - Direct Standardization (**DS**)

Transformation Methods



- Both transformation methods **determine** the **difference** between the dry and field spectral data
- **EPO** – Difference at **specific locations**
- **DS** – **Average** difference across the data

Optimization of Transformation Methods

	Dry Spectra	Field Spectra Before Transformation	Field Spectra After DS	Field Spectra After EPO
	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$
1st Derivative + Gap				
PLSR	0.92	0.90	0.89	0.34
Cubist	0.89	0.89	0.82	0.29
RF	0.90	0.85	0.81	0.12
ELM	0.92	0.89	0.41	0.34
2nd Derivative + Gap				
PLSR	0.89	0.85	**0.92**	0.44
Cubist	0.91	0.79	**0.88**	0.44
RF	0.91	0.81	**0.86**	0.20
ELM	0.87	0.80	0.54	0.42
SNV				
PLSR	0.93	0.91	0.74	0.42
Cubist	0.92	0.90	0.73	0.40
RF	0.86	0.85	0.68	0.11
ELM	0.89	0.81	0.46	0.36

Can we predict soil properties in-situ using vis-NIR spectroscopy?

Lab Measurements
- Processed samples

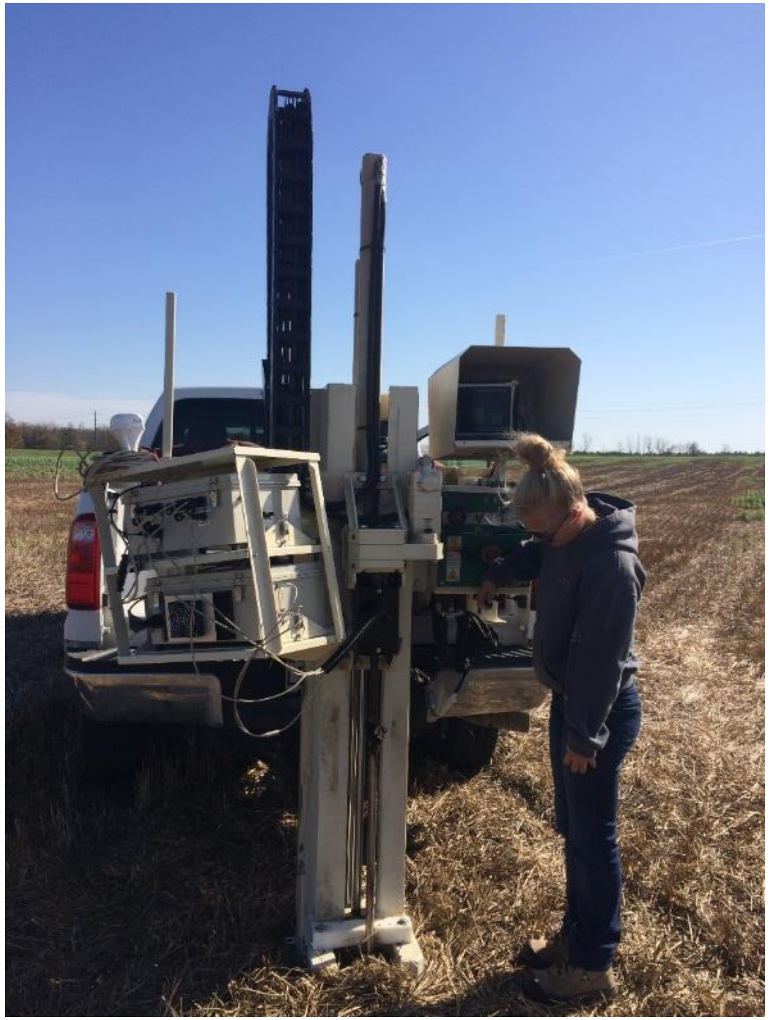
Lab measurements
- Unprocessed samples

Field measurements
- In-situ, unprocessed samples

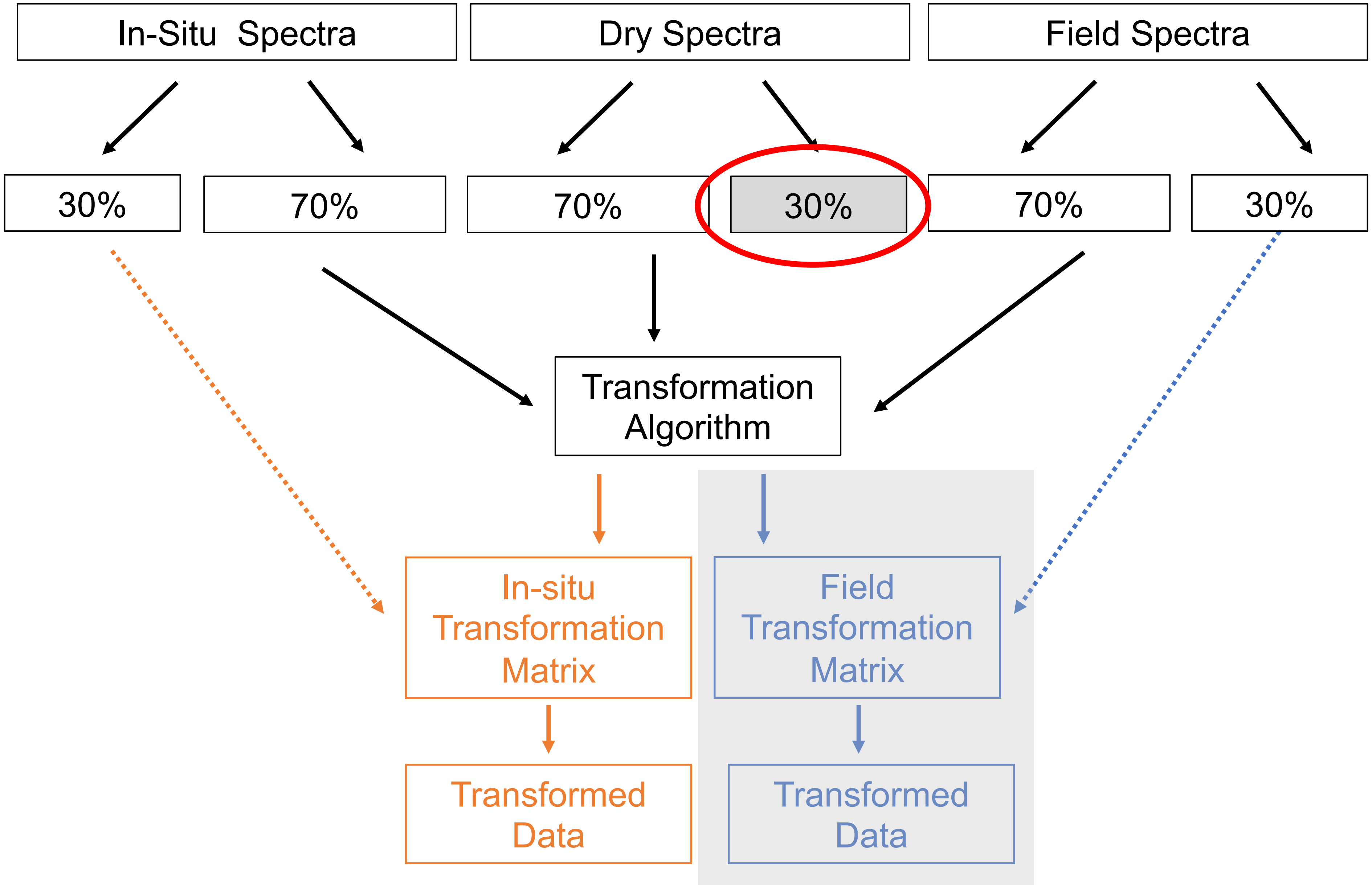
Digital Soil Mapping

In-situ Spectra Collection

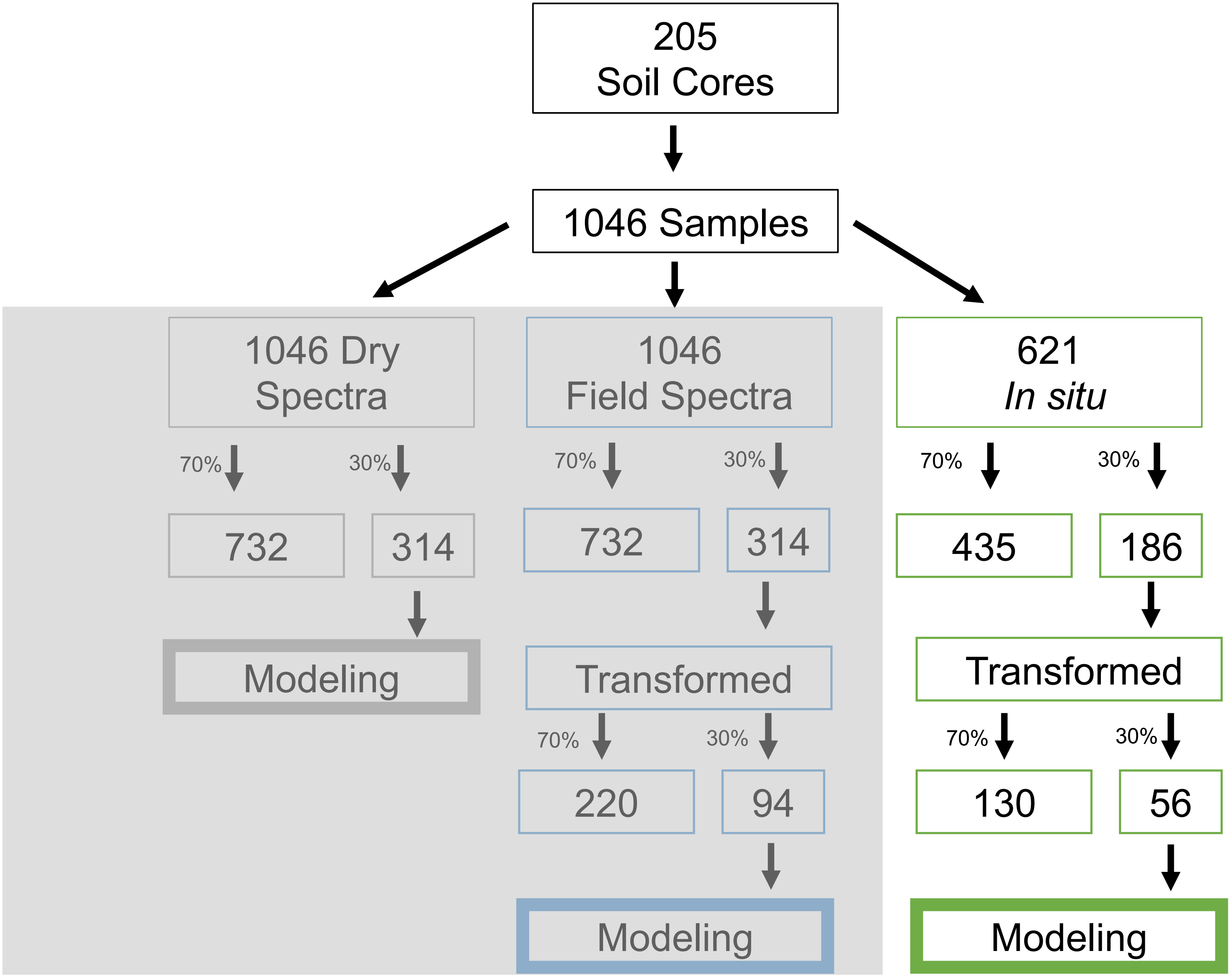
- 3 replications spectral data were collected **in-situ** at each soil sample location
- **DS** and **EPO** for transformation
  - 2 different matrix were used for each = 4 transformations
- **Previously optimized** preprocessing and modeling algorithms



Transformation Methods

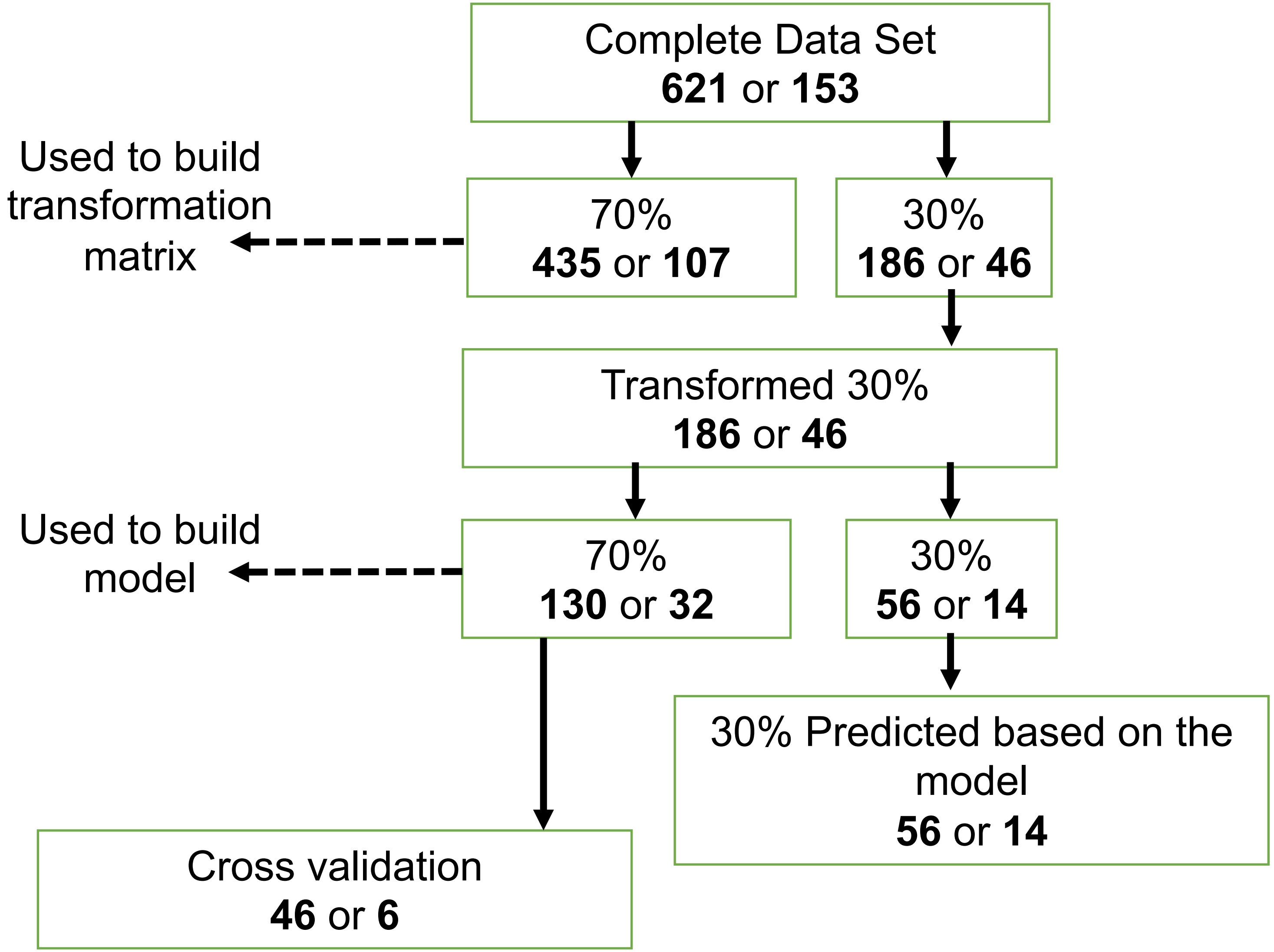


Datasets



**These values may vary between soil properties

Dataset Size



	Before Transformation			After Transformation			
	Dry	Field	In situ	DS Field Matrix	DS In-Situ Matrix	EPO Field Matrix	EPO In-Situ Matrix
	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$	$_{Adj}R^2$
			1st Derivative + Gap				
PLSR	0.92	0.86	0.59	0.99	0.96	0.53	0.41
Cubist	0.92	0.78	0.51	0.98	0.85	0.59	0.49
RF	0.95	0,84	0.57	0.83	0.49	0.42	0.51
ELM	0.95	0.83	0.56	0.33	0.13	0.34	0.53
			2nd Derivative + Gap				
PLSR	0.87	0.78	0.62	0.99	0.96	0.46	0.45
Cubist	0.89	0.78	0.61	0.98	0.85	0.50	0.43
RF	0.89	0.82	0.70	0.86	0.53	0.54	0.37
ELM	0.89	0.79	0.60	0.27	0.38	0.44	0.45
			SNV				
PLSR	0.88	0.69	0.75	0.97	0.80	0.32	0.49
Cubist	0.93	0.77	0.69	0.97	0.84	0.40	0.55
RF	0.88	0.74	0.61	0.79	0.69	0.29	0.29
ELM	0.80	0.62	0.26	0.20	0.69	0.11	0.60

In-Situ Spectral Prediction

DS Field Matrix												
	1st Derivative + Gap				2nd Derivative + Gap				SNV			
	PLSR	Cubist	RF	ELM	PLSR	Cubist	RF	ELM	PLSR	Cubist	RF	ELM
	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2
OM(%)	**0.99**	0.98	0.83	0.33	**0.99**	0.98	0.86	0.27	0.97	0.97	0.79	0.20
pH	**0.95**	0.79	0.43	-0.02	0.94	0.72	0.53	0.29	0.91	0.68	0.35	0.42
%Sand	**0.99**	**0.99**	0.95	0.75	**0.99**	**0.99**	**0.99**	0.86	0.95	0.97	0.86	0.69
%Silt	**0.99**	**0.99**	**0.99**	**0.99**	**0.99**	**0.99**	0.97	0.95	0.98	0.91	0.89	0.72
%Clay	**0.96**	0.86	0.74	0.95	**0.96**	0.84	0.84	0.80	0.91	0.81	0.24	0.20
DS In-Situ Matrix												
	1st Derivative + Gap				2nd Derivative + Gap				SNV			
	PLSR	Cubist	RF	ELM	PLSR	Cubist	RF	ELM	PLSR	Cubist	RF	ELM
	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2	$_{Adj}$ R^2
OM(%)	**0.96**	0.85	0.49	0.13	**0.96**	0.85	0.53	0.38	0.80	0.84	0.69	0.69
pH	0.76	0.28	0.32	0.28	0.85	0.57	0.47	0.10	0.83	0.60	0.31	0.38
%Sand	0.99	0.99	0.99	0.73	**0.99**	**0.99**	0.88	0.93	0.95	0.64	0.87	-0.25
%Silt	0.97	0.98	0.98	0.91	**0.99**	**0.99**	0.97	0.89	0.97	**0.99**	0.92	0.18
%Clay	**0.99**	0.98	0.83	0.89	**0.99**	0.97	0.96	0.49	**0.99**	0.95	0.90	-0.18

- All soil properties were predicted well by DS transformed *in-situ* spectral data
  - May suggest model overfitting

Can we leverage vis-NIR spectroscopy to fill data gaps in digital soil mapping?

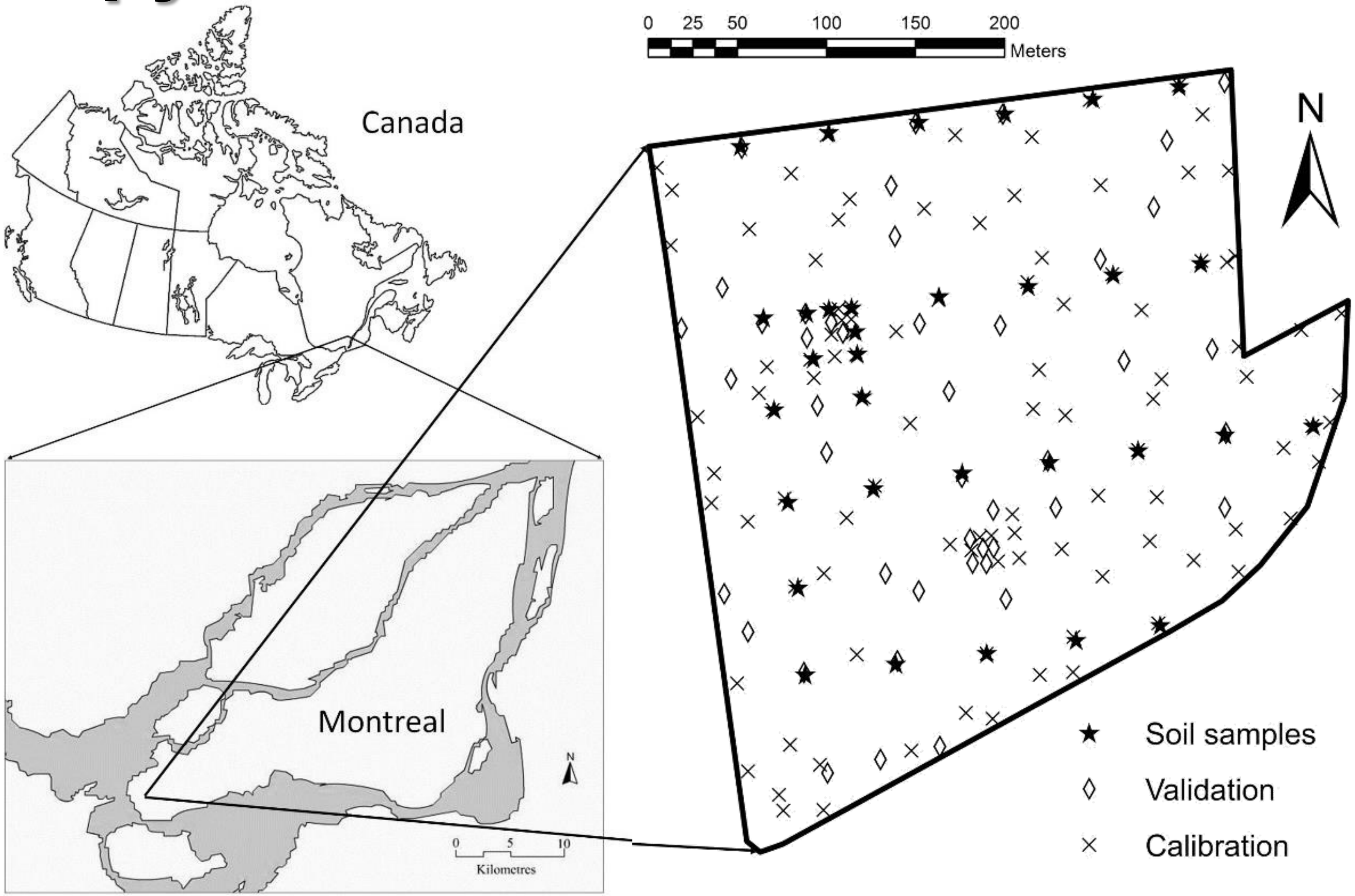
Lab Measurements
- Processed samples

Lab measurements
- Unprocessed samples

Field measurements
- In-situ, unprocessed samples

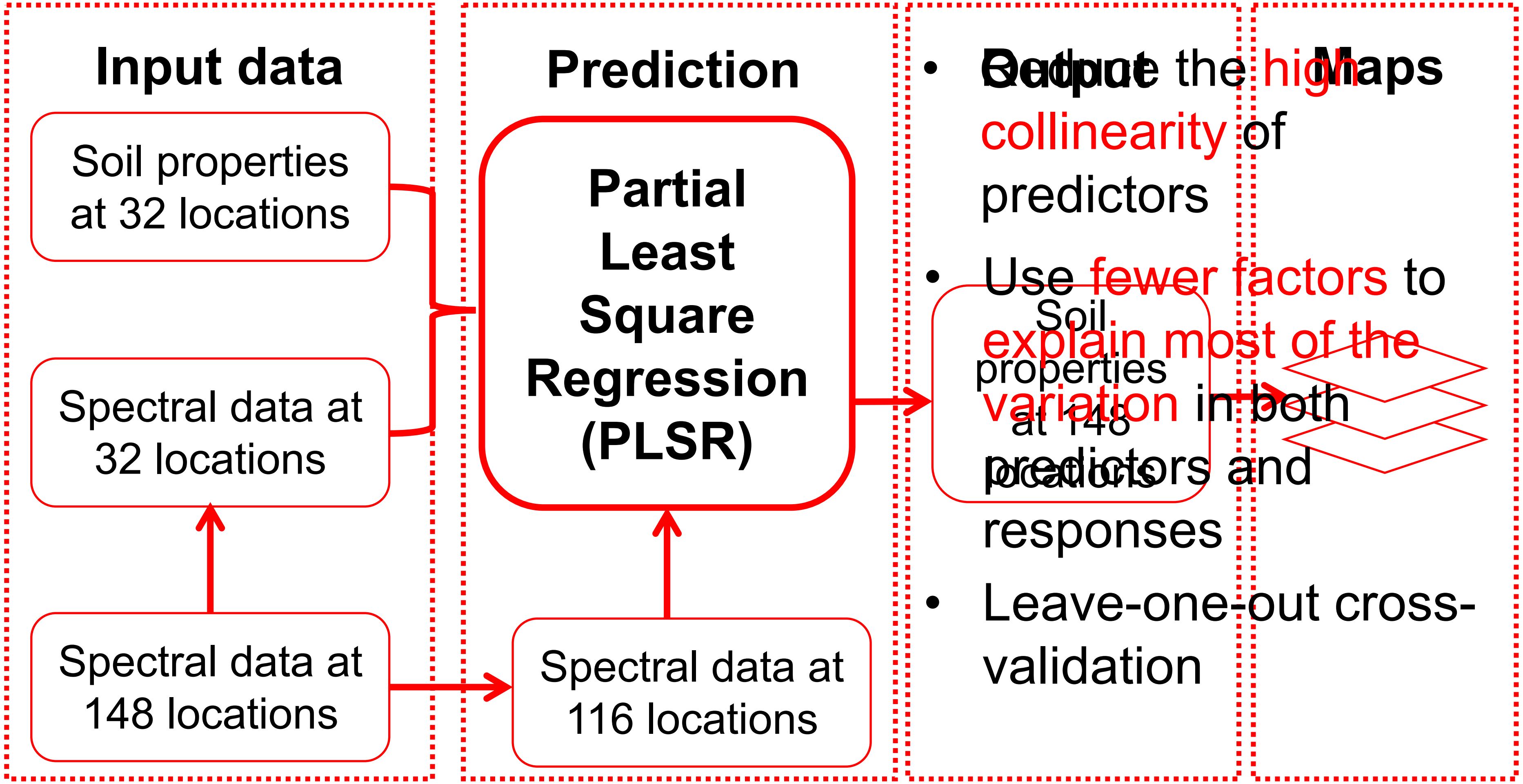
Digital Soil Mapping

Spectroscopy and DSM



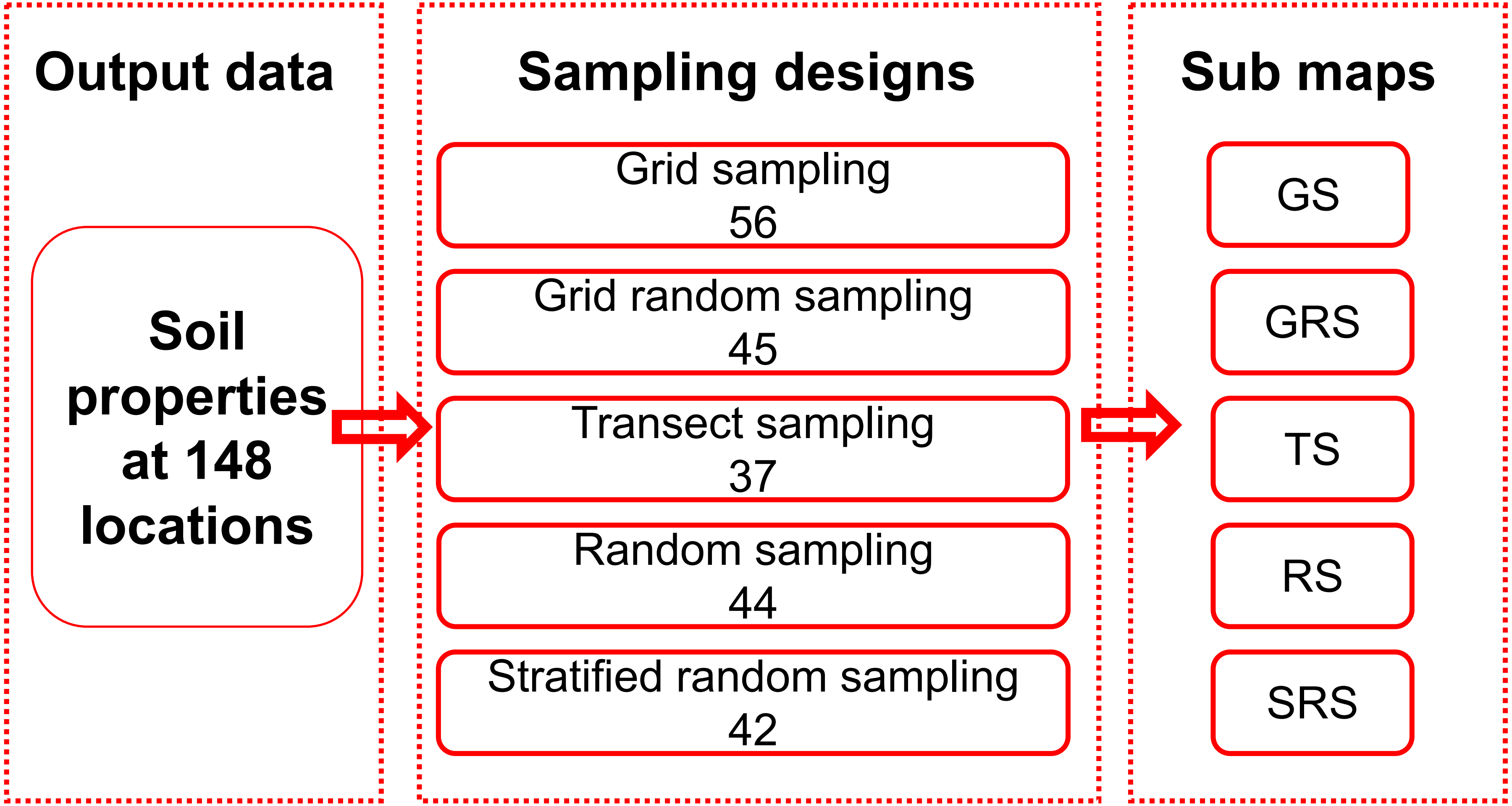
Field Data Collection

Profile and Profile Spectra



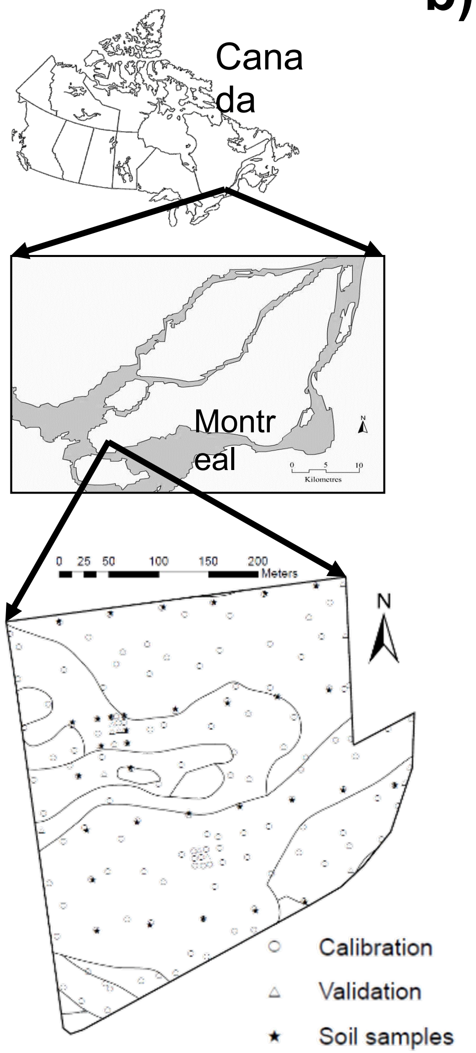
- Reduce the high collinearity of predictors
- Use fewer factors to explain most of the variation in both predictors and responses
- Leave-one-out cross-validation

Comparing Sampling Designs

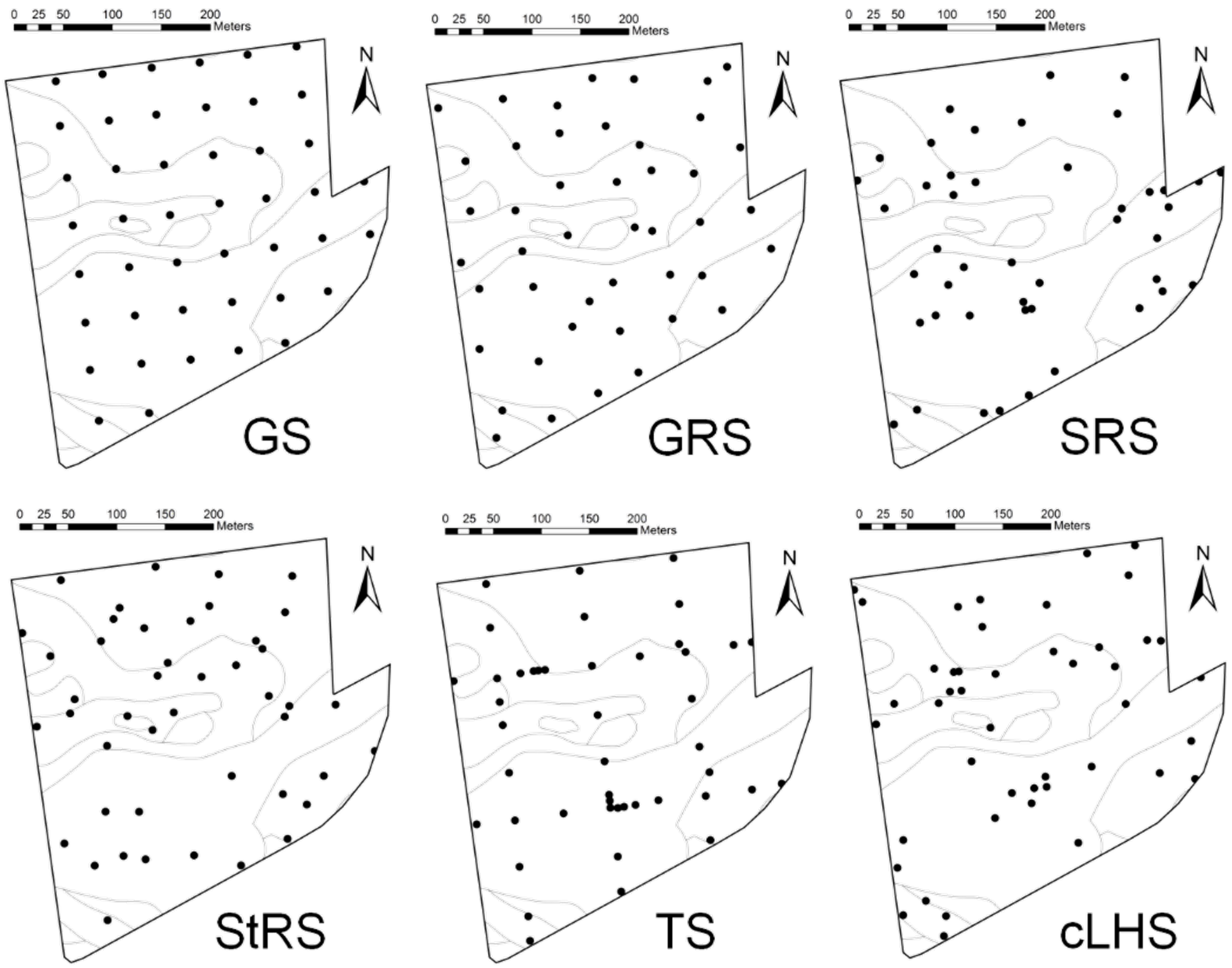


Soil Sampling Designs

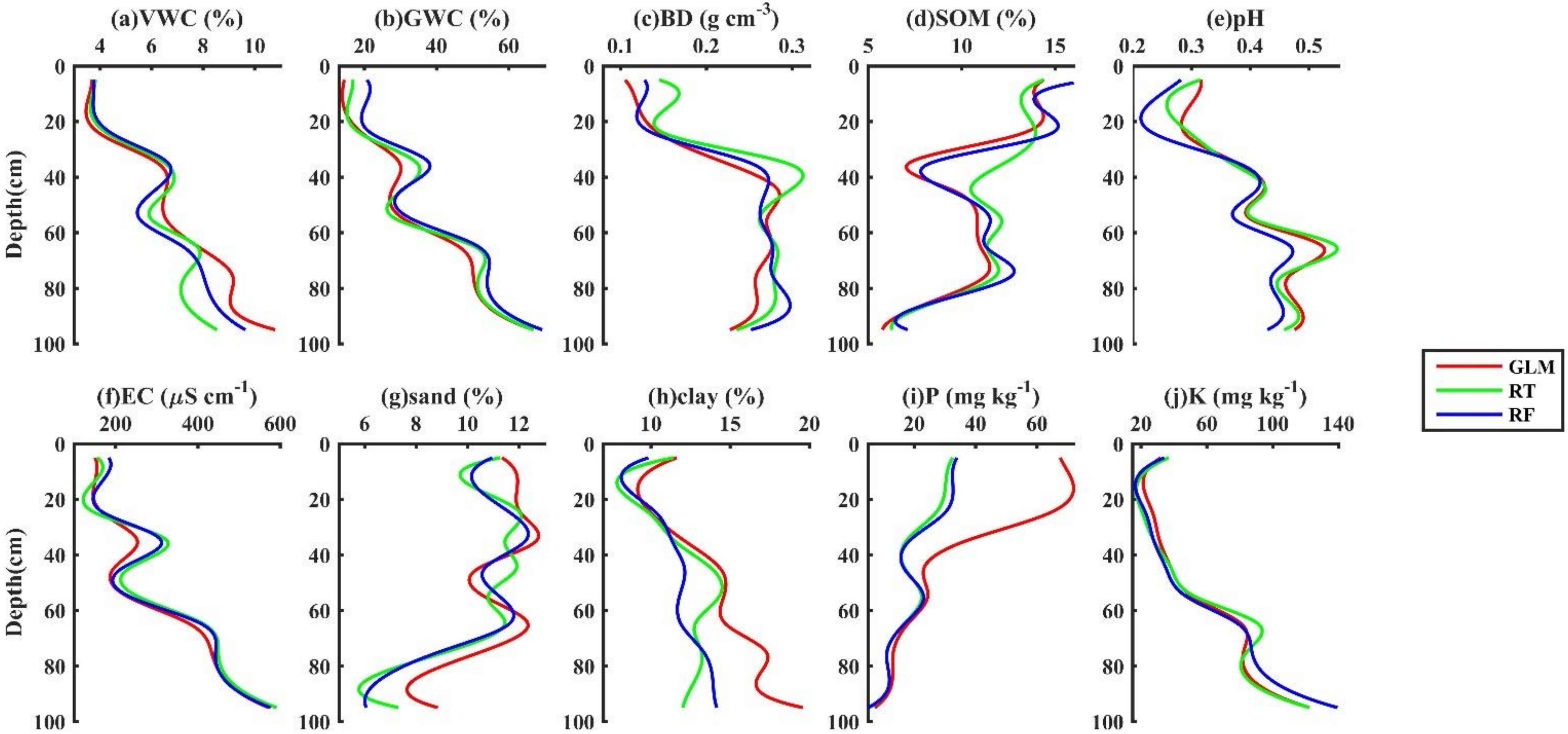
a)



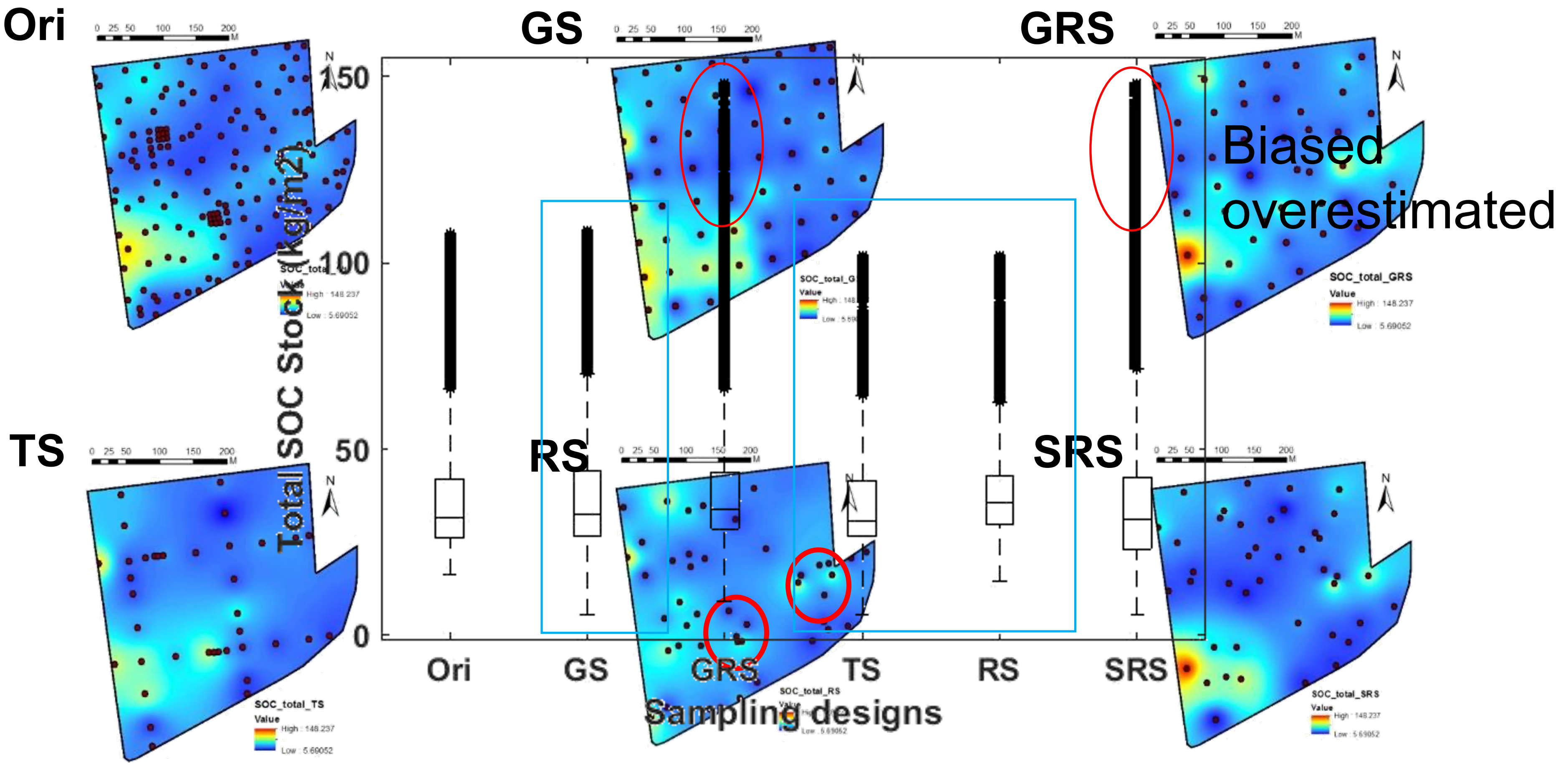
b)



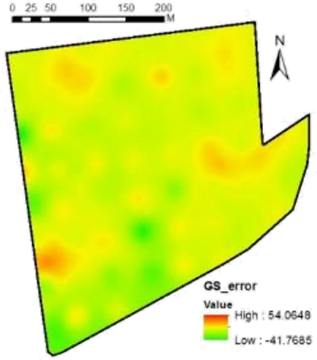
Depth-wise RMSE



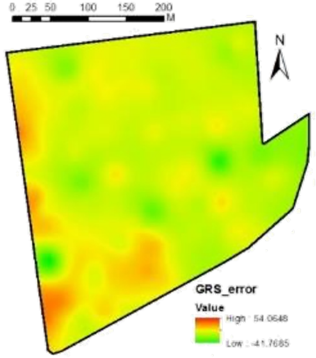
Comparing C Stock (0-1 m)



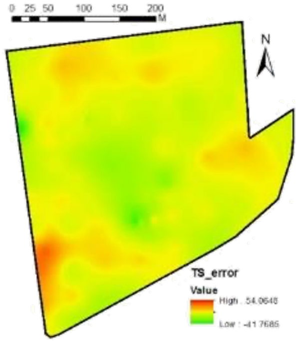
Comparing Error (0-1 m)



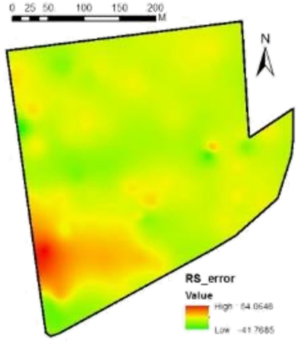
GS



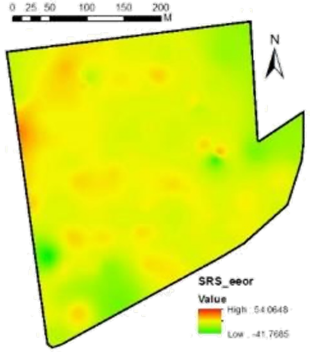
GRS



TS



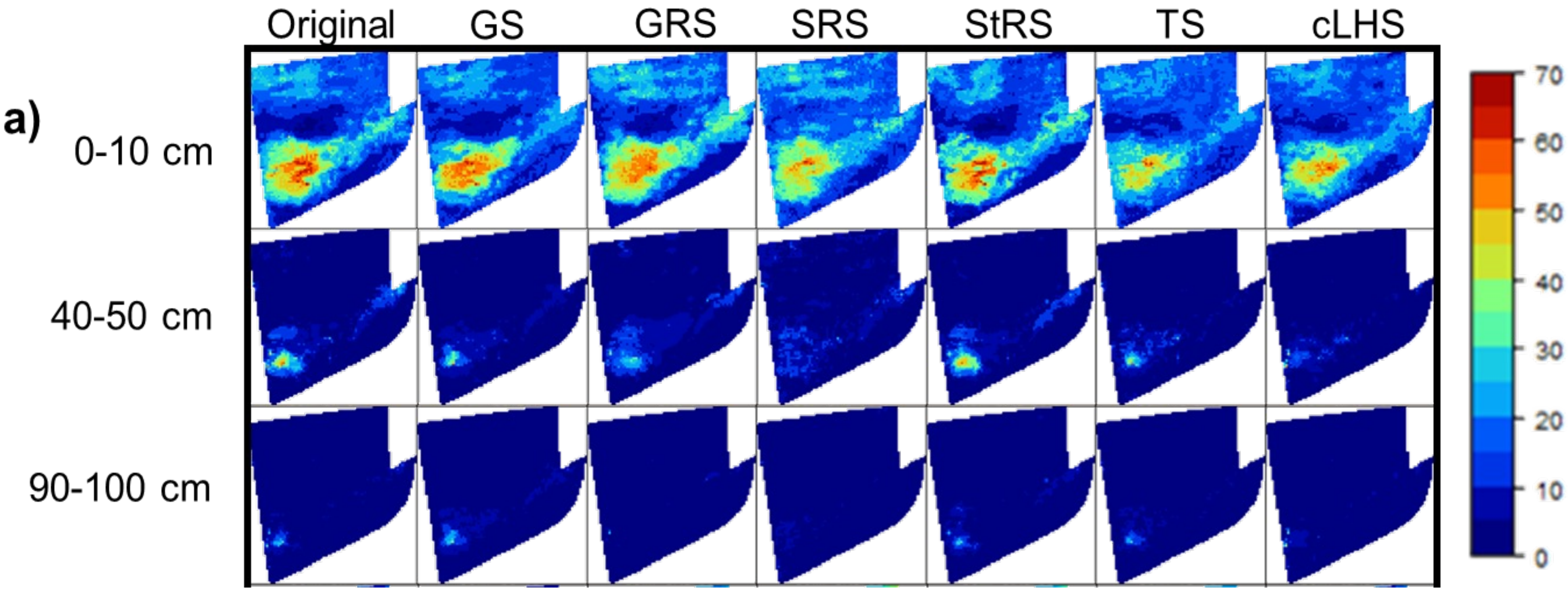
RS



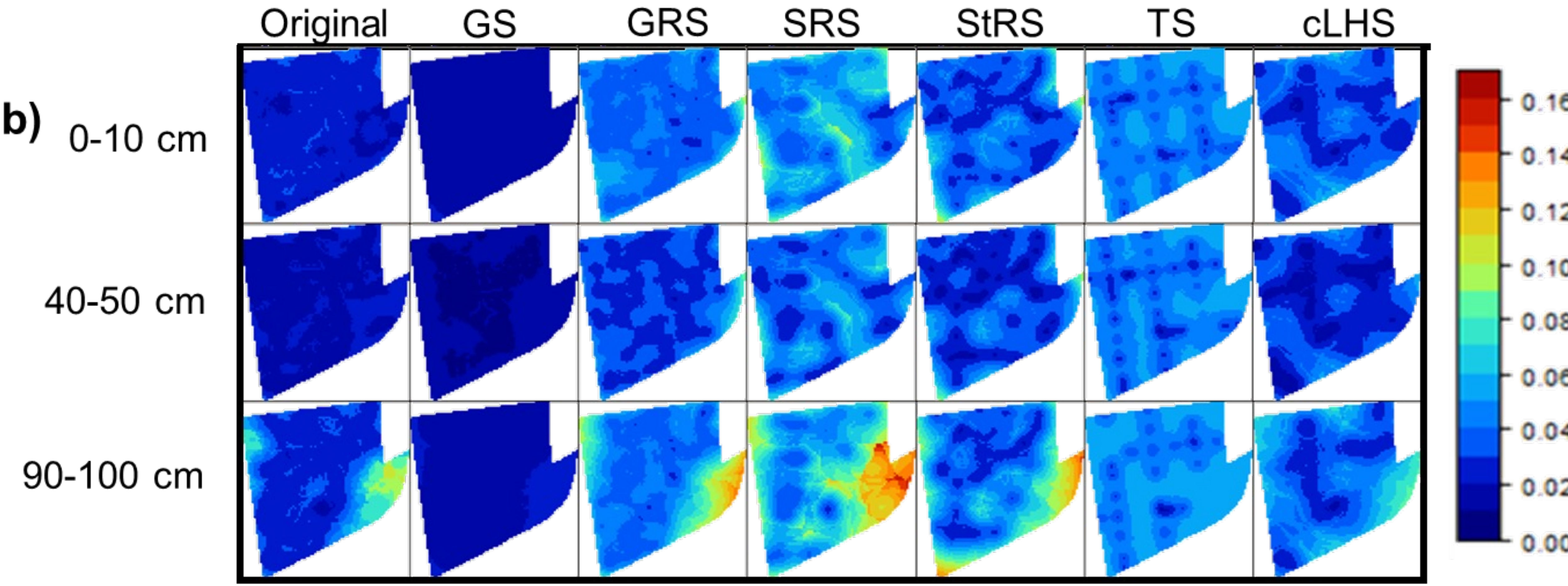
SRS

	GS	GRS	TS	RS	SRS
RMSE	8.94	10.32	8.75	11.38	8.47

3D Digital Soil Maps



3D Digital Soil Maps (uncertainty)



Take-Home Message

- Can we use spectroscopy for soil?
  - Yes- as good as we have seen globally
- Can we take spectroscopy to field?
  - Yes, additional information recommended
  - Additional data processing required
- Should we do field moist or in-situ?
  - No significant difference in predictability
  - In-situ can reduce resources but need specialized equipment
- Can we leverage field spectroscopic data for digital soil mapping?
  - Yes, show promise
  - Need specialized equipment

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Canadian Geophysical Union Union Géophysique Canadienne

AGU American Geophysical Union

CSIRO

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BAYER

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Biswas Soil Lab

Thank You

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