

Food and Agriculture Organization of the United Nations GLOSOLAN Soil spectroscopy training workshops

# WEBINAR 3

Online webinars



#### Acknowledgment of Country

We would like to acknowledge the Gadigal people of the Eora Nation, the traditional custodians of the land from which we are webcasting this presentation.

We recognise their continuing connection to land, waters and culture. We pay our respects to the Elders past, present and emerging.

#### A future for soil spectral inference



#### Alex M<sup>c</sup>Bratney

#### The University of Sydney

Webinar 3 0800-0930 CET Sep 23 2021 FAO Global Soil Partnership GLOSOLAN Working Group on Soil Spectroscopy

### CONTRIBUTORS

Mario Fajardo **Ed Jones Budiman Minasny** Wartini Ng **Jose Padarian Alexandre Wadoux** 







### Partially DIDACTIC

### Partially PROGNOSTIC

# RECOLLECTION



### **SOIL SPECTROSCOPY**

# 1960s first work? 1980s digital, chemometrics 2000s NIR, MIR, spectral libraries 2020s field spectroscopy, inference

### WHAT IS A SPECTRUM?

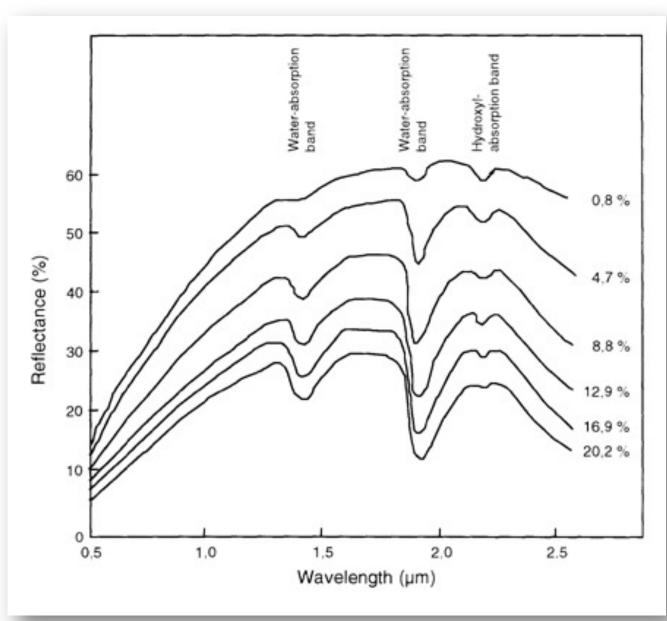
Spectrum singular noun Spectra plural noun Spectral adjective

## WHAT IS A SPECTRUM?

**Response (reflectance, absorbance,** conductivity etc.) as function of some systematic portion of a continuum (wavelength, frequency) **Digital spectrum – spectrum sampled** at fixed wavelengths or frequencies.

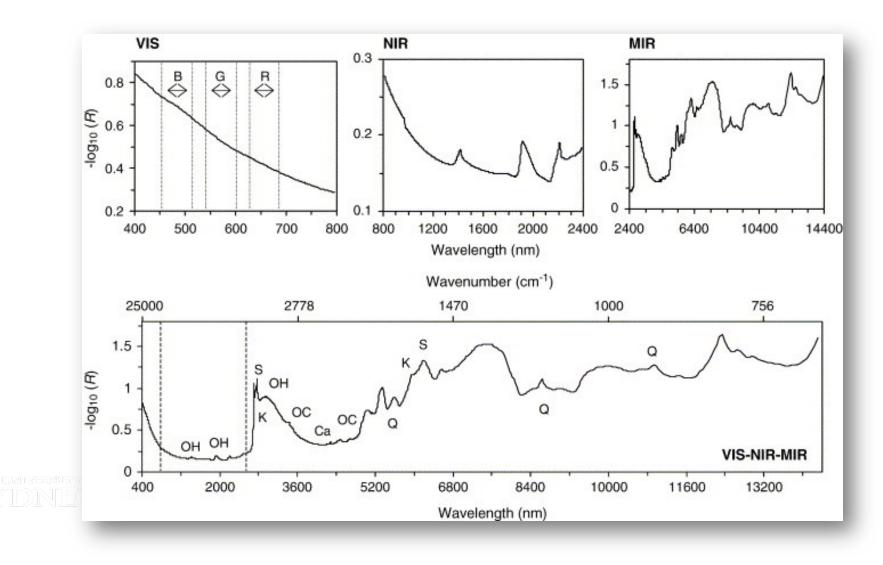
#### Vis-NIR reflectance spectrum – Newtonia silt loam

Bowers, S.A. & Hanks, R.J. 1965 Reflection of radiant energy from soils. Soil Science 100, 130-138.



#### Vis-NIR-MIR absorption spectrum

R.A. Viscarra Rossel, D.J.J. Walvoort, A.B. McBratney, L.J. Janik & J.O. Skjemstad 2006 Visible, near infrared, mid infrared or combined diffuse reflectance spectroscopy for simultaneous assessment of various soil properties. Geoderma 131, 59-75.



#### SOIL CONDITION & <u>CAPACITY</u> Indicators and MIR spectrometry

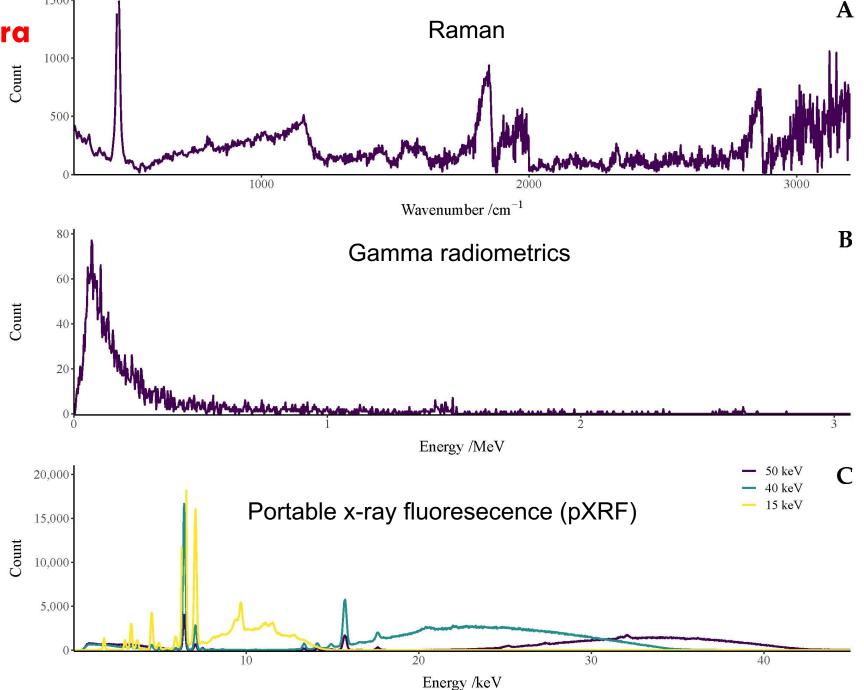
Biological	Chemical	Physical	
Microbial Biomass	рН	Rooting Depth	McProtney A.R. Field D
Mycorrhiza populations	CEC	Stoniness	<ul> <li>McBratney, A.B., Field, D.,</li> <li>Morgan, C.L.S. &amp; Huang, J.</li> <li>(2019). On soil</li> <li>capability,capacity and</li> <li>condition. Sustainability 11(12),</li> </ul>
Particulate Organic Matter	Heavy Metals	<u>Texture</u>	
Respiration	EC	Aggregate Stability	
Potential N mineralization	Organic C & N	Slaking Index	3350.
Fatty Acid profiles	Extractable macronutrients	Water holding capacity	
Soil enzymes	Total elements,	Bulk Density	
	Micronutrients		
	CaCO <sub>3</sub>	Infiltration	
	<u>P retention</u>	Penetration resistance	

Poorly Estimated by MIR, Reasonably Estimated by MIR, Well Estimated by MIR

#### Other kinds of soil spectra

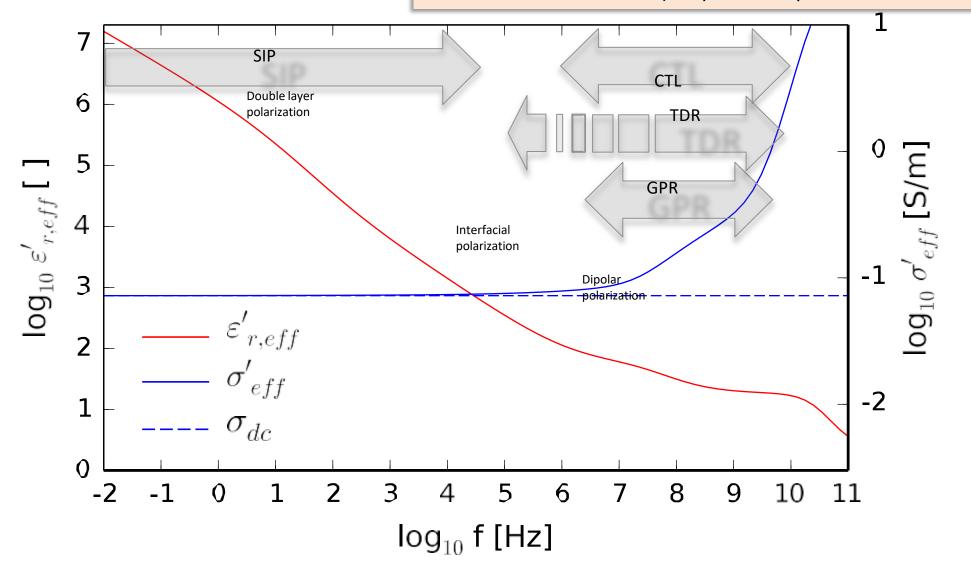
1500-

Wadoux, A.M.J-C., Malone, B., Minasny, B., Fajardo, M. & McBratney, A.B. (2021). *Soil Spectral Inference with R: Analysing Digital Soil Spectra Using the R Programming Environment*. Springer Nature. Chapter 1 Fig 1



#### SOIL ELECTRIC SPECTRUM

Revil, A. (2013). Effective conductivity and permittivity of unsaturated porous materials in the frequency range 1 mHz-1 GHz. Water Resour. Res., 49(W02517):306–327.



#### McBratney, Minasny, Mendonca Santos 2003 On digital soil mapping. Geoderma 117, 3-52.

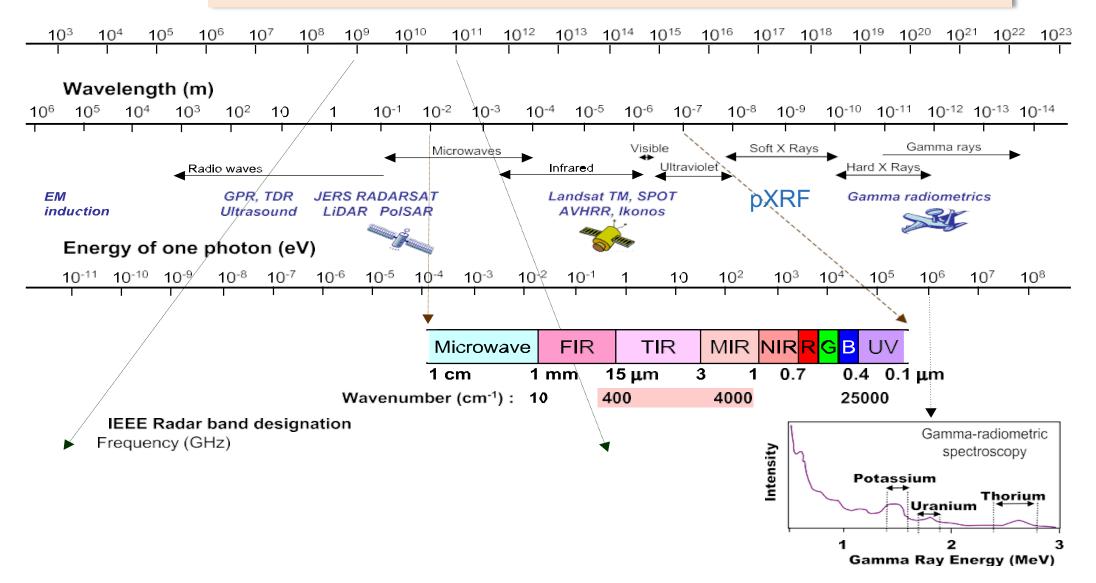
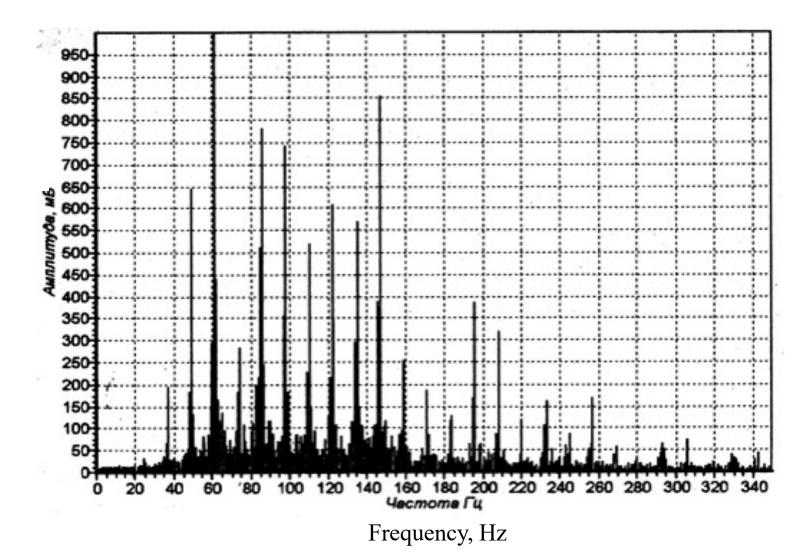


Fig. 1. The electromagnetic spectrum, highlighting the useful parts for obtaining information on soil and environmental variables through remote and proximal sensing. The boundaries for the infrared spectrum (NIR, MIR and FIR) are not consistent and vary between the chemical and remote-sensing literatures. The terms in this figure are based on remote-sensing literature, while the other literature defines the wavelength as: NIR: 0.7 to (2.5 - 5) Am, MIR: (2.5 - 5) to (25 - 40) Am and FIR: (25 - 40) to 1000 Am.

S I Evtushenko et al 2020 Identification of soils, grounds and lands strata using the acoustic spectral analysis. *IOP Conf. Ser.: Mater. Sci. Eng.* **913** 052043

#### SOIL ACOUSTIC SPECTRUM



Amplitude, VHF

#### MANY NEW KINDS OF SOIL SPECTRA REMAIN TO BE EXPLORED



Soil inference

The prediction of a property or properties from other soil property or properties

# **SOIL SPECTRAL INFERENCE** Soil spectral inference The prediction of a property or properties from a spectrum or spectra (direct) or from other soil property or properties predicted from the spectrum or spectra (indirect)

### Soil inference system

### A software engine for the systematic prediction of a property or properties from other soil properties

Soil spectral inference system

A software engine for the systematic prediction of a property or properties from a spectrum or spectra (direct) or from other soil property or properties predicted from the spectrum or spectra (indirect)

### Soil spectral inference system

### (Simpler definition)

# A soil inference system driven (solely or mainly) from soil spectra

McBratney, A.B., Minasny, B. Viscarra Rossel R.A. 2006. Spectral soil analysis and inference systems: A powerful combination for solving the soil data crisis. Geoderma 136, 272-278.

#### EXPLANATION & DEMONSTRATION OF SOIL INFERENCE SYSTEM & SOIL SPECTRAL INFERENCE SYSTEM



Combination of Spectroscopy and Pedotransfer Functions in a Soil Spectral Inference System can improve predictability

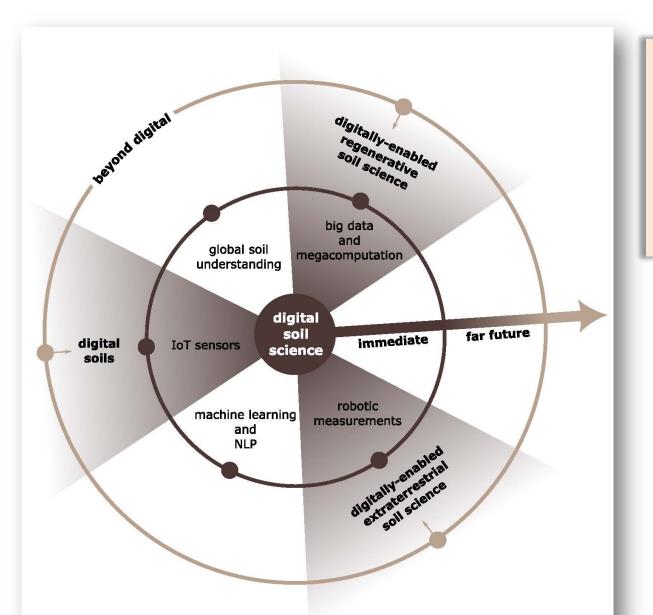
SOIL CONDITION & <u>CAPACITY</u> Indicators and MIR spectrometry

Biological	Chemical	Physical
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Poorly Estimated by MIR, Reasonably Estimated by MIR, Well Estimated by MIR



#### **SOIL SPECTRA & DIGITAL SOIL SCIENCE**



Wadoux, A.M.J-C., & McBratney, A.B. Digital soil science and beyond. (2021) Soil Science Society of America Journal. <u>https://acsess.onlinelibrary.wiley.com/doi/full</u> /10.1002/saj2.20296 Fig 3

# **Routine Lab Spectroscopy**

Laboratory spectroscopy (on whole soil samples)

UV Vis NIR MIR /(FTIR) XRF LIBS LIFS Raman

Issues

Sample preparation Calibration

#### **Sample preparation**

UV Vis NIR MIR /(FTIR) XRF LIBS LIFS Raman

Drying

Grinding (size?)

#### Calibration

UV Vis NIR MIR /(FTIR) XRF LIBS LIFS Raman



James Hutton Institute, Scotland

How local? How global? How many?

# **Routine Field Spectroscopy**

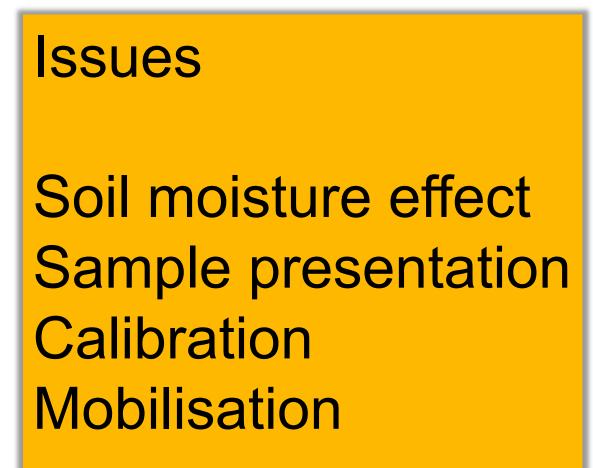
#### "Soil Sensing" Principle

Given real and significant natural soil variation in the field, a plethora of low cost, low precision soil data can produce high-value spatialised soil information

# Spectroscopy is one way of generating such data

#### Mobile field spectroscopy (many possibilities)

Gamma radiometrics Ground-penetrating radar Portable NIR Portable XRF MIR EMI?/ mag sus **UV Vis NIR** MIR /(FTIR) XRF LIBS LIFS Raman



#### Soil moisture effect

Gamma radiometrics Ground-penetrating radar Portable NIR Portable XRF MIR EMI?/ mag sus UV Vis NIR MIR /(FTIR) XRF LIBS LIFS Raman

# Likely to offer most interference

Affects some more than others

Remove effect by various algorithmic means

### Sample presentation

Gamma radiometrics Ground-penetrating radar Portable NIR Portable XRF MIR EMI?/ mag sus **UV Vis NIR** MIR /(FTIR) XRF LIBS LIFS Raman

A 44 A 44

### In situ or Ex situ

### Homogenisation

Lateral or Vertical travel



Gamma radiometrics Ground-penetrating radar Portable NIR Portable XRF MIR EMI?/ mag sus UV Vis NIR MIR /(FTIR) XRF LIBS LIFS Raman

More challenging than lab

Is global calibration feasible?

### **Mobilisation**

Gamma radiometrics Ground-penetrating radar Portable NIR Portable XRF MIR EMI?/ mag sus UV Vis NIR MIR /(FTIR) XRF LIBS LIFS Raman

### **Vertical probe**

### Autonomous vehicle

Autonomous very low flying aircraft

Endochoric soil probe



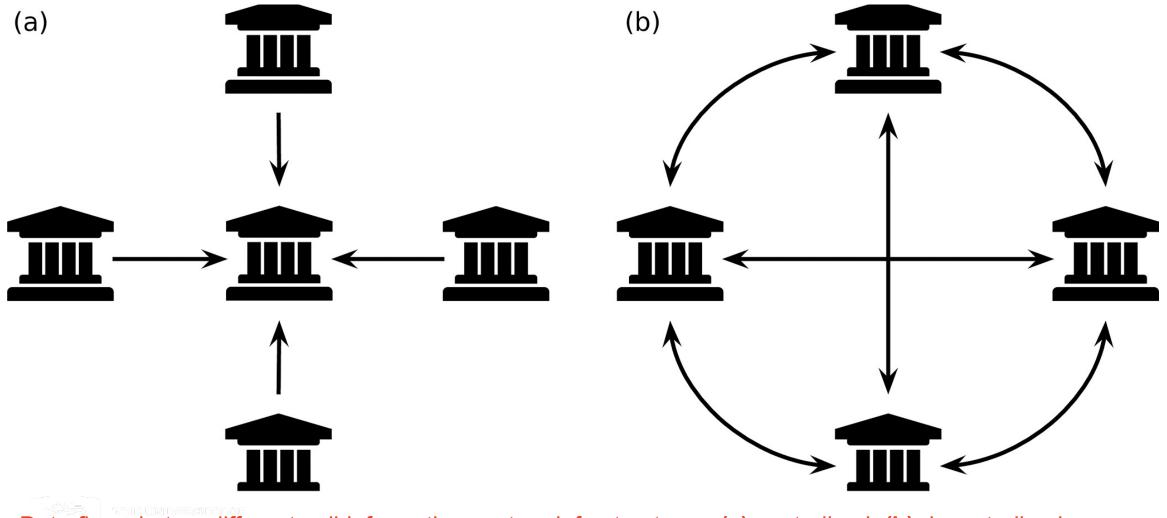
## organo-digital

## Chemometrics/Pedometrics Interface

### Spectral Data Sharing & Calibration



#### José Padarian and Alex B. McBratney 2020. A new model for intra- and inter- institutional soil data sharing. Soil 6, 89–94.

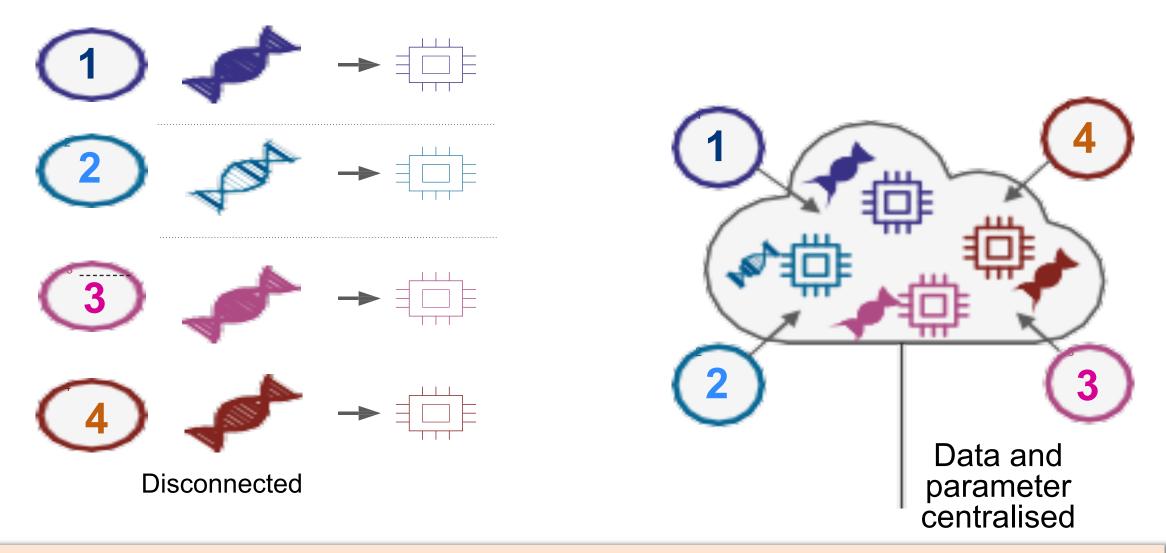


Data flows in two different soil information system infrastructures: (a) centralised; (b) decentralised.

Potential use case discussed: global soil spectral library

### Local learning

### **Central learning**

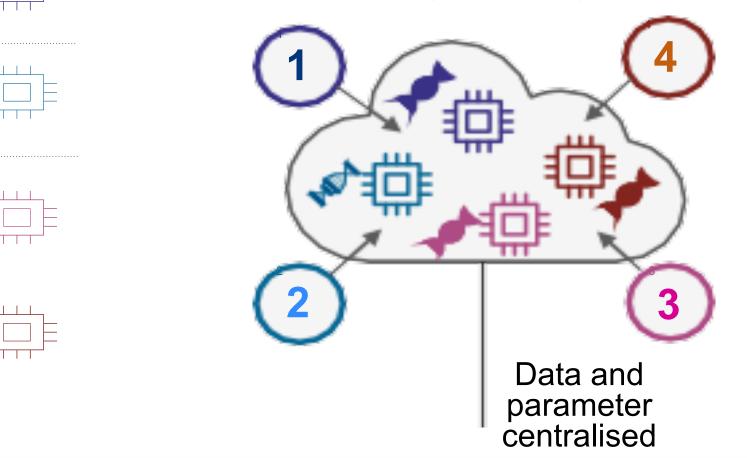


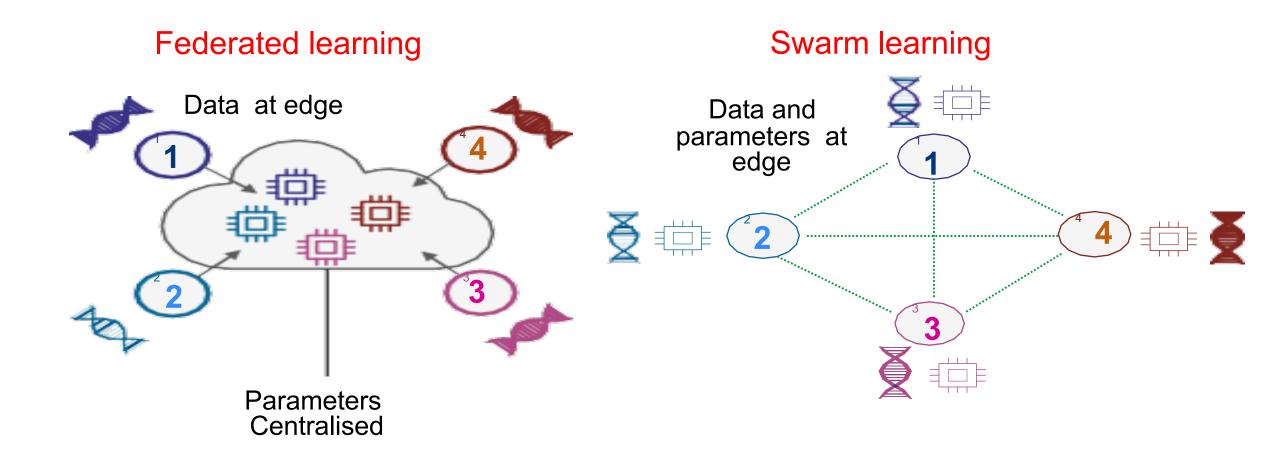
### Local learning

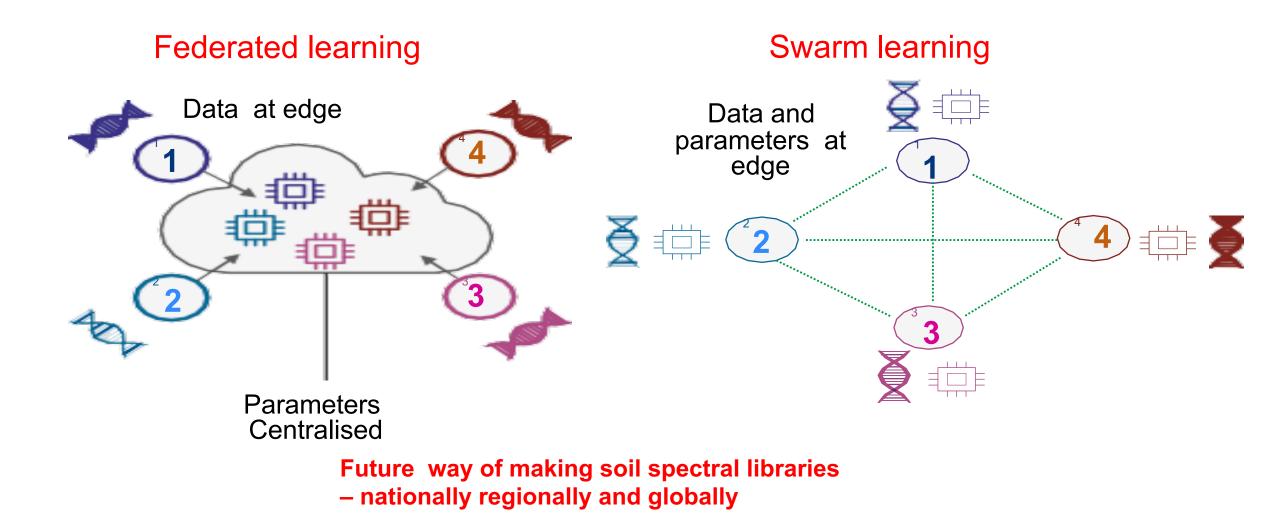
Disconnected

### **Central learning**

Current way of making soil spectral libraries – nationally regionally and globally







### **Spectra for Soil Classification & Identification**

The biggest challenge for the future in which soil spectroscopy can play a crucial role

## A formal global digital quantitative system of soil classification

We don't have it

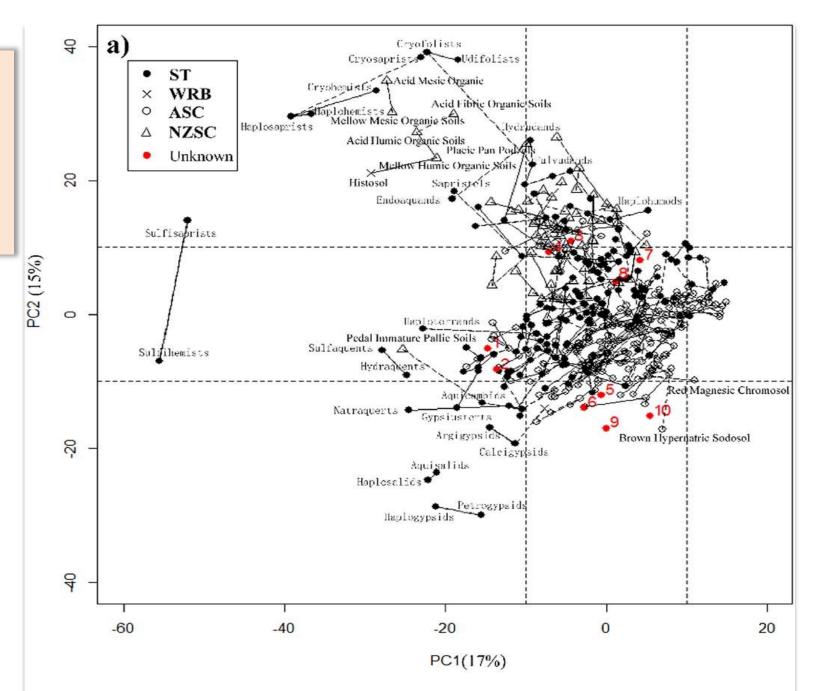
### 23 soil variables

Category	Variable
Physical (7)	coarse fractions, clay, silt and sand contents, water content, ice content, bulk density
Chemical (13)	organic carbon content, carbonate content, pH, cation exchange capacity, exchangeable cations (Ca, Na, Mg, K), acid saturation, base saturation, exchangeable sodium percentage, electrical conductivity, and gypsum content
Morphological (3)	soil colour expressed in L, a, b or red, green and blue

## All derivable (in the field\* or lab) from MIR/NIR soil spectra



Hughes, P. et al 2017. Creating a novel comprehensive soil classification system by sequentially adding taxa from existing systems. Geoderma Regional 11, 123-140.



## CAVEAT EMPTOR

## Danger Will Robinson



### ARTIFICIAL INTELLIGENCE

A field of science that is primarily concerned with getting computers to do tasks that would normally require human intelligence.



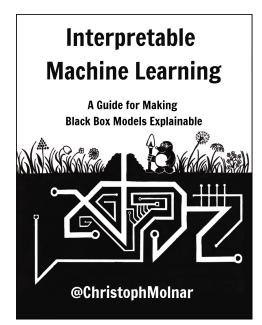
### MACHINE LEARNING

A set of algorithms that allow computers to learn from data without being explicitly programmed



A more recently developed set of learning techniques

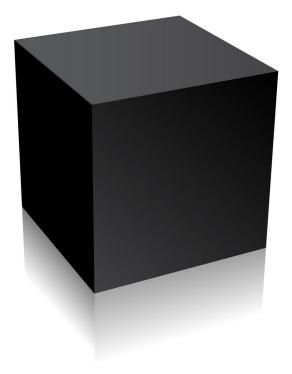
> Phote Credit; From Noun Project by ImageCatalog, Becris and Dispitivust



## Interpretation of the machine-learned spectral soil prediction models

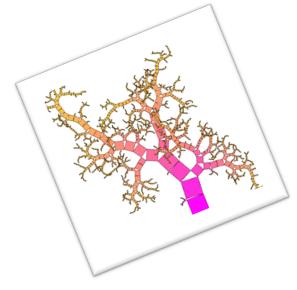
Can we interpret the models? If we can't then ...?

### **Proprietary soil prediction**



### AgTech SoilTech ENVTECH

### **Proprietary soil prediction**



Do we need to know what is inside the black box?

**Does it make sense?** 

AgTech SoilTech ENVTECH

### **Doing too much with too little?**

Please don't overfit or overstretch the data

Spectral predictions calibrated with too few observations are not predictive

Spectral predictions using calibrations models with too many parameters with respect to the data are not predictive



 There are many kinds of spectroscopy that are potentially useful for the rapid generation of soil information on whole soil – many are largely un-investigated.

2. MIR, NIR pXRF and Gamma radiometry are the most deployable at present for whole soil

 Soil spectral inference systems will be the principal mode of operation – applicable to laband field-based systems

4. In the lab, calibrations will be developed for many hundreds of soil properties using federated and swarm learning

5. In the field, spectrometers of various kinds will be deployed on autonomous platforms to update a wide array of dynamic soil properties important for monitoring soil condition ('health')

6. Principal applications will be for real-time agronomic and environmental decision-making including soil classification and diagnosis, soil monitoring Would you like to say something new? We would like to hear it

Publish in the new soil security journal

https://www.sciencedirect.com/journal/Soil-Security

We are currently developing a Special Issue on Soil Spectroscopy for Soil Condition and Capability

Contact alexandre.wadoux@sydney.edu.au





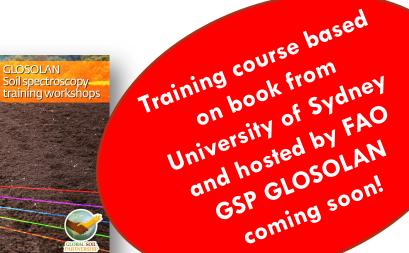
# SCURITY



### Training Course coming soon...

An overview of techniques for inferring information from soil spectroscopic data supported by a suite of software coded in R for performing these analyses.





#### **Progress in Soil Science**

Alexandre M.J.-C. Wadoux Brendan Malone · Budiman Minasny Mario Fajardo · Alex B. McBratney

### Soil Spectral Inference with R

Analysing Digital Soil Spectra using the R Programming Environment

Springer

https://github.com/AlexandreWadoux/soilspec



### THE PEAK BODY FOR THE WORLD'S SOIL SCIENTISTS



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Food and Agriculture Organization of the United Nations GLOSOLAN Soil spectroscopy training workshops

## THANK YOU 0

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Online webinars



## **Questions?**