INFRARED SPECTROSCOPY FOR RAPID AND ACCURATE MEASUREMENT OF SOIL PROPERTIES

Budiman Minasny

Wartini Ng, Edward Jones, Alex. McBratney, José Padarian, Alexandre Wadoux



FAO GLOSOLAN Webinar 16 September 2021



ACKNOWLEDGEMENT OF THE COUNTRY

I would also like to acknowledge the Gadigal People of the Eora Nation on who's land I am standing today. As the traditional custodians of Australia, they have a long and rich history of caring for the country.







CONTENTS

- (Vis) NIR Applications
- NIR in the field
- Some words about calibration and accuracy
- MIR for accurate lab measurements



NIR APPLICATIONS IN Soll Science

Potential of Low Cost Infrared Spectrometer





Evaluating low-cost portable near infrared sensors for rapid analysis of soils from South Eastern Australia Y Tang, E Jones, B Minasny - Geoderma Regional, 2020



Evaluating low-cost portable near infrared sensors for rapid analysis of soils from South Eastern Australia Y Tang, E Jones, B Minasny - Geoderma Regional, 2020



Developing a soil spectral library using a low-cost NIR spectrometer for precision fertilization in Indonesia



Wartini Ng ^{a,*}, Husnain ^c, Linca Anggria ^b, Adha Fatmah Siregar ^b, Wiwik Hartatik ^b, Yiyi Sulaeman ^c, Edward Jones ^a, Budiman Minasny ^a



Table 4

	Calibration		Validation			
Properties	R ²	RMSE	bias	R ²	RMSE	bias
Sand (%)	0.62	12.59	-1.1	0.45	15.2	-0.28
Silt (%)	0.38	11.49	-0.46	0.22	13.14	-0.26
Clay (%)	0.67	11.63	-0.15	0.52	14.22	0.57
pH _{H₂O}	0.71	0.61	-0.02	0.6	0.72	0
pH _{KCl}	0.68	0.58	-0.04	0.54	0.69	-0.01
C _{Organic} (%)*	0.73	0.23	-0.01	0.57	0.29	0
Total N (%)*	0.69	0.04	0	0.52	0.05	0
C/N	0.3	2.69	-0.33	0.12	3.15	-0.01
Potential P (mg 100 g ⁻¹)*	0.62	0.63	0.04	0.47	0.74	0.01
Potential K (mg 100 g ⁻¹)*	0.56	0.74	-0.06	0.44	0.84	0.01
Available P Olsen (mg kg ⁻¹)*	0.33	0.78	-0.04	0.09	0.94	0.02
Available P Bray (mg kg ⁻¹)*	0.42	0.74	-0.08	0.3	0.82	0.01
Available K Morgan (mg kg $^{-1}$)*	0.24	0.81	-0.05	0.08	0.9	-0.03
P retention (%)	0.89	10.55	0.28	0.75	16.14	-0.66
Exchangeable Ca $(cmol(+) kg^{-1})$	0.81	6.75	-0.7	0.71	8.32	0.17
Exchangeable Mg (cmol(+) kg ⁻¹)	0.72	3.08	-0.38	0.59	3.66	0.1
Exchangeable K (cmol(+) kg ⁻¹)	0.29	0.34	-0.08	0.19	0.35	0.01
Exchangeable Na $(cmol(+) kg^{-1})$	0.45	1.8	-0.23	0.24	2.16	0
Sum of bases $(cmol(+) kg^{-1})$	0.83	7.85	-0.5	0.72	9.99	0.2
$CEC(cmol(+) kg^{-1})$	0.66	5.79	-0.4	0.54	6.77	0.14
Base saturation (%)	0.74	15.64	0.95	0.57	20.38	0.85

Predictive performance of the NeoSpectra NIR spectrometer using the Cubist model.

 R^2 – coefficient of determination, RMSE – root mean squared error.

Subjected to log-transformation.

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Smart Soil Sensor Kit Ver 1.1



Canning Data Unsur Info Lok	asi Observasi Rekomendasi Punuk Export Data	
No Form	No Obs	
Mapping Unit	Tahun	
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Pengirim	Kecamatan	
Koordinat	Provinsi	
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Chemometric predictions	
Sand (%)	78.1
Silt (%)	2.6
Clay (%)	19.3
$pH_{H_{2}O}$	5.91
Organic carbon (%)	0.46
Total N (%)	0.1
P retention (%)	18.92
$CEC(cmol(+)kg^{-1})$	9.21
Potential P (mg 100 g ⁻¹)	Low
Potential K (mg 100 g ⁻¹)	Low
Available P Bray (mg kg ⁻¹)	Low
Available K Morgan (mg kg ⁻¹)	Low
Exchangeable K (cmol(+) kg ^{-1})	Low



Smart Soil Sensing Kit Ver 1.1

- S3K Ver 1.1 launched in 2021.
- This new version is built with android system-based program.





From Spectra to Fertilizer Recommendation







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NEAR INFRARED FOR FIELD SOIL INFERENCE



(Dematte er al. 2004)

SCANNING IN-SITU USING VISNIR SPECTROMETER





Predict



E.Jones. Proximal sensing in soil profiles

SOIL SPECTRAL INFERENCE SYSTEM

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E.Jones. Proximal sensing in soil profiles



MINERAL COMPOSITION

Site A Site **B** Site C 0 0 Quartz 25 25 25 Smectite 50 50 50 e Kaolinit CaCO₃ 75 75 75

Legend Ka 🗖 Sm 🗆 II 📕 He 🗖 Go 🗆 Ca 🗖 Q

SPEC-SINFERS PREDICTED VOLUMETRIC RELATIONS.



Unavailable water Available water Air-filled porosity Soil solids

E.Jones. Proximal sensing in soil profiles



E.Jones. Proximal sensing in soil profiles

NIR PENETROMETER





Murad et al. (The University of Sydney) A VisNIR Penetrometer System For Predicting Soil Carbon Under Australian Conditions





Murad et al. (The University of Sydney) A VisNIR Penetrometer System For Soil Carbon AUDIT Under Australian Conditions



MIR FOR LAB Soll Analysis

MIR SPECTROSCOPY FOR LAB ANALYSIS





(Zhang et al. 2019)

NIR

MIR



Robust field use, spectra not affected too much by field conditions

Overtone, broad & diffuse peaks

Suitable for field analysis

Not robust for field use, spectra affected too much by the environment & surface roughness

Fundamental molecular vibrations, well-defined peaks

Suitable for lab analysis



Nguyen et al. (1991)

MIR SPECTROSCOPY FOR LAB ANALYSIS

After 23 years

Australian Journal of Experimental Agriculture, 1998, 38, 681-96

Can mid infrared diffuse reflectance analysis replace soil extractions?

L. J. Janik^{AB}, R. H. Merry and J. O. Skjemstad^A

^A CSIRO, Land and Water, PMB No. 2, Glen Osmond, SA 5064, Australia.
^B Corresponding author; e-mail: les.janik@adl.clw.csiro.au

Summary. Recent developments in infrared spectroscopy and computer software, together with decreasing spectrometer costs, have resulted in an increase in the potential for soil analysis. Infrared spectroscopy in both the near and mid infrared ranges allows rapid acquisition of soil information at quantitative and qualitative, or indicator, levels for use in agriculture and environmental monitoring. In this paper, we describe how mid infrared diffuse reflectance analysis can provide results comparable in accuracy

with many traditional extractive and digestion laboratory methods in soil studies, with the possibility of either replacing or enhancing them. Examples are given for estimation of lime requirement, organic carbon, exchangeable cations, air-dry moisture, clay content and biological indicators. Infrared methodology appears to have advantages in facilitating some soil analyses that are otherwise very time-consuming or expensive, or where spatially dense data is required.

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CALIBRATION & ACCURACY

CALIBRATION

Spectra

Calibration Functions

İ()

Soil properties



Soil texture pH OC CaCO₃ CEC K, Ca, Mg N,P

. . .

CALIBRATION

Relating spectra to soil properties

If the Beer Lambert's law was observed :



Univariate Calibration $a = a_0 + kC + e$

CALIBRATION METHODS



Since the Beer Lambert's law is not observed,

The shape of the spectra Is more meaningful than Reflectance at particular wavelengths

Multivariate Calibration

(using the whole spectra)

CALIBRATION

Linear models



MULTIVARIATE CALIBRATION

• Problems :

- The spectra are highly correlated
- There can be more variables than number of samples (large p, small n)
- Some solutions:
 - Reducing the dimension of X via calculation of latent variables
 - Variables selection
- Methods:
 - Linear multivariate methods, e.g. PLS
 - Machine learning methods



PCA

Principal component analysis





Spectra

Residuals scores (new descriptors)

PARTIAL LEAST SQUARES (PLS)

- PLS regression decomposes both X and Y as a product of a common set of orthogonal factors and a set of specific loadings (Wold, 1960)
- Then set up a regression model between the scores and **Y**.

ACURACY ASSESSMENT

Statistics

Root-mean square error (accuracy)

In the NIR literature it is called SEP (standard error of prediction)

$$MSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}$$

Mean error (bias)

 $ME = \sum_{i=1}^{n} (y_i - \hat{y}_i)$



STANDARD ERROR OF PREDICTION



Std Err of Prediction (SEP)=RMSE

95% of the errors are in [BIAS-2*SEP; BIAS+2*STD]

COEFFICIENT OF DETERMINATION, R²

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$$R^{2} = 1 - \frac{SS_{residual}}{SS_{total}}$$

$$SS_{total} = \sum_{i} (y_i - \bar{y})^2$$

$$SS_{residual} = \sum_{i} (y_i - \hat{y}_i)^2$$

PREDICTION QUALITY

Lin's Concordance correlation coefficient

- Lin (1989)
- Evaluates agreement between pairs of observations by measuring variation from the 45° line

$$\rho_c = \frac{2 \sigma_{12}}{\sigma_1^2 + \sigma_2^2 + (\mu_1 - \mu_2)^2}$$



Be careful when you only Read conclusions...

Reference: The Anscombe's quartet, 1973

Designed by @YLMSportScience



THESE FOUR DATASETS HAVE IDENTICAL MEANS, VARIANCES & CORRELATION COEFFICIENTS

Property	Value
Mean of x	9
Sample variance of x	11
Mean of y	7.50
Sample variance of y	4.125
Correlation between x and y	0.816
Linear regression line	y = 3.0 + 0.5x
Coefficient of determination R ²	0.667
Lin's concordance correlation coefficient between x and y	0.633

https://en.wikipedia.org/wiki/Anscombe%27s_quartet



Std. dev = 0.72 RMSE = 0.74 RPD = 0.97 CCC = 0.41 N=23

HOW TO LIE WITH RPD & R²



Std. dev = 4.55 RMSE = 1.60 RPD = 2.83 CCC = 0.89 N=25

MIR FOR ACCURATE Soll measurements

USDA-KSSL DATABASE



- Kellogg Soil Survey Laboratory (KSSL) database.
- Contained measurements of>17,000 pedons from the USA with welldocumented and precise standard operating procedures.
- MIR & Soil analysis

MODEL CALIBRATION

• Memory Based Learning (Local) PLS Regression Method



Ng, W., Minasny, B., Montazerolghaem, M., Padarian, J., Ferguson, R., Bailey, S. and McBratney, A.B., 2019. Convolutional neural network for simultaneous prediction of several soil properties using visible/near-infrared, mid-infrared, and their combined spectra. *Geoderma*, *352*, pp.251-267.

DEEP LEARNING: CNN





WHAT OTHER SOIL PROPERTIES THAT CAN BE WELL PREDICTED?

- \sim 200 soil physical, chemical & biological properties

• WE ONLY MODEL MINERAL SOILS!

ACCURACY ASSESSMENT

Accuracy	\mathbf{R}^2	Concordance	RPIQ	St. Bias
	0.901		2.353	
A	(0.82-0.99)	0.946	(0.82-1.85)	0.001
	0.847		1.263	
В	(0.76-0.86)	0.915	(0.54-1.71)	0.001
	0.665		0.821	
С	(0.58-0.74)	0.800	(0.20-1.34)	0.007
	0.486		0.490	
D	(0.10-0.60)	0.659	(0.02-1.10)	0.029

Multiple criteria:

R² = variance explained Concordance: agreement at 1:1 line RPIQ = Interquartile range/RMSE

St. Bias = Bias/Interquartile range

SOIL CHEMICAL PROPERTIES

Proposition

- Properties related to soil mineral components and surface chemistry can be well predicted (infrared-responsive chromophores)
- Properties related to soil solution (extraction) chemistry cannot be well predicted
- Elements in high concentration and related to soil minerals can be well predicted



MEHLICH EXTRACTION

Properties	units	Accuracy	R 2	RMSE	1						
Calcium, Element Mehlich3 Extractable	mg/kg	В	0.928	1056.672	0 9					• ,	•
Aluminum, Element Mehlich3 Extractable	mg/kg	A	0.948	157.099	0.5					•	
Magnesium, Element Mehlich3 Extractable	mg/kg	В	0.869	149.077	0.0		•				
Barium, Element Mehlich3 Extractable	mg/kg	В	0.810	26.118	0.7	• • •	•••		•	•	
Silicon, Element Mehlich3 Extractable	mg/kg	С	0.688	122.599					•		
Potassium, Element Mehlich3 Extractable	mg/kg	D	0.502	65.888	20.5						
Iron, Element Mehlich3 Extractable	mg/kg	С	0.582	42.124	0.4	•					
Sodium, Element Mehlich3 Extractable	mg/kg	С	0.614	102.009	0.3						
Manganese, Element Mehlich3 Extractable	mg/kg	С	0.663	32.772	0.2						
Strontium, Element Mehlich3 Extractable	mg/kg	С	0.793	9.918	0.1						
Phosphorus, Element Mehlich3 Extractable	mg/kg	D	0.502	13.779	0						
Copper, Element Mehlich3 Extractable	mg/kg	С	0.718	0.858	C C) 1	1	10	100	1000	10000
Zinc, Element Mehlich3 Extractable	mg/kg	С	0.665	0.697		/. L	Ŧ	10	100	1000	10000
Arsenic, Element Mehlich3 Extractable	mg/kg	С	0.611	0.790				IQ	R		
Lead, Element Mehlich3 Extractable	mg/kg	С	0.671	0.432			Inte	rquar	tile ra	ange	
Cobalt, Element Mehlich3 Extractable	mg/kg	С	0.662	0.308	(nnm)						
Nickel, Element Mehlich3 Extractable	mg/kg	С	0.647	0.290	(ppm)						
Cadmium, Element Mehlich3 Extractable	mg/kg	С	0.654	0.061							
Chromium, Element Mehlich3 Extractable	mg/kg	D	0.516	0.046							
Molybdenum, Element Mehlich3 Extractable	mg/kg	D	0.346	0.045							

PHOSPHORUS

Properties	units	Accuracy	R2	RMSE
Phosphorus, P Retention	%	A	0.928	6.750
Phosphorus, Water Soluble	mg/kg	D	0.387	0.130
Phosphorus, Bray-1 Extractable	mg/kg	С	0.590	12.902
Phosphorus, Olsen Extractable	mg/kg	D	0.562	7.499
Phosphorus, Mehlich3 Extractable	ma/ka	D	0.524	12.842



ELEMENTAL CONCENTRATION



Properties	units	Accuracy	R2	RMSE
Siligon Major Flomont	ma/ka	π	0 991	20205 514
Aluminum Major Flomont	mg/kg	Π	0.001	5060 //9
Potossium Major Element	mg/kg	π	0.090	2020.005
Sodium Major Element	mg/kg	π	0.004	1701.000
Vanadium Traco Flomont	mg/kg	Л	0.001	0.274
Parallium Trace Element	mg/kg	Π	0.010	0.166
Iron Major Flomont	mg/kg	P	0.010	5014 026
Coloium Major Element	mg/kg	D	0.910	1020 720
Magnagium Major Element	mg/kg	D	0.900	1719 701
Titanium Major Floment	mg/kg	D	0.000	011 616
Deepherus Major Element	mg/kg	D	0.011	167.015
Priosphorus, Major Element	mg/kg	D	0.190	101.010
Strentium Major Floment	mg/kg	D	0.104	44.400
Zirzenium Major Element	mg/kg	D	0.040	41.002
Zincomuni, Major Element	mg/kg	D	0.011	12 752
Streptium Trace Element	mg/kg	D	0.010	10.100
Strontium, Irace Element	mg/kg	B	0.831	16.493
Chromium, Trace Element	mg/kg	B	0.840	0.020
Nickel, Trace Element	mg/kg	В	0.195	5.236
	mg/kg	В	0.802	4.819
Lead, Trace Element	mg/kg	В	0.760	3.565
Cobalt, Trace Element	mg/kg	В	0.829	1.955
Tin, Trace Element	mg/kg	В	0.792	0.238
Manganaga Majar Flomont	ma/lta	C	0.654	022 720
Solonium Traco Flomont	ng/kg	C	0.004	176 124
Manganaga Traga Floment	ug/kg	C	0.002	172 076
Manganese, mace Element		C	0.000	16.416
	ug/ kg	G	0.001	10.410
Arsenic, Trace Element	mg/kg	C	0.713	1.953
Molybdenum, Trace Element	mg/kg	C	0.609	0.434
Cadmium, Trace Element	mg/kg	C	0.647	0.093
Silver, Trace Element	mg/kg	C	0.708	0.039
Antimony, Trace Element	mg/kg	D	0.458	0.148
Tungsten, Trace Element	mg/kg	D	0.442	0.029

GEOCHEMICAL CONCENTRATION

Total Silica



Landré, A., Saby, N.P.A., Barthès, B.G., Ratié, C., Guerin, A., Etayo, A., Minasny, B., Bardy, M., Meunier, J.D. and Cornu, S., 2018. Prediction of total silicon concentrations in French soils using pedotransfer functions from mid-infrared spectrum and pedological attributes. *Geoderma*, 331, pp.70-80.

SATURATION EXTRACT

Properties	units	Accuracy	R2	RMSE
Electrical Conductivity, Saturation Extract	dS/m	С	0.685	2.065
Electrical Conductivity, Predict, 1:2 (w/w)	dS/m	D	0.783	0.887
Acetate, Saturation Extract	mmol(-)/L	D	0.290	0.151
Bicarbonate, Saturation Extract	mmol(-)/L	С	0.628	1.003
Bromide, Saturation Extract	mmol(-)/L	D	0.079	0.026
Calcium, Saturation Extract	mmol(+)/L	С	0.645	5.602
Chloride, Saturation Extract	mmol(-)/L	D	0.675	13.132
Fluoride, Saturation Extract	mmol(-)/L	D	0.195	0.085
Magnesium, Saturation Extract	mmol(+)/L	С	0.668	8.818
Nitrate, Saturation Extract	mmol(-)/L	D	0.392	2.168
Nitrite, Saturation Extract	mmol(-)/L	D	0.286	0.458
Ammonium, Saturation Extract	mmol(+)/L	D	0.364	0.405
Potassium, Saturation Extract	mmol(+)/L	D	0.408	0.454
Sodium, Saturation Extract	mmol(+)/L	D	0.703	17.386
Sulfate, Saturation Extract	mmol(-)/L	С	0.653	18.416

Carbon, Total NCS

SOIL ORGANIC MATTER

Properties	units	Accuracy	R ²	RMSE
Carbon, Total	% wt	A	0.97	0.42
Organic C	% wt	A	0.93	0.65
C, KMnO ₄ extract	mg kg ⁻¹	A	0.92	84.47
Nitrogen, Total	% wt	В	0.90	80.0
Sulfur, Total	% wt	D	0.64	0.10
Carbon, hpom	% wt	В	0.90	0.18
Nitrogen, hpom	% wt	С	0.71	0.03
Sulfur, hpom	% wt	С	0.72	< 0.01
ß-Glucosidase	mg kg ⁻¹ hr ⁻¹	В	0.81	32.78



observed



ttps://www.nrel.colostate.edu/investigator/francesca-cotrufo-homepage/francesca-cotrufo-research.



SOIL PHYSICAL PROPERTIES

Proposition

- Properties based on the soil solid composition and surfaces can be predicted well predicted
- Properties based on pore-space relationships cannot be well predicted



^bDepartment of Environment and Climate Change, Cowra, New South Wales 2794, Australia

AGGREGATE & BULK DENSITY

Properties	units	Accuracy	R 2	RMSE
Aggregate Stability, 0.5-2mm Aggregates	% wt	С	0.656	18.331
Bulk Density, <2mm Fraction, 1/3 Bar	g/cc	С	0.683	0.106
Bulk Density, <2mm Fraction, Ovendry	g/cc	С	0.694	0.114
Bulk Density, Core, <2 mm fraction, Field				
Moist	g/cc	С	0.616	0.212



Field



MIR Lab analysis

Bulk Density, <2mm Fraction, Ovendry



observed

WATER RETENTION

Properties	units	Accuracy	R2	RMSE
Water Retention, 0.06 Bar, <2mm Clod	% wt	С	0.587	4.594
Water Retention, 1/10 Bar, <2mm Clod	% wt	С	0.694	6.287
Water Retention, 1/3 Bar, <2mm Clod	% wt	С	0.715	4.287
Water Retention, 0.06 Bar, <2mm Sieve	% wt	A	0.808	4.971
Water Retention, 1/10 Bar, <2mm Sieve, Air-dry	% wt	A	0.836	4.489
Water Retention, 1/3 Bar, <2mm Sieve	% wt	A	0.892	3.205
Water Retention, 1 Bar, <2mm Sieve, Air-dry	% wt	A	0.912	2.408
Water Retention, 2 Bar, <2mm Sieve, Air-dry	% wt	A	0.905	2.278
Water Retention, 5 Bar, <2mm Sieve, Air-dry	% wt	A	0.864	2.585
Water Retention, 15 Bar, <2mm, Air-dry	% wt	A	0.907	1.854
Volumetric water content at 1/3 Bar	% vol	С	0.653	4.327
Volumetric water content at 15 Bar	% vol	В	0.851	3.493
Field Water Content, <2mm	% wt	В	0.755	4.569
Field Water Content, Core	% wt	С	0.681	25.177







Water Retention, 1/3 Bar, <2mm Clod

SOIL QUALITY INDICATORS

Biological	Chemical	Physical
Microbial Biomass	pH	Rooting Depth
Mycorrhiza populations	CEC	Stoniness
Particulate Organic Matter	Heavy Metals	Texture
Respiration	EC	Aggregate Stability
Potential N mineralization	Organic C & N	Slaking Index
Fatty Acid profiles	Extractable macronutrients	Water holding capacity
Soil enzymes	Total elements,	Bulk Density
	Micronutrients	
	CaCO ₃	Infiltration
	P retention	Penetration resistance

Poorly estimated, reasonably estimated, Well Estimated

Quantitative Evaluation of Soil Functions: Potential and State

		inherent							affected										
		bydrol site				soil					nhysics				chem h		hi	ol	
											pity	5105		CIIC		DI			
	ES	tion period	tion period																
	SOIL & SITE ATTRIBUTI	water balance (vegeta	depth to groundwater	temperature	slope aspect	slope gradient	soil depth (rootable)	texture	mineralogy	caCO ₃	coarse fragments	oulk density	air capacity	olant available water	nydraulic conductivity	soc	Н	earthworm abundance	species diversity
SOIL FUNCTIONS											_								
Production (fertility)																			
Nutrient cycling – mobilization & buffering																			
Carbon storage																Х			
Water storage & filtering												Х							
Habitat for biological activity																			X

https://www.frontiersin.org/articles/10.3389/fenvs.2019.00164/full

SUMMARY

- MIR offers a rapid and highly accurate measurement of many soil physical and chemical properties
- Properties related to soil mineral components and surface chemistry can be well predicted (infrared-responsive chromophores)
- Properties related to soil solution (extraction) chemistry cannot be well predicted.
- Properties based on soil solid composition and surfaces can be predicted well predicted.
- Properties based on pore-space relationships cannot be well predicted. However MIR can be used as a better alternative to PTFs

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

JUST PUBLISHED

Soil Spectral Inference with R

• Springer (2020)



ACKNOWLEDGEMENT

Indonesian Center for Agricultural Land Resources Research and Development(ICALRD)

United States Department of Agriculture Natural Resources Conservation Service Soil and Plant Science Division National Soil Survey Center Kellogg Soil Survey Laboratory

