Cost-efficient spectroscopy for soil analyses

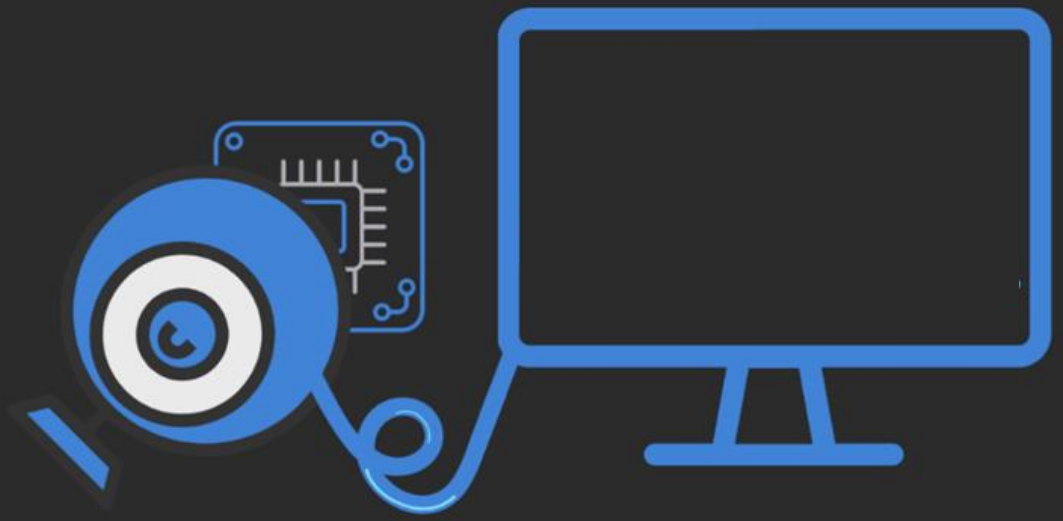
TropiRes – Summer School – Uganda, 2024

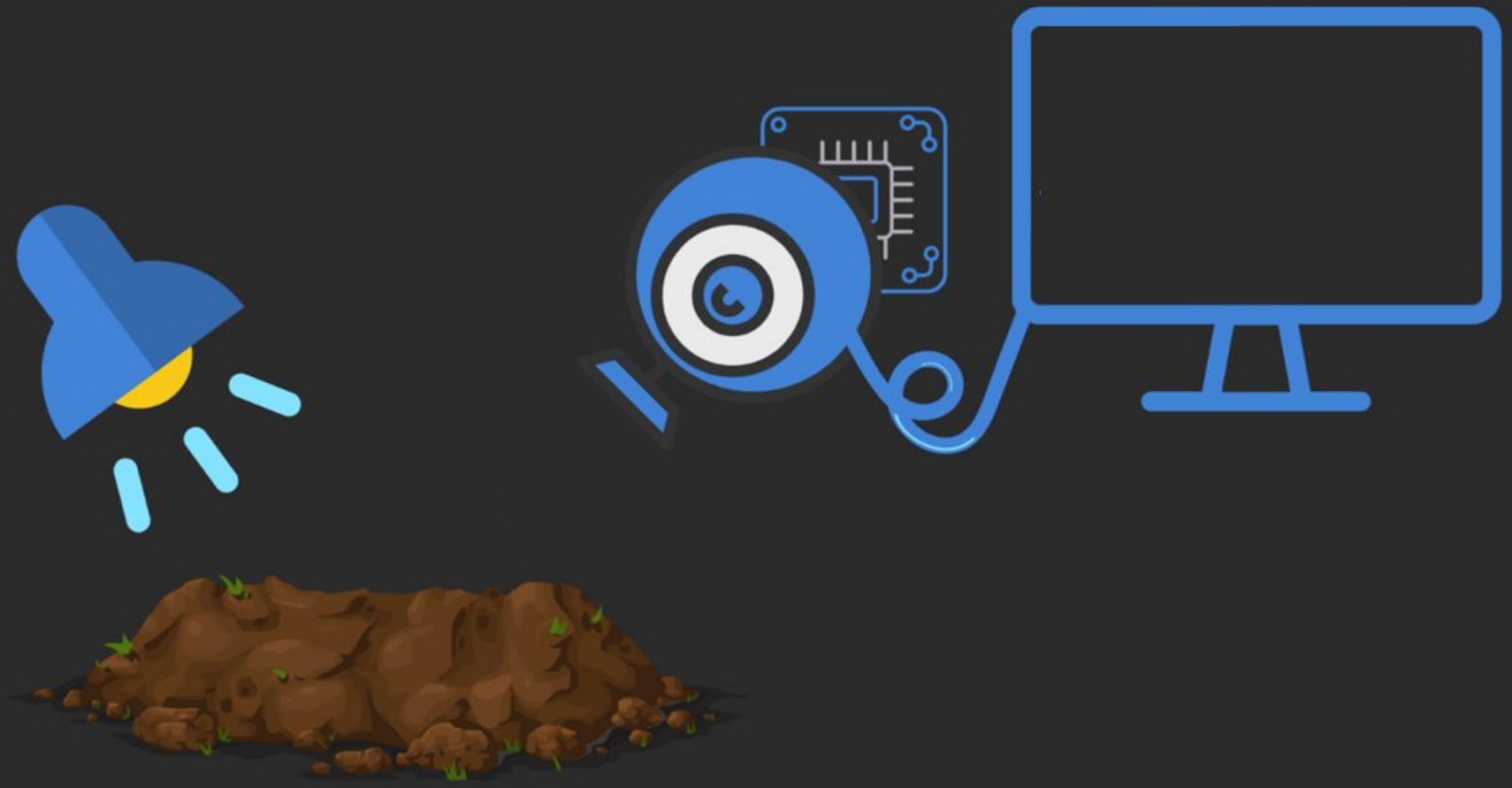
Workshop II

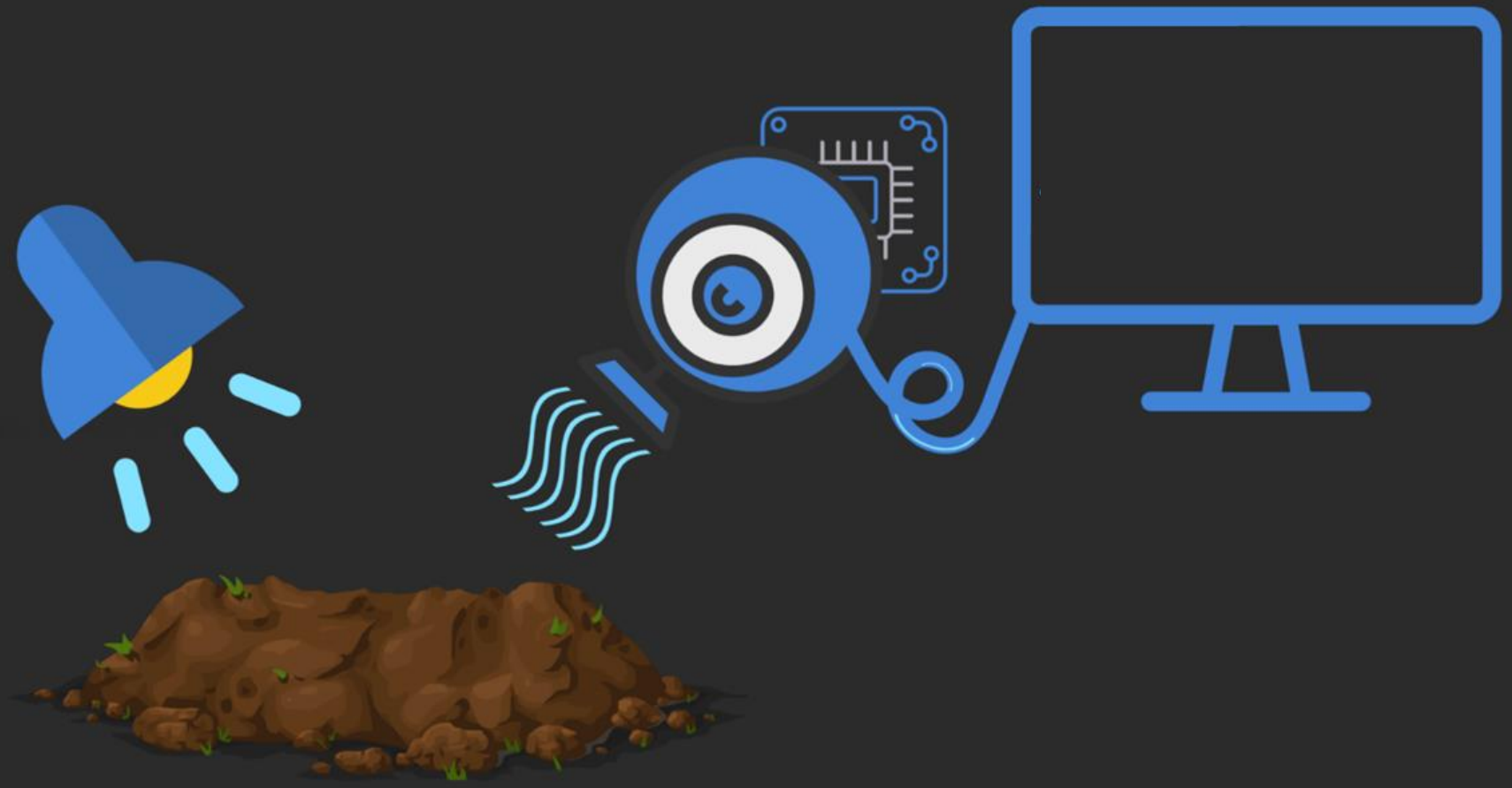
Leo Ramirez-Lopez, Laura Summerauer, Moritz Mainka

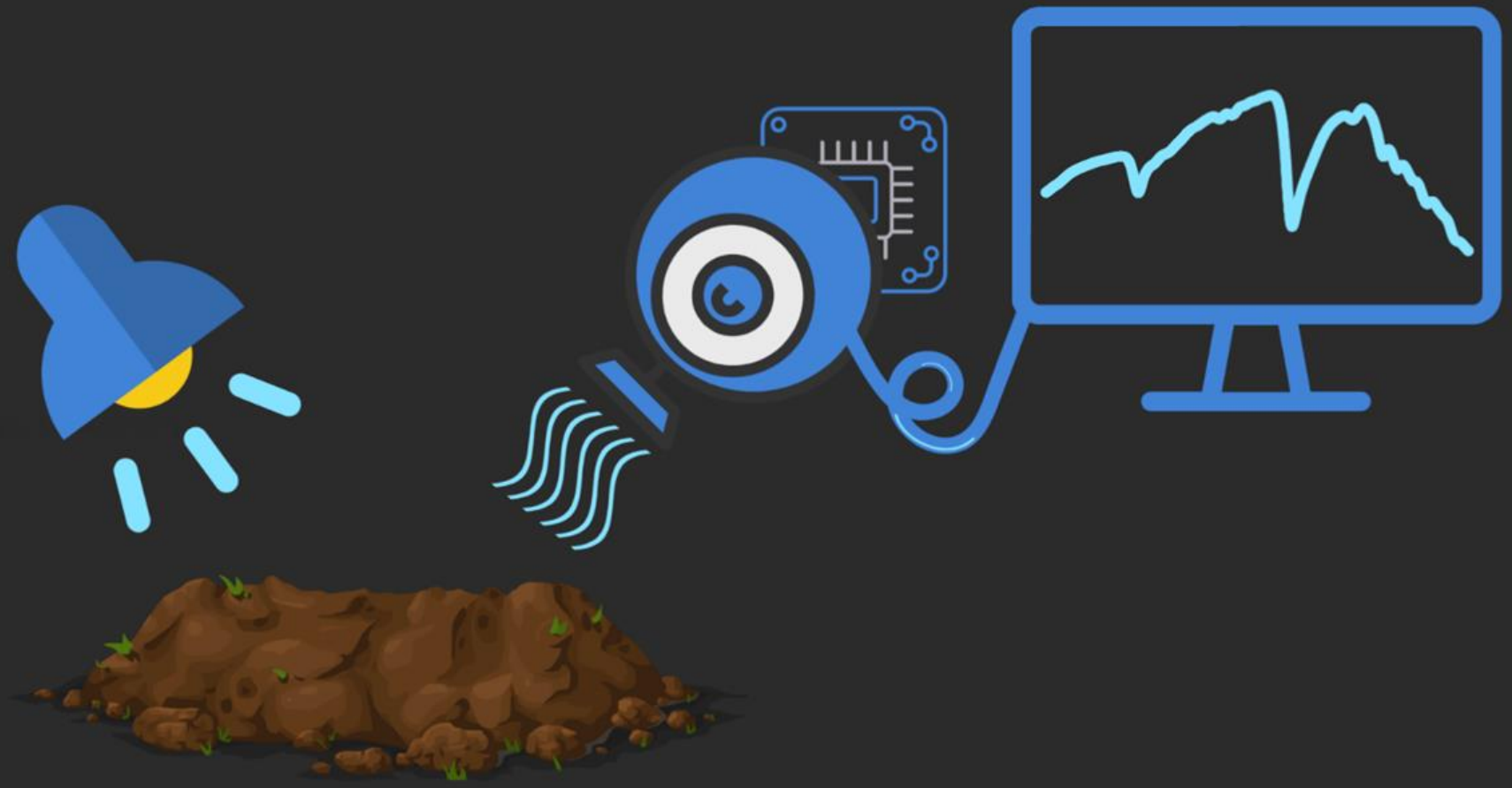
NIR/IR Spectroscopy – An equation for success

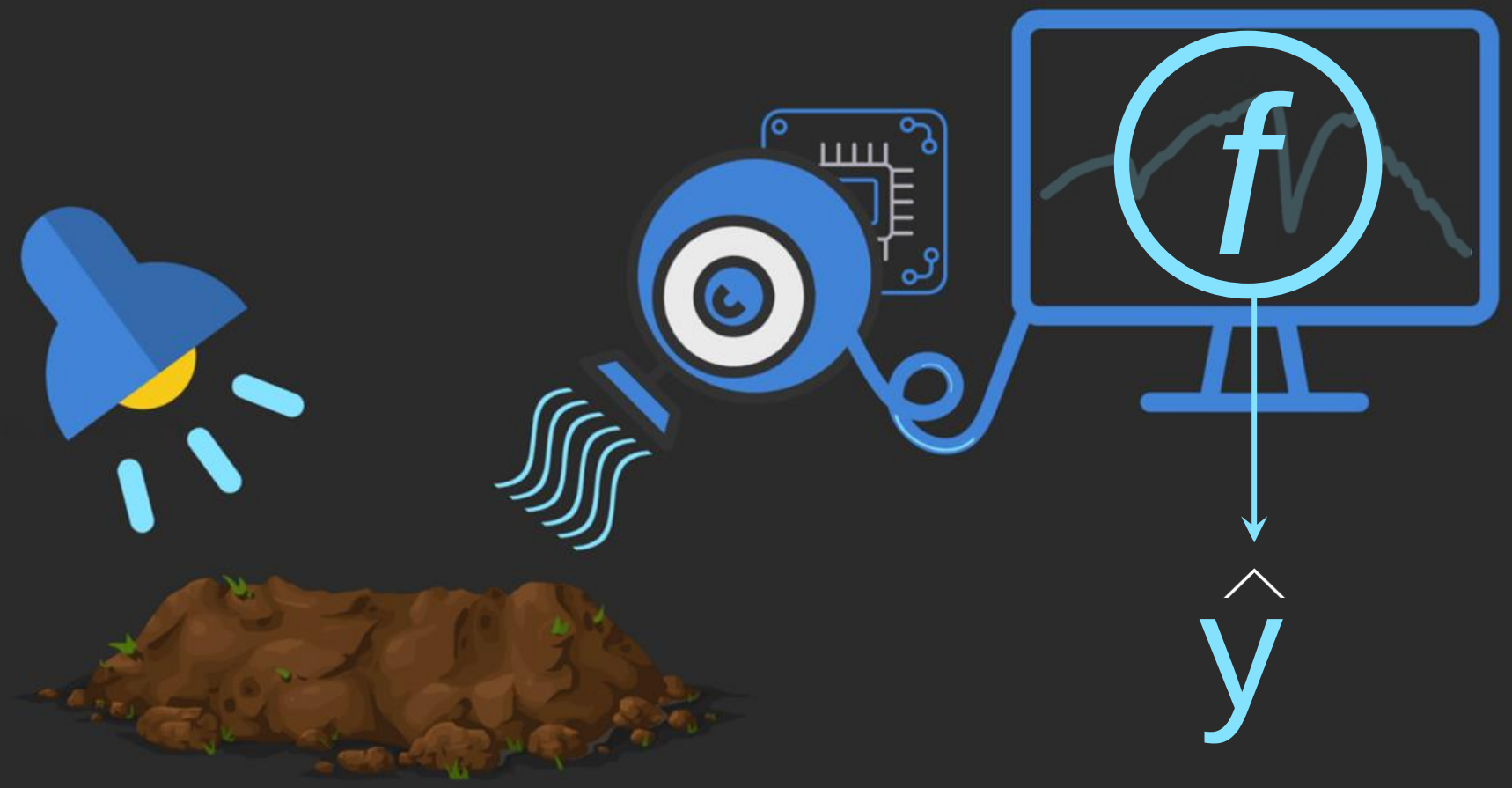
Success = f (hardware, software, data, models, people, automation, ...)





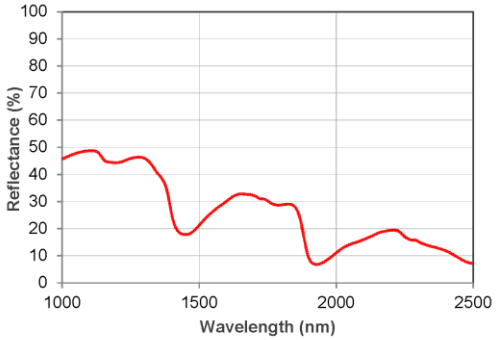




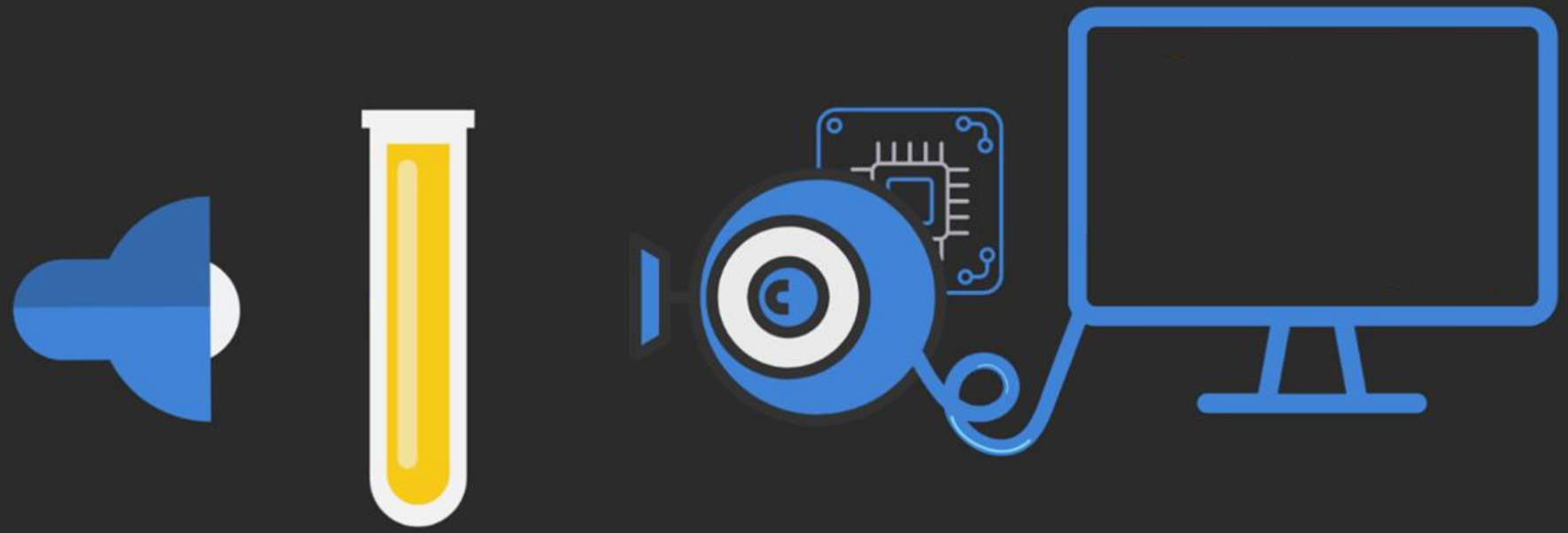

f
ŷ

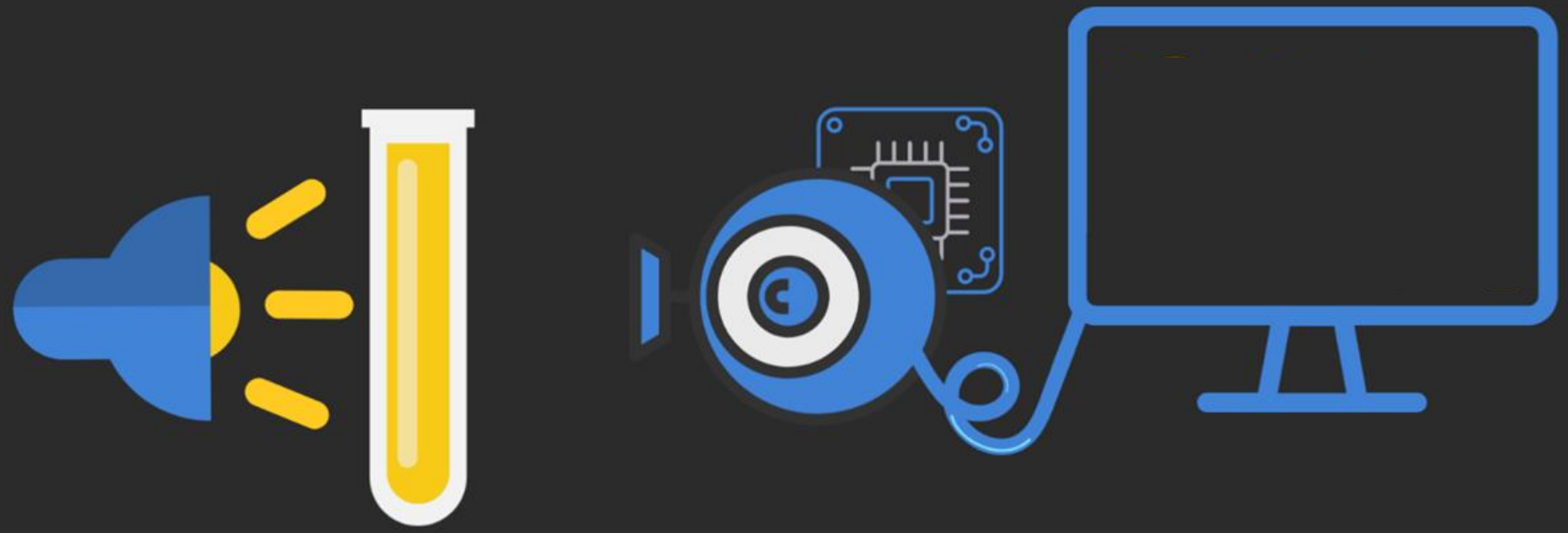
translating spectral information that we have into chemical information that users need!

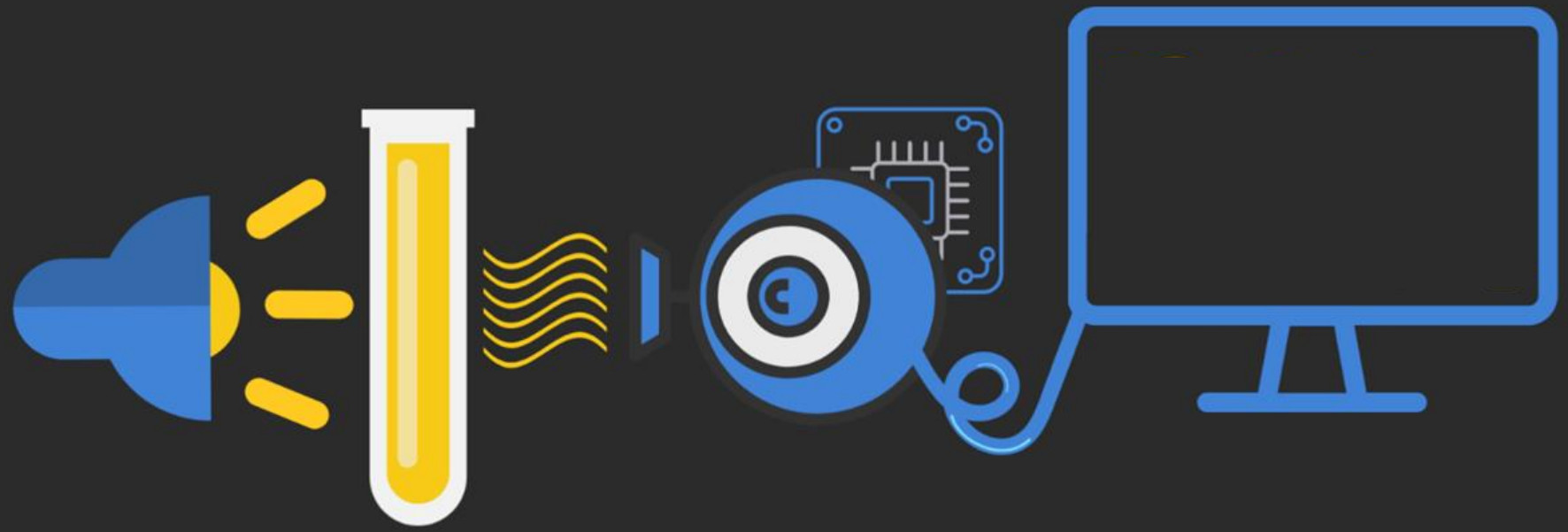
$$\hat{y} = f\Big(\text{[spectrum]}, \ldots \Big) + \varepsilon$$

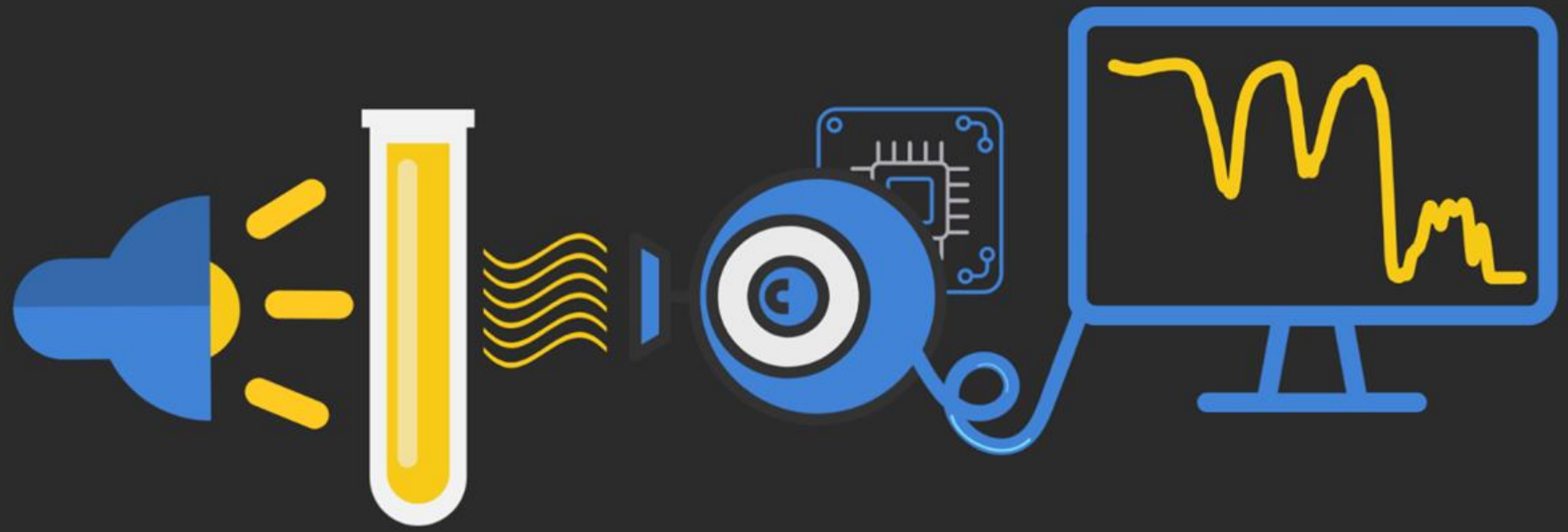


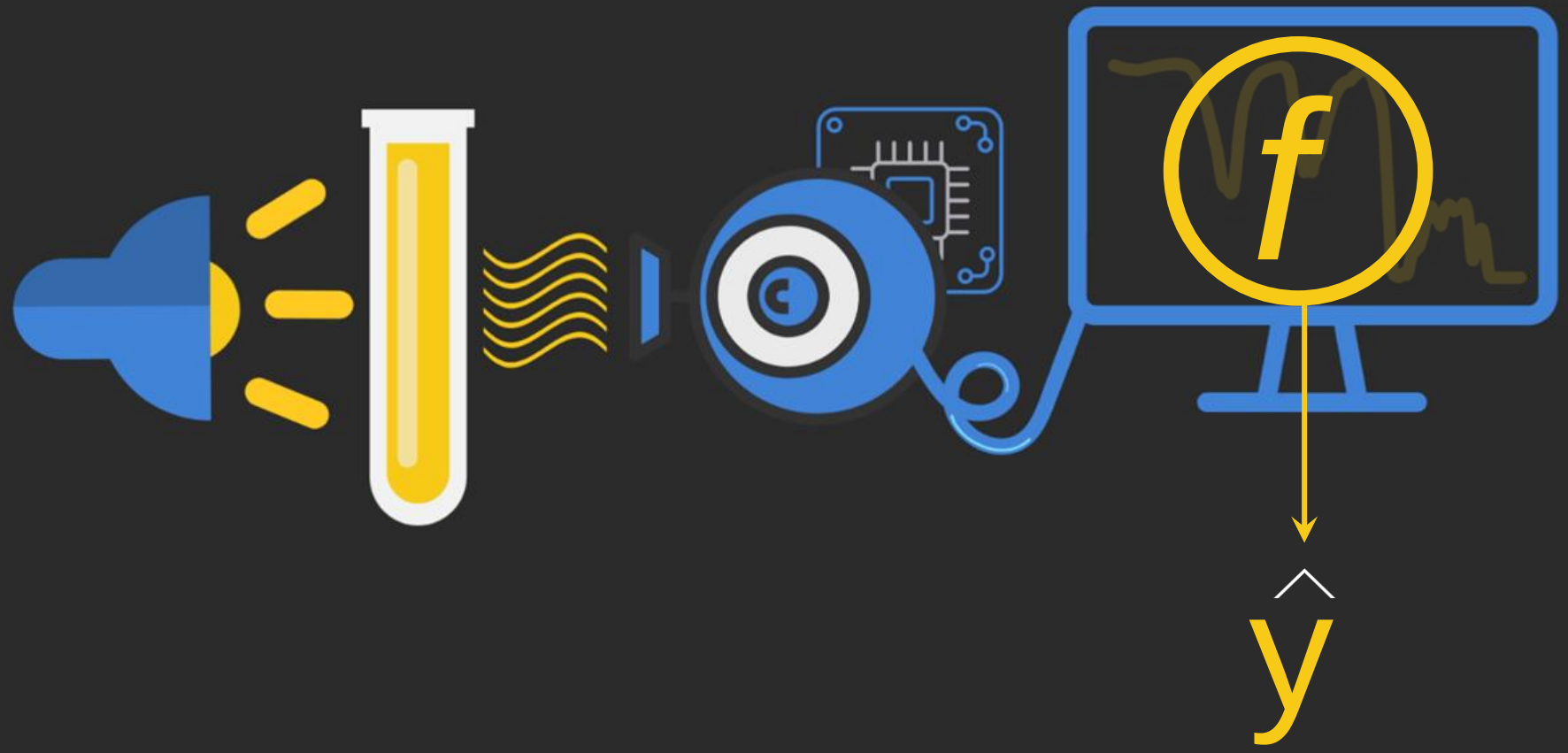
Function that can be approximated by using chemometrics/machine learning







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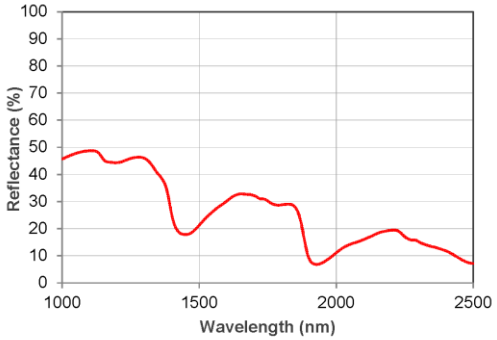


Function that can be approximated by using chemometrics/machine learning

transmission

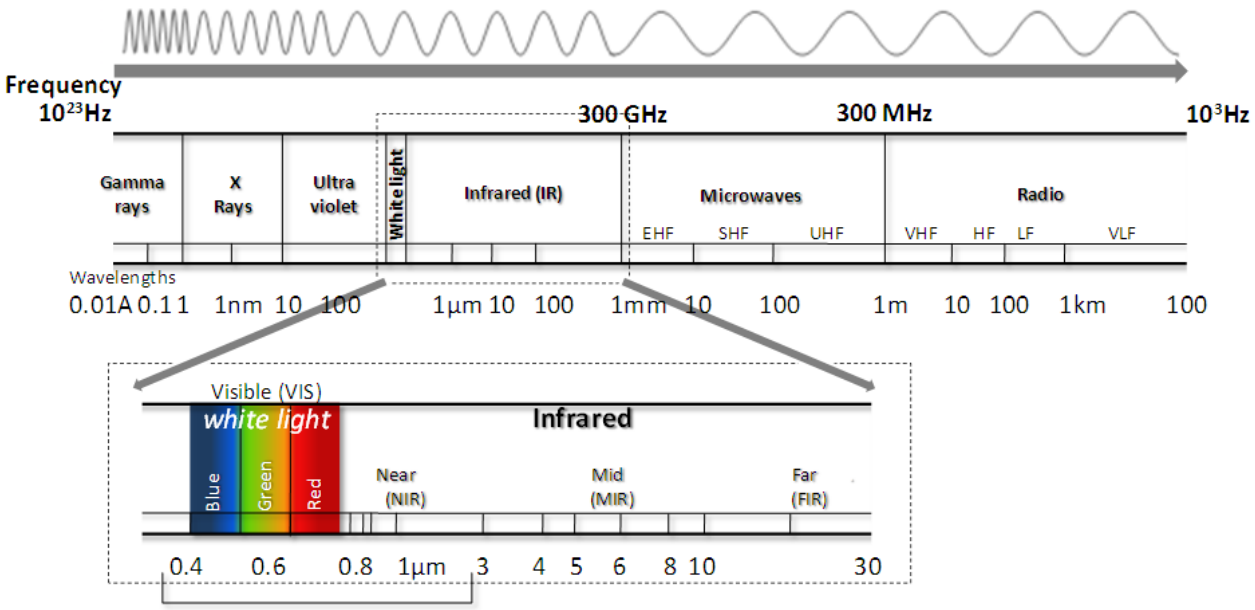
reflection

absorbance

transmission

reflection

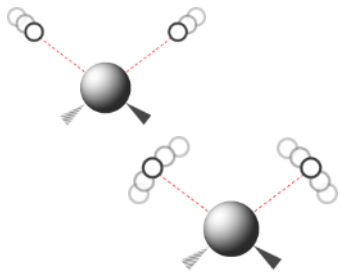
absorbance [$\log_{10}(1/\text{reflection})$]



NIR/IR spectroscopy is based on the measurements of the spectral response of objects in the infrared region of the electromagnetic spectrum.

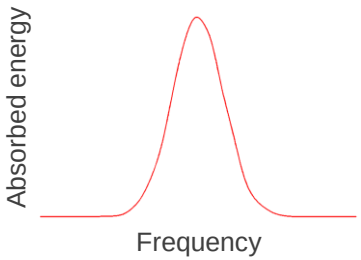
Near-infrared spectroscopy (NIR)…

How does it work?



A given molecule absorbs energy (light) if the frequency of the light energy matches the vibrational frequency of the functional group of the molecule.

The amount of energy absorbed can be different for each frequency (wavenumber). This usually results in energy absorption peaks.



ProxiMate

NIR-Online

ASD
TerraSpec

TANGO

7.9
13.3

MPA II
BRUKER

FOSS

Device name	Manufacturer	Spectral range (nm)	Price (USD)
		Bechtop	
ASD FieldSpec*	Malvern Panalytical	350 – 2500	~68100
NIRS DS2500 L	FOSS Analytics	400 – 2500	~75000
		Handheld	
SR-3500	Spectral Evolution	350 - 2500	~49700
MicroNIR 1700	VIAVI Solutions	950 - 1650	~20000
trinamiX	trinamiX/BASF	1450 - 2450	~8733
NeoSpectra	Si-Ware Systems	1300 - 2600	~3550
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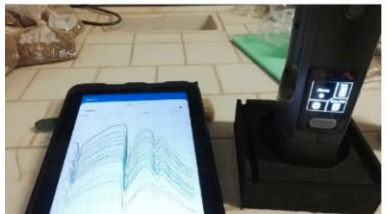
STS-VIS	Ocean Insight	350 - 830	~3408
NIRONE Sensor S	Spectral Engines	1750 - 2150	~3635
microPHAZIR	Thermo Fisher	1596 - 2396	?
SCiO	Consumer Physics	740 - 1070	~450
NIRscan	Texas Instruments	900 - 1700	~3000
Tellspec	Tellspec	900 - 1700	~320 - 1500

*a portable option is also available



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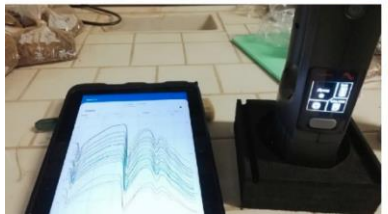
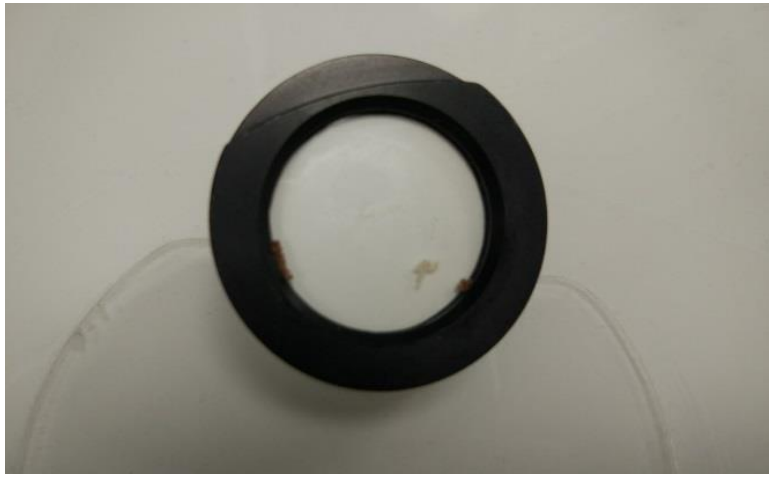


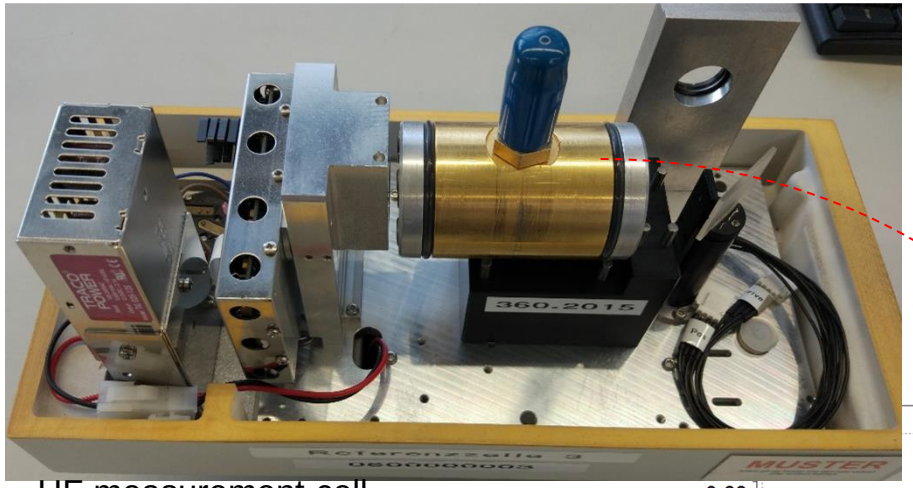


Photometric alignment/calibration

Wavelength alignment

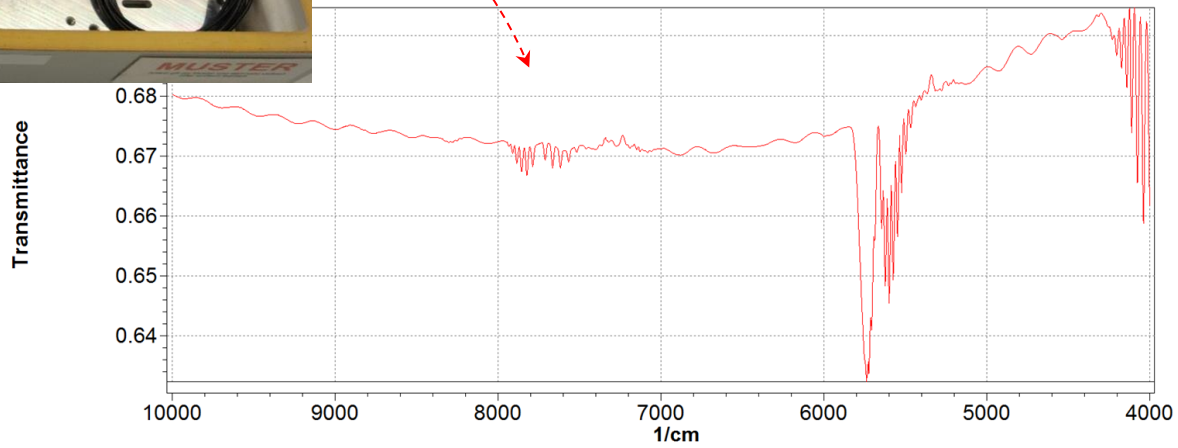
1. Hydrogen fluoride alignment

Some instruments are factory standardized using a wavelength standardization cell containing Hydrogen Fluoride (HF) gas. The spectral signature of this gas consist in very well defined peaks which can be measured with high precision and accuracy.



HF measurement cell

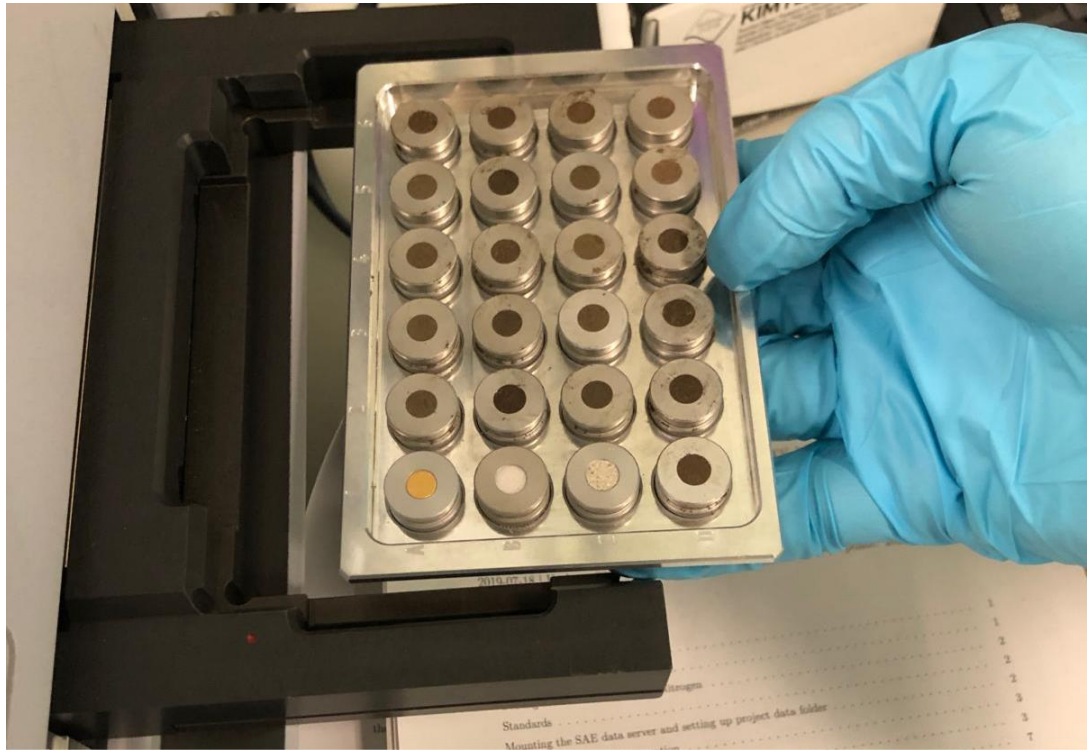
HF spectrum for wavelength alignment



Let’s scan our first samples

Download SI-WARE COLLECT

Scanning in the IR spectrometer…



NIR Applications

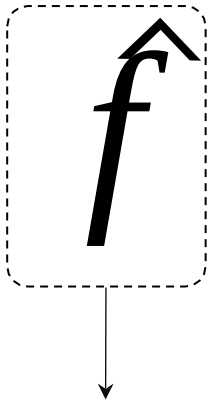
$\hat{f}$

Function that can be approximated by using chemometrics/machine learning

We currently use our own BUCHI software for that!

These **functions are device-, product- and property-specific.**

NIR Applications



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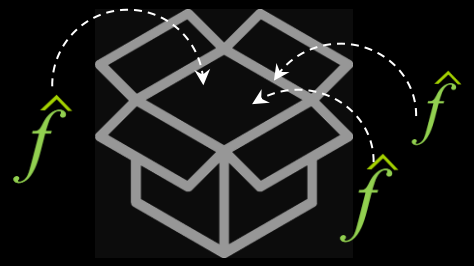
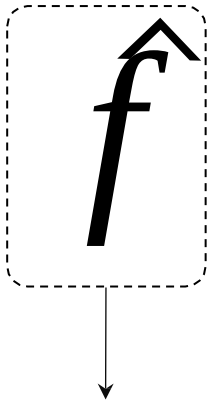
For each product we build and group a set of functions that quantify relevant product properties (e.g. moisture, protein, fat). **This group of functions is called application.**



NIR Applications



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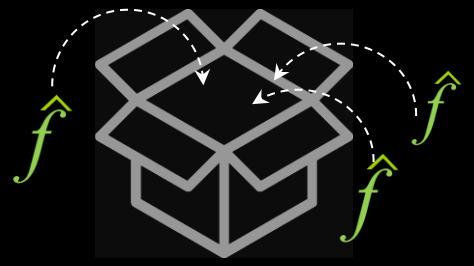


From average user's perspective, **a NIR device without an application can be perceived as useless.**

Samples

Measurements…

Lab measurements for obtaining reference property values (y)

Spectral measurements (x)

Calibration…

The poupose is to obtain a predictive model and quantify its accuracy

$$y = f(x) + \varepsilon$$

This is the error of the predictions. It is obtained by using model validation methods

This function (or model) translates spectral data onto property values. This can be obtained by partial least squares (pls) regression

Is the accuracy of the model acceptable?

Application development…

Define application information and calibration model constraints. For example:

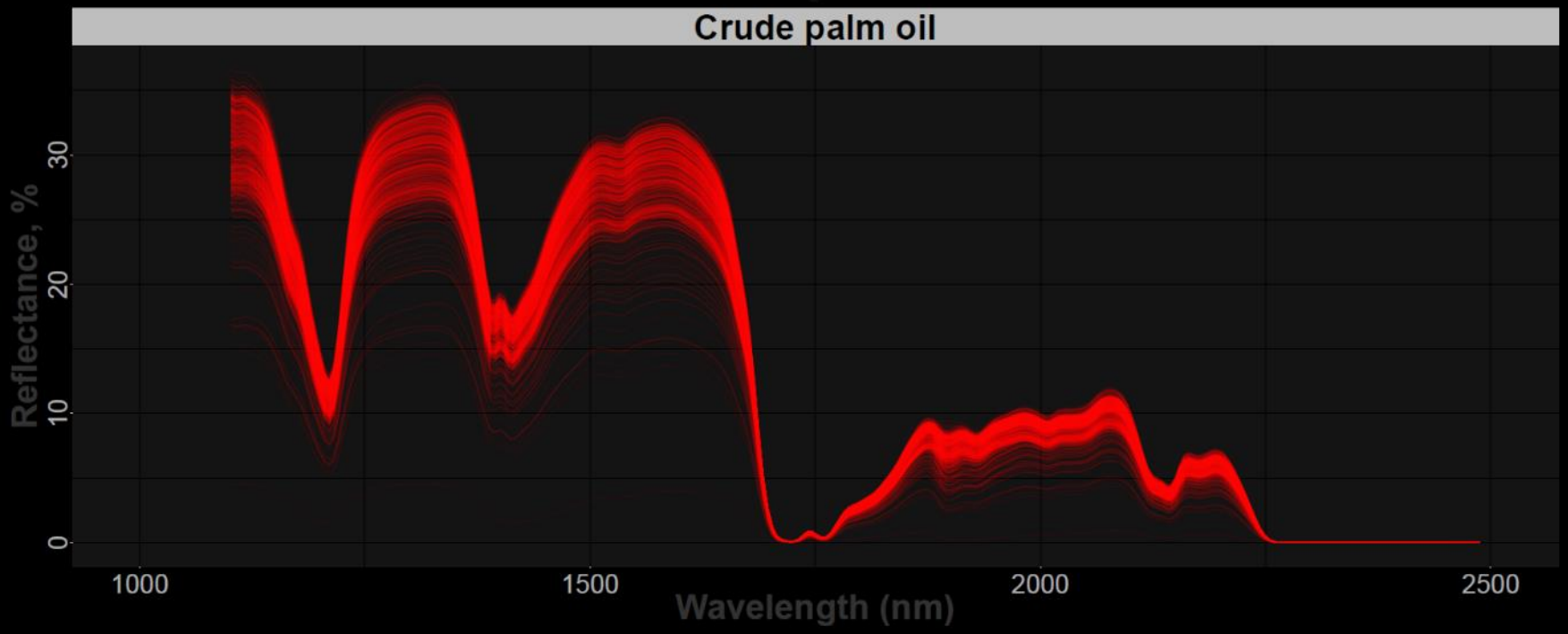
- Prediction and warning limits for each calibration model
- Spectra transformations required by each model
- Instruments
- Number of spectral measurements to obatin the final spectrum of a sample
- etc

Note: an application can contain multiple calibration models

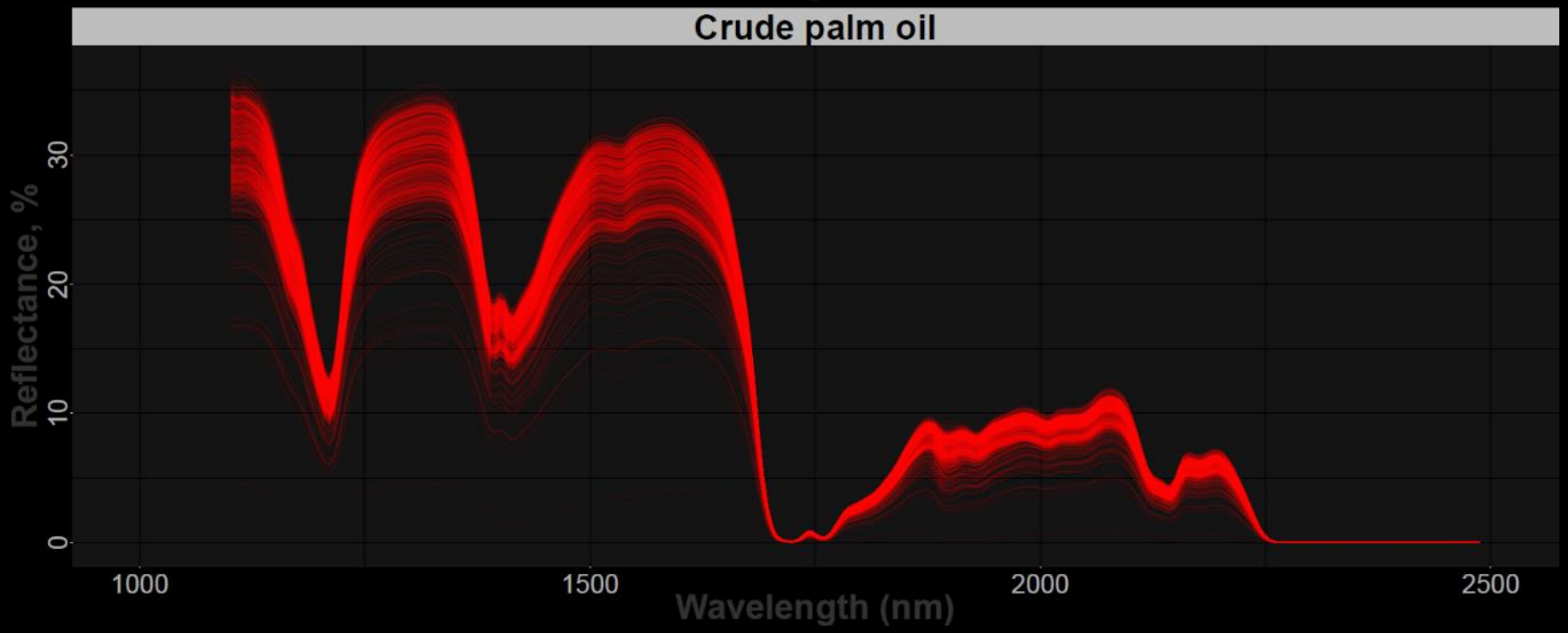
Using the application…

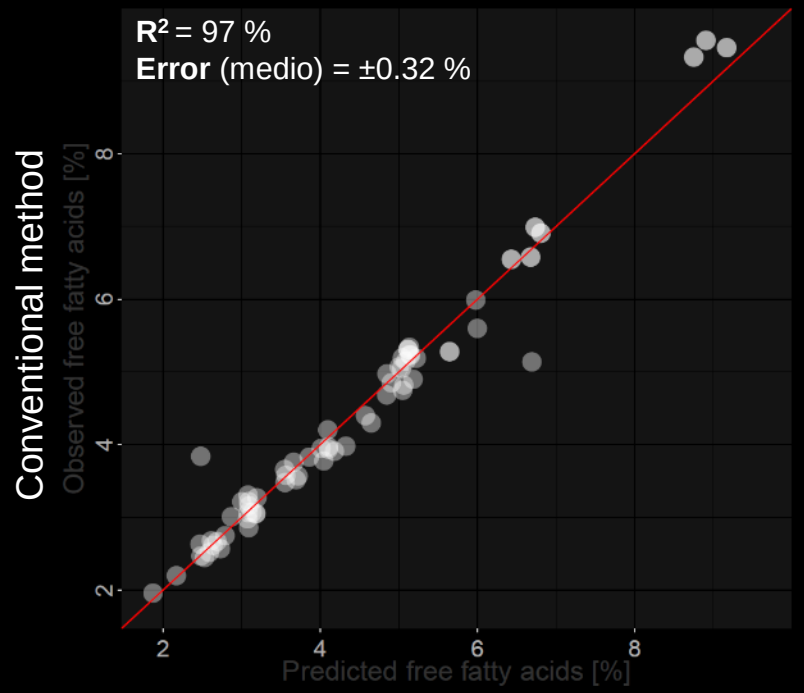
This consist in using the calibration models inside the application to predict the property values of new samples based only on their spectra.
For a single sample (and applying a single calibration model) the process is as follows:

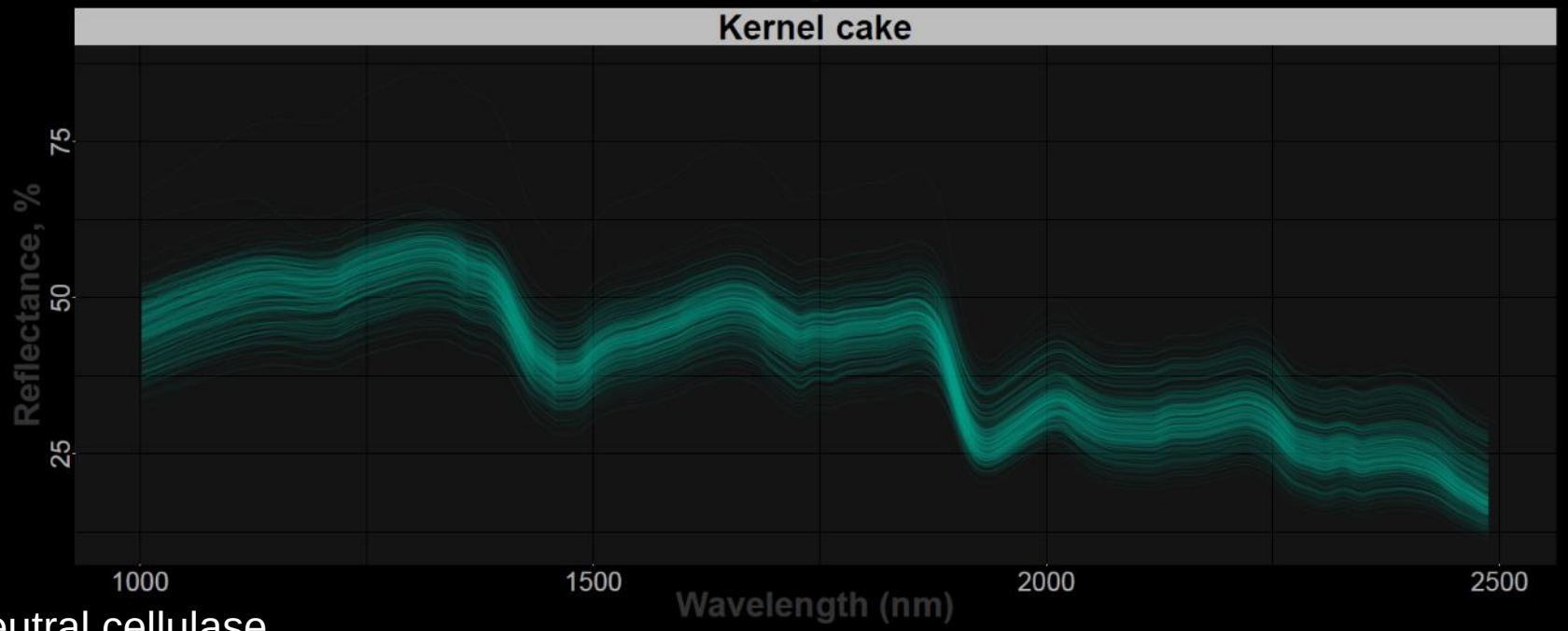
Measue the spectrum → apply the required transformations → apply the calibration model → predict the property value → calculate additional information (e.g. out of calibration range?)


Crude palm oil
Reflectance, %
0
10
20
30
1000
1500
2000
2500
Wavelength (nm)

Free fatty acids

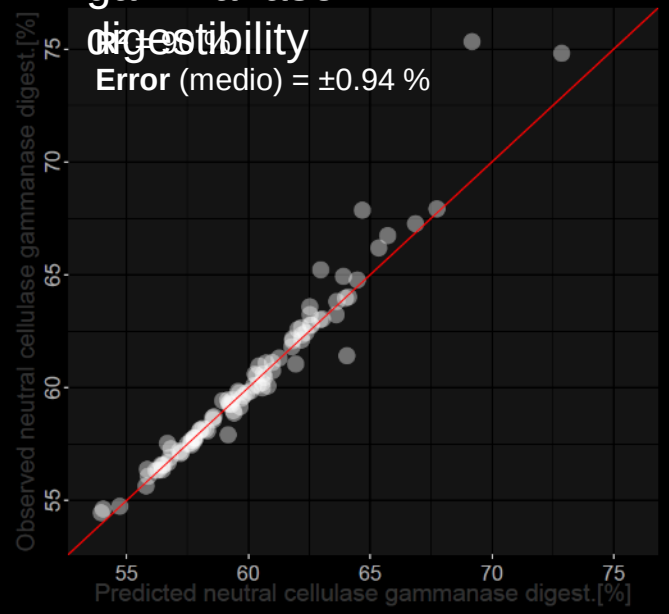




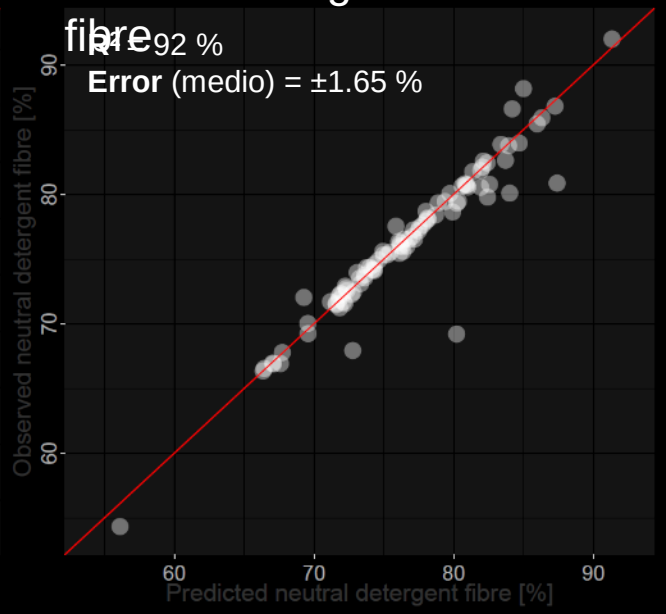


Conventional method

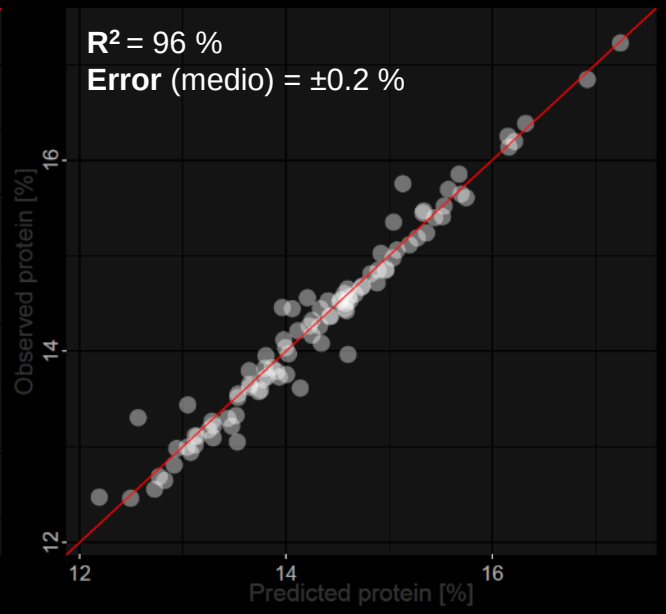
Neutral cellulase gammanase digestibility



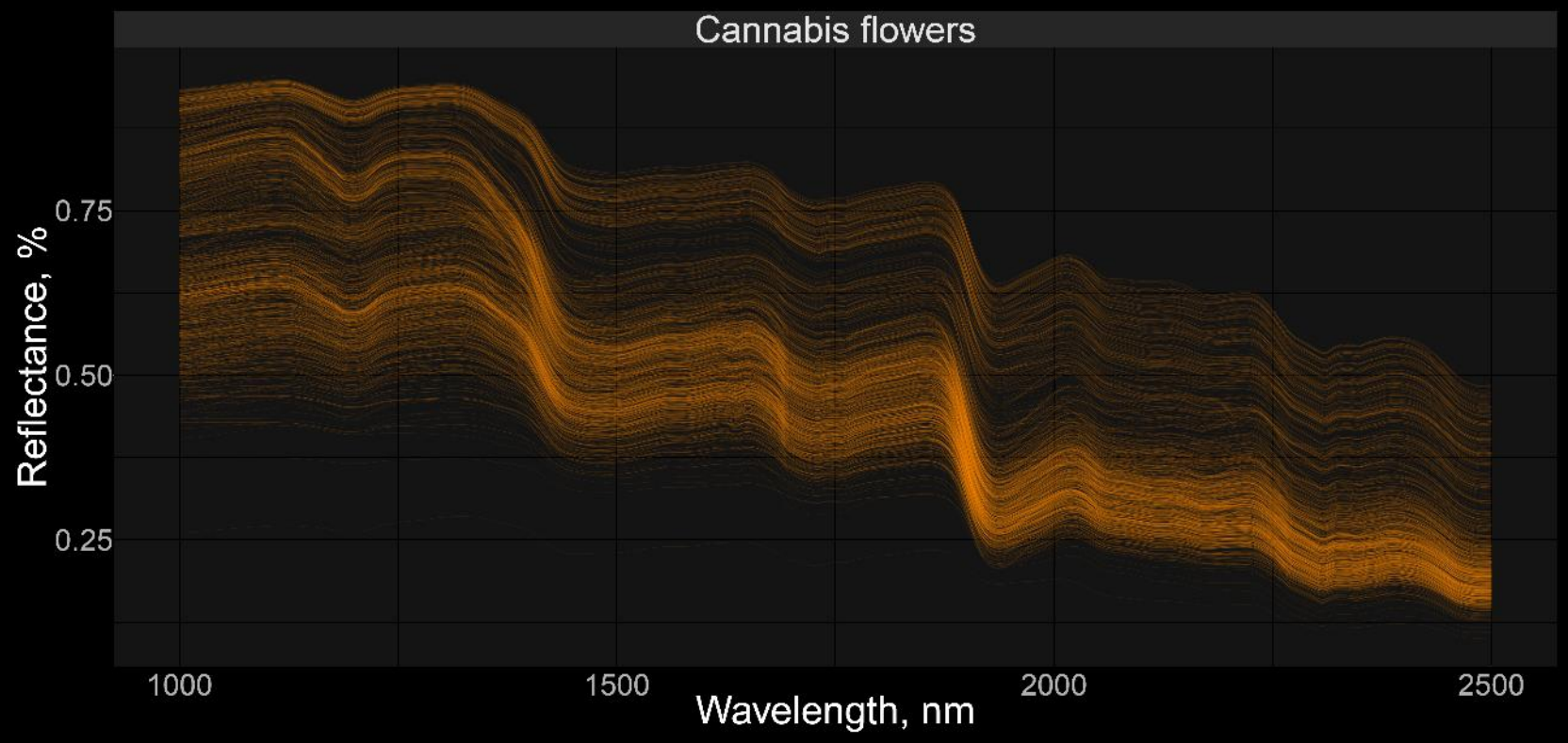
Neutral detergent fibre

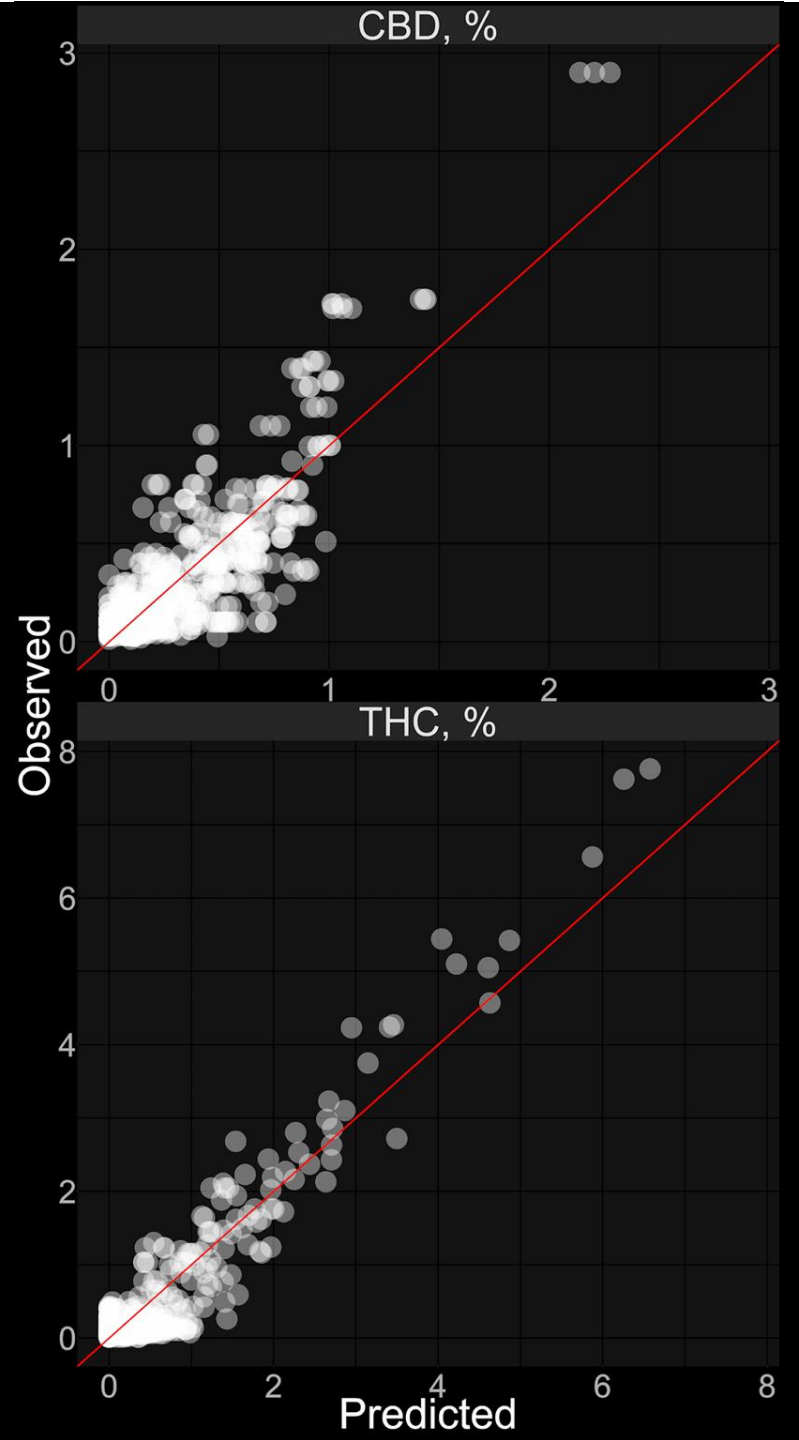


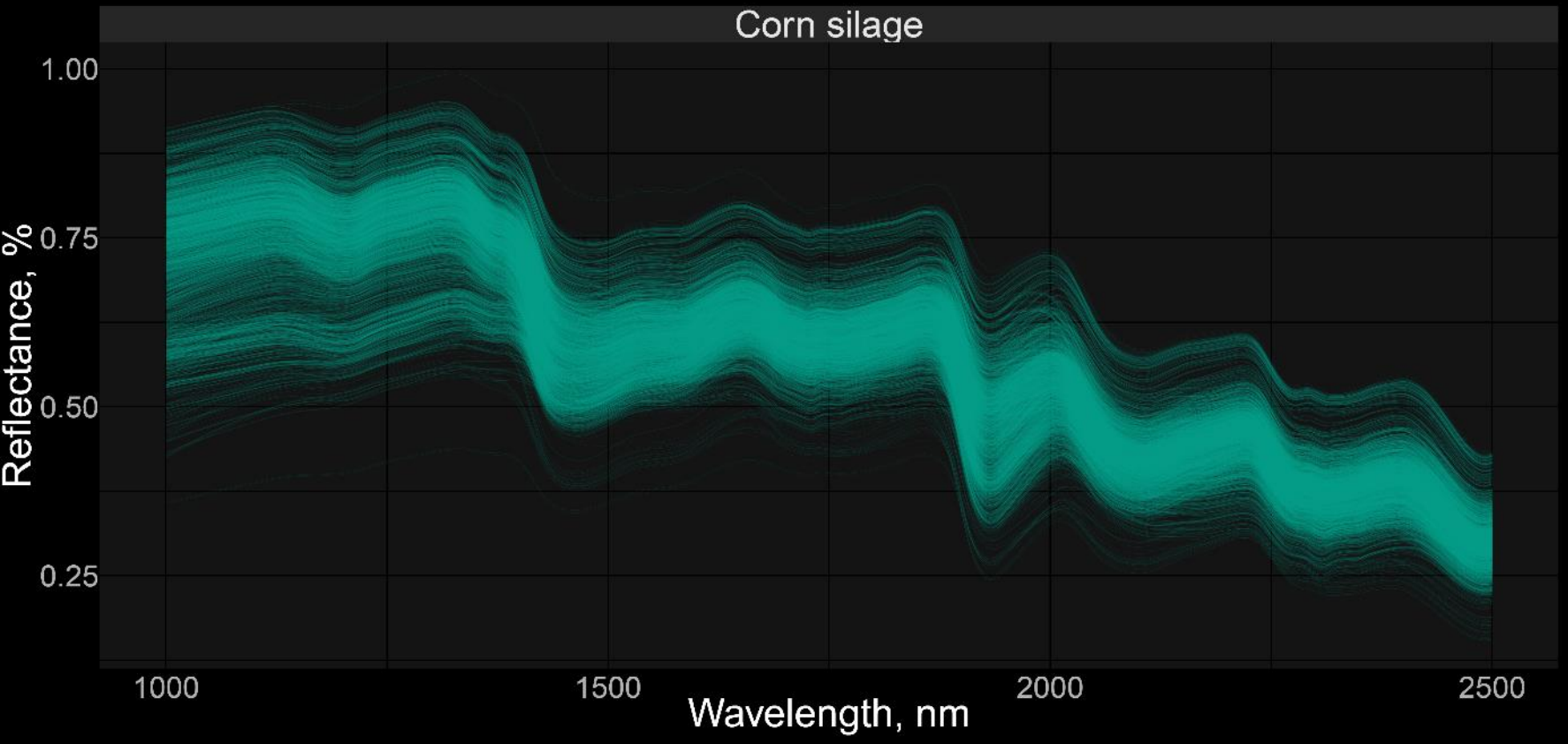
Protein

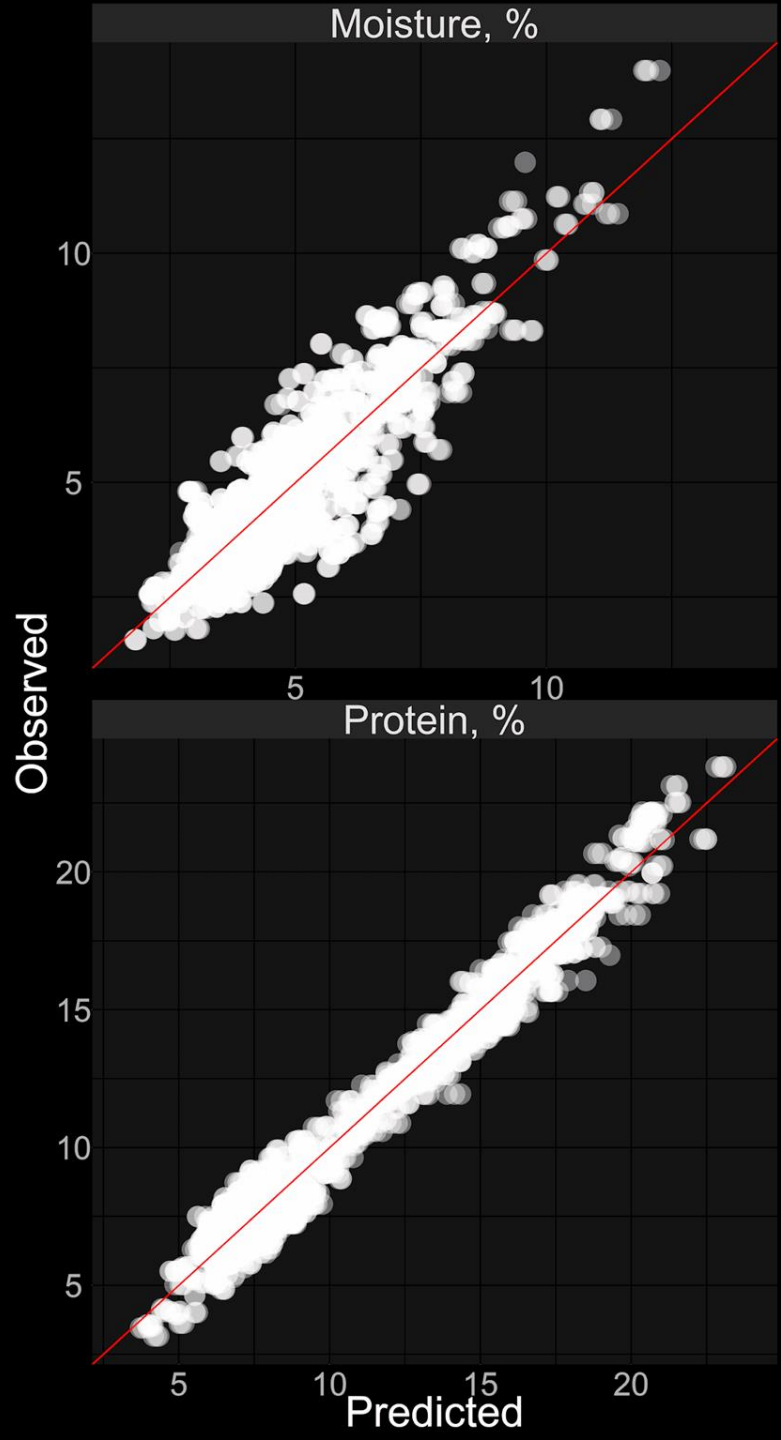


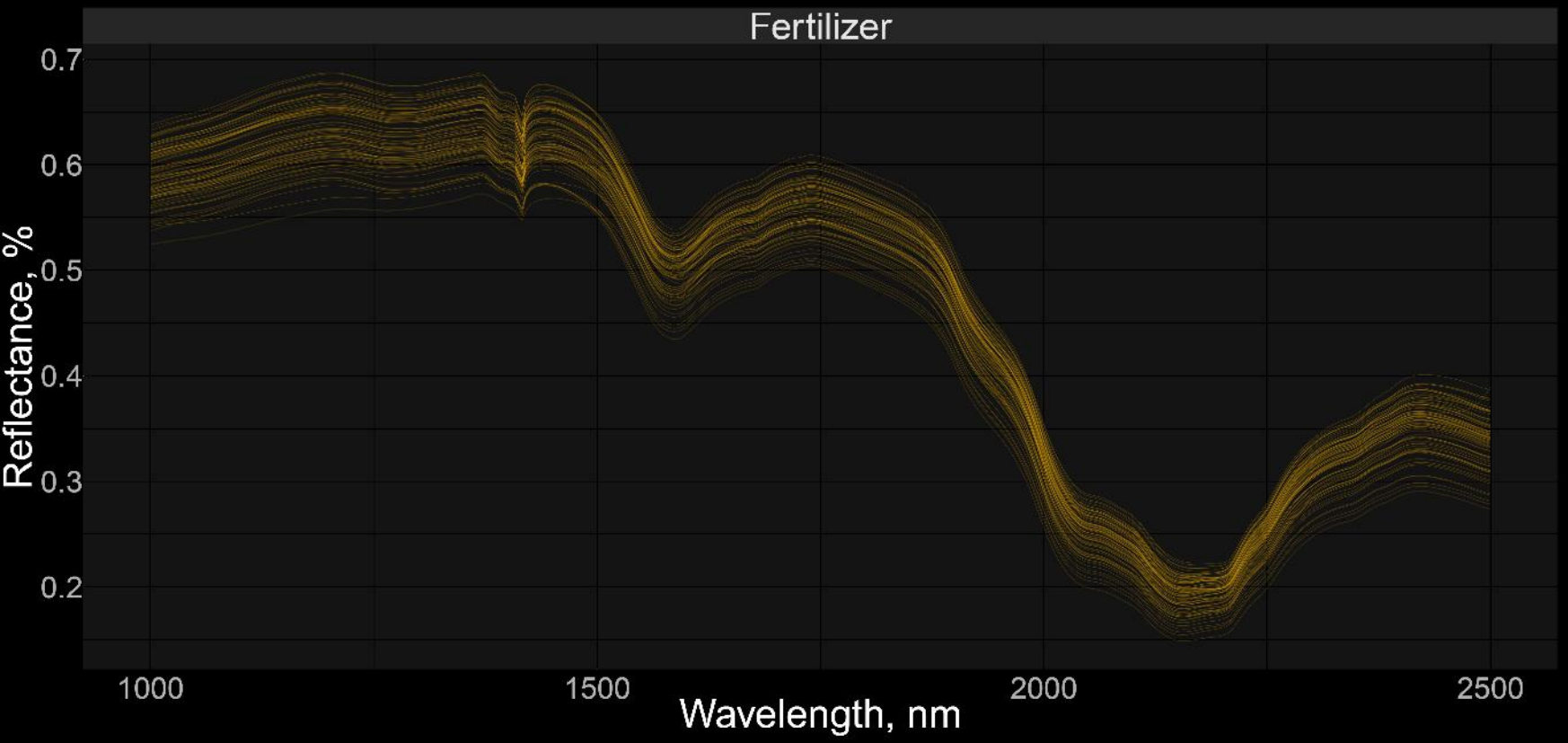
NIR spectroscopy

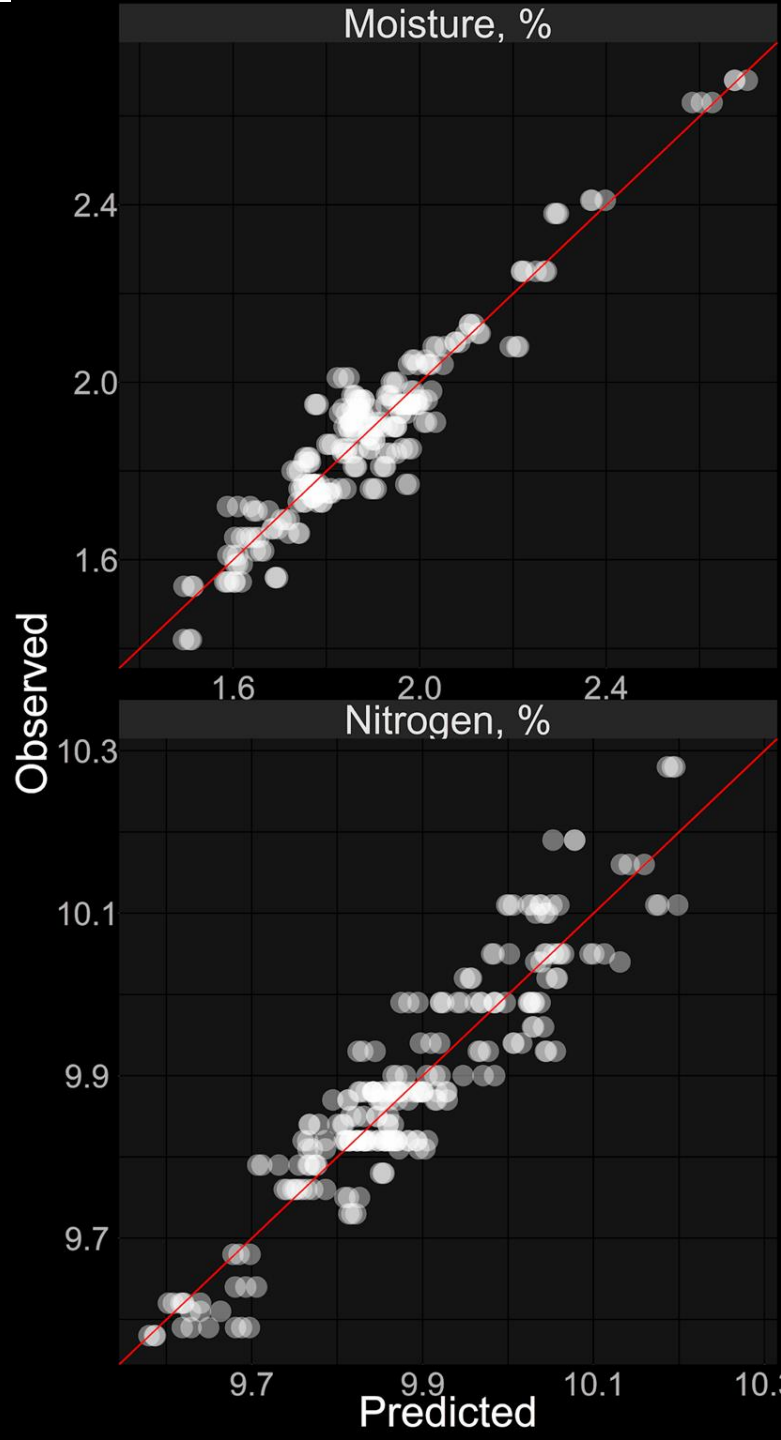

Cannabis flowers
Reflectance, %
0.75
0.50
0.25
1000
1500
2000
2500
Wavelength, nm

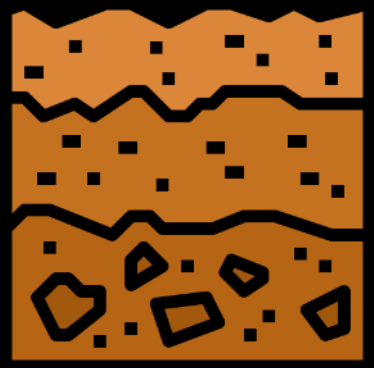

CBD, %
THC, %
Observed
Predicted
0
1
2
3
0
2
4
6
8

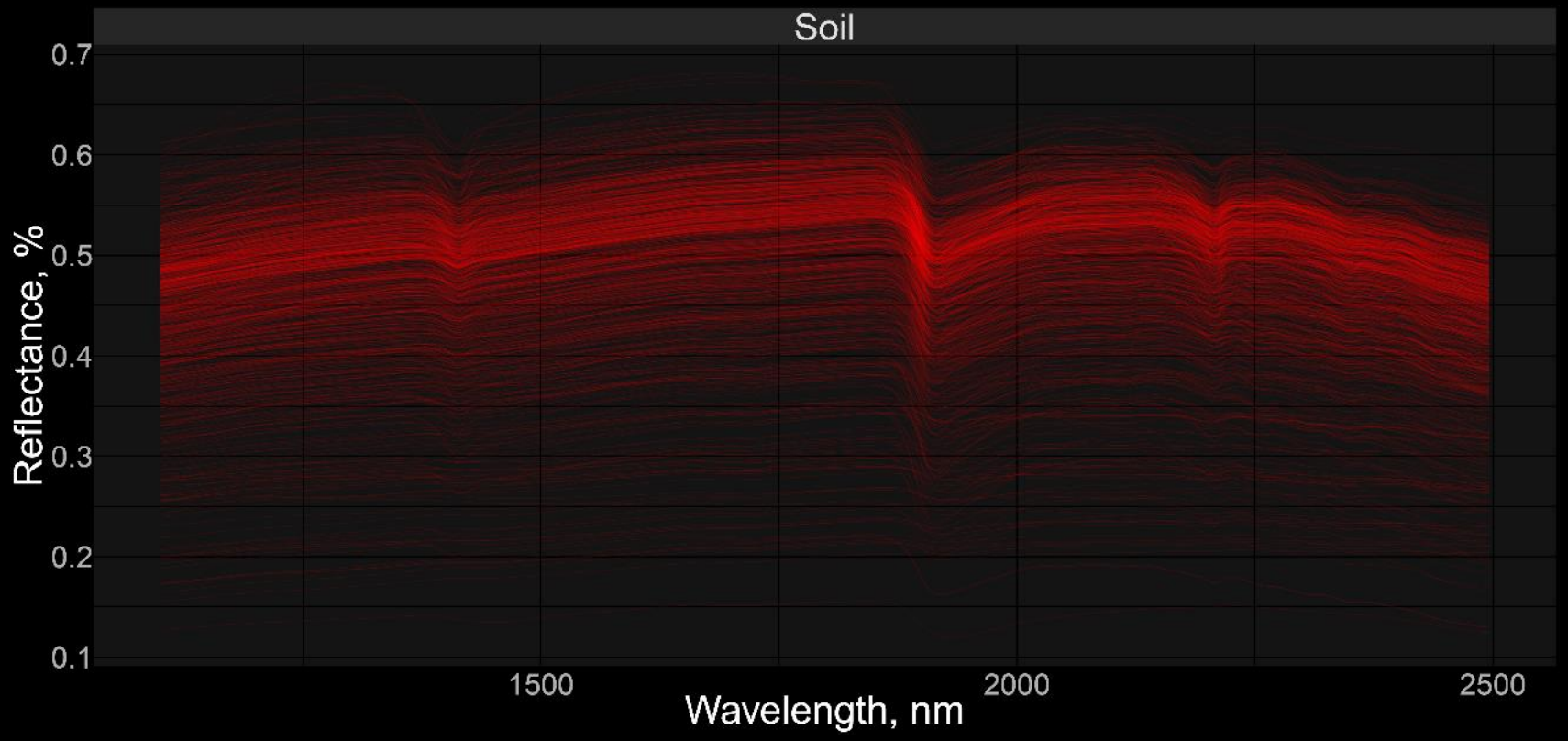

Corn silage
1.00
0.75
0.50
0.25
Reflectance, %
1000
1500
2000
2500
Wavelength, nm

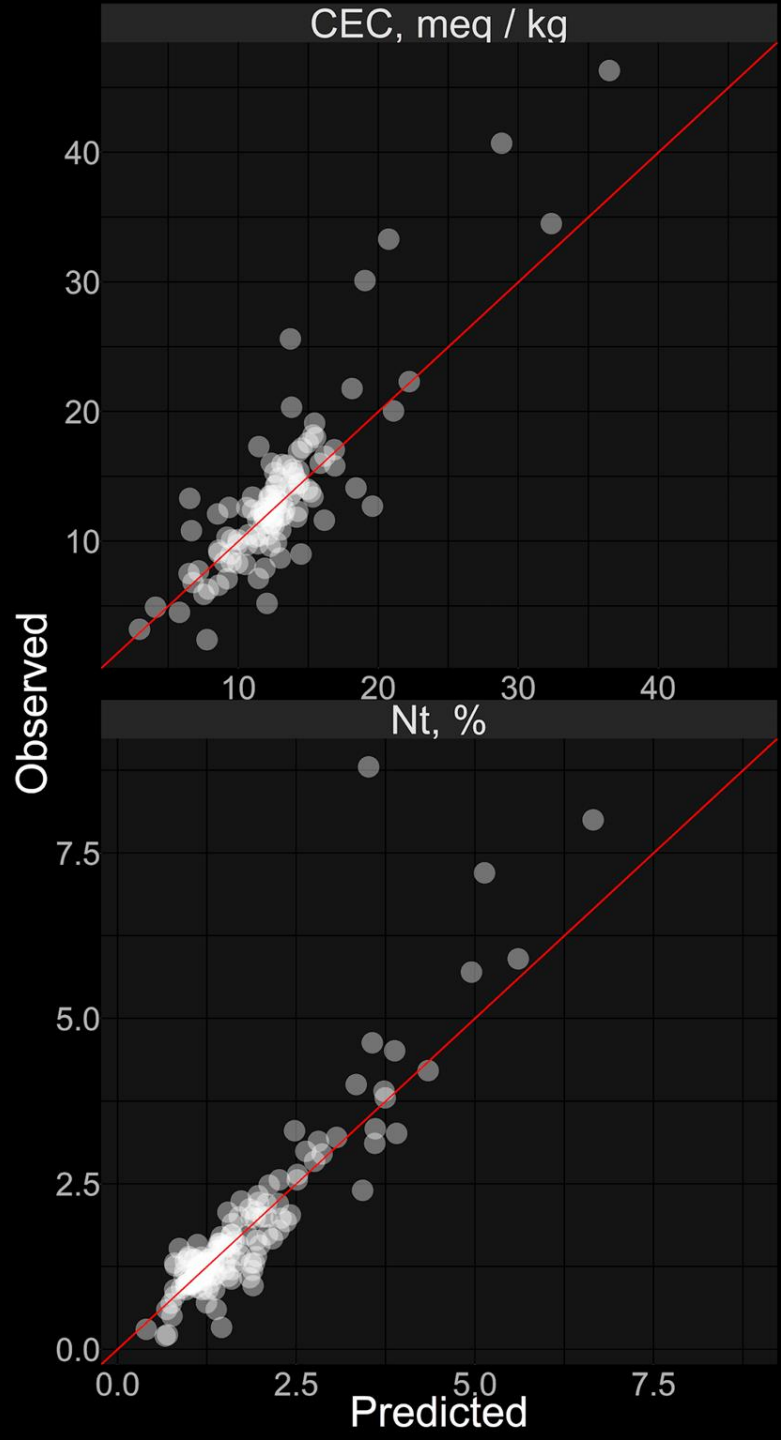

Moisture, %
10
5
5
10
Protein, %
20
15
10
5
5
10
15
20
Observed
Predicted


Fertilizer
Reflectance, %
0.7
0.6
0.5
0.4
0.3
0.2
1000
1500
2000
2500
Wavelength, nm


Moisture, %
2.4
2.0
1.6
1.6
2.0
2.4
Nitrogen, %
10.3
10.1
9.9
9.7
9.7
9.9
10.1
Observed
Predicted




Soil
Reflectance, %
0.7
0.6
0.5
0.4
0.3
0.2
0.1
1500
2000
2500
Wavelength, nm


CEC, meq / kg
40
30
20
10
10
20
30
40
Nt, %
7.5
5.0
2.5
0.0
0.0
2.5
5.0
7.5
Observed
Predicted

NIR/IR Spectroscopy – An equation for success

Success = *f*(hardware, software, data, models, people, automation, …)

Application Development Roadmap

Collect calibration data

Legacy and/or new data to develop calibrations is collected.

1

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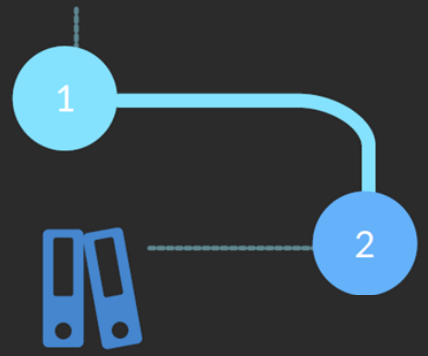
Collect calibration data

Legacy and/or new data to develop calibrations is collected.



Organize data

cleaning/filtering, sorting, harmonizing, pooling, storing and document all the calibration data gathered.

Application Development Roadmap

Collect calibration data

Legacy and/or new data to develop calibrations is collected.

1

2

Organize data

cleaning/filtering, sorting, harmonizing, pooling, storing and document all the calibration data gathered.

3

Calibrate spectral models

Use the calibration data to calibrate the models of the multiple properties of the target product. For each model, several data processing methods are empirically tested to optimize the accuracy and precision of the models.

The training/calibration set

Property
(response)

NIR signals (predictors)

Application Development Roadmap

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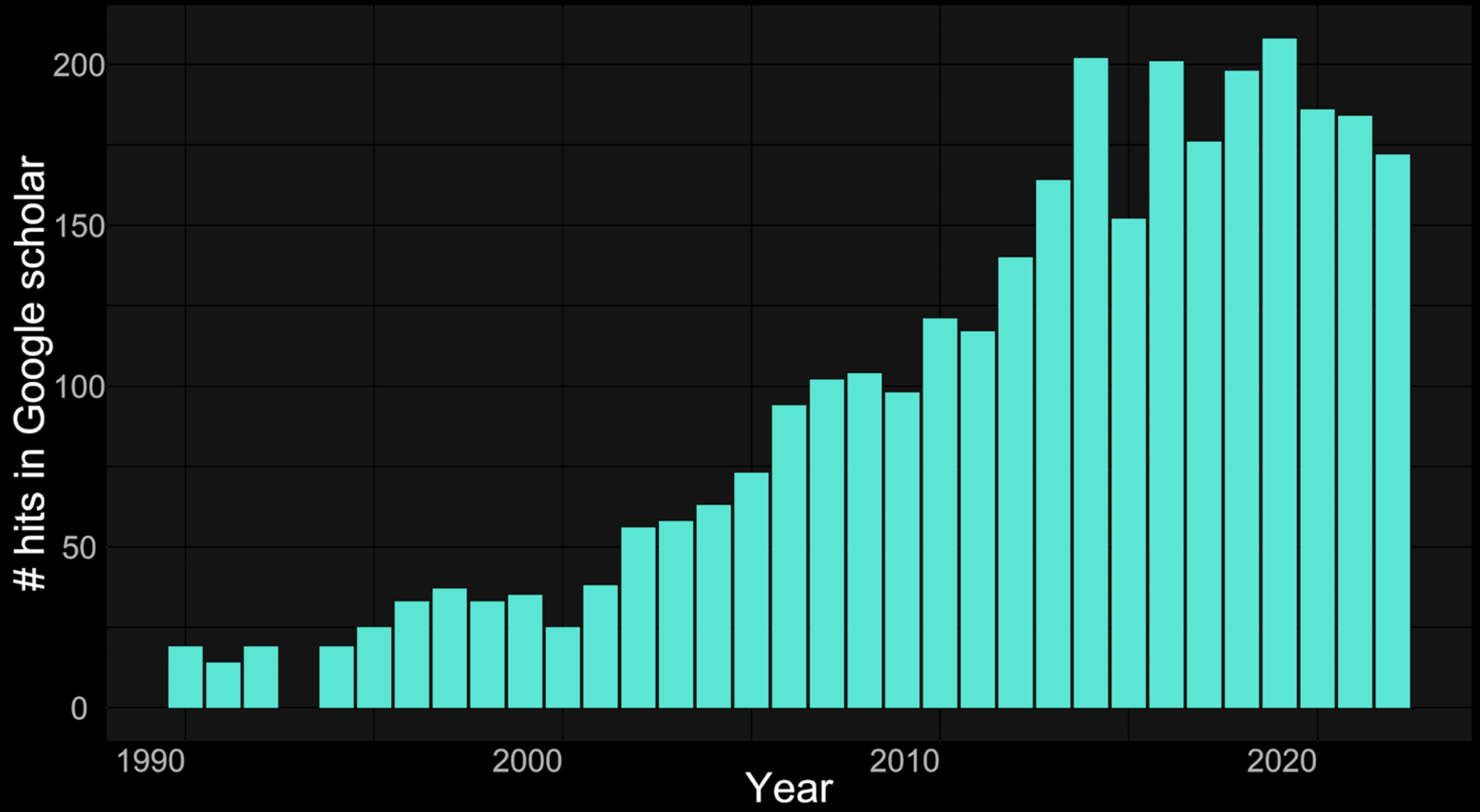
The training/calibration set

Property
(response)

NIR signals (predictors)

The calibration model $\hat{f}$

33 years
~3166 scientific publications



Search terms:
`Soil + spectroscopy` (in the title of the paper)

Application Development Roadmap

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Legacy and/or new data to develop calibrations is collected.

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and then?

Application Development Roadmap

Pack into a predictive application

All the spectral models are packed into an application. All the technical and user-required documentation is generated along with the necessary licensing information.

Collect calibration data

Legacy and/or new data to develop calibrations is collected.

1

2

3

4

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cleaning/filtering, sorting, harmonizing, pooling, storing and document all the calibration data gathered.

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All the spectral models are packed into an application. All the technical and user-required documentation is generated along with the necessary licensing information.

5

Validation test

A specialist (different from the application developer), test that the application can be used. In this step the application is also tested with real samples to verify if reasonable results returned.

Application Development Roadmap

1 Collect calibration data

Legacy and/or new data to develop calibrations is collected.

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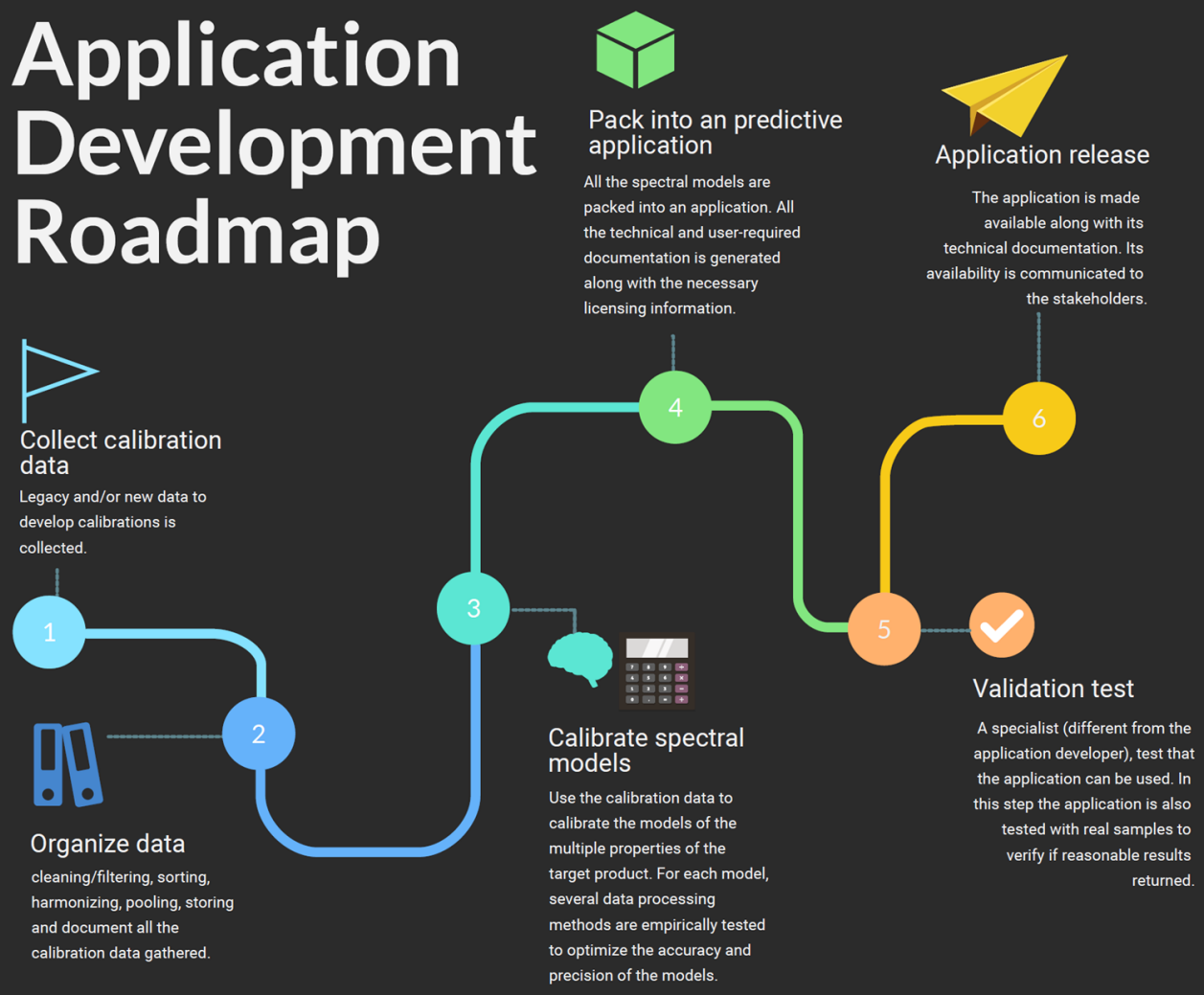
A specialist (different from the application developer), test that the application can be used. In this step the application is also tested with real samples to verify if reasonable results returned.

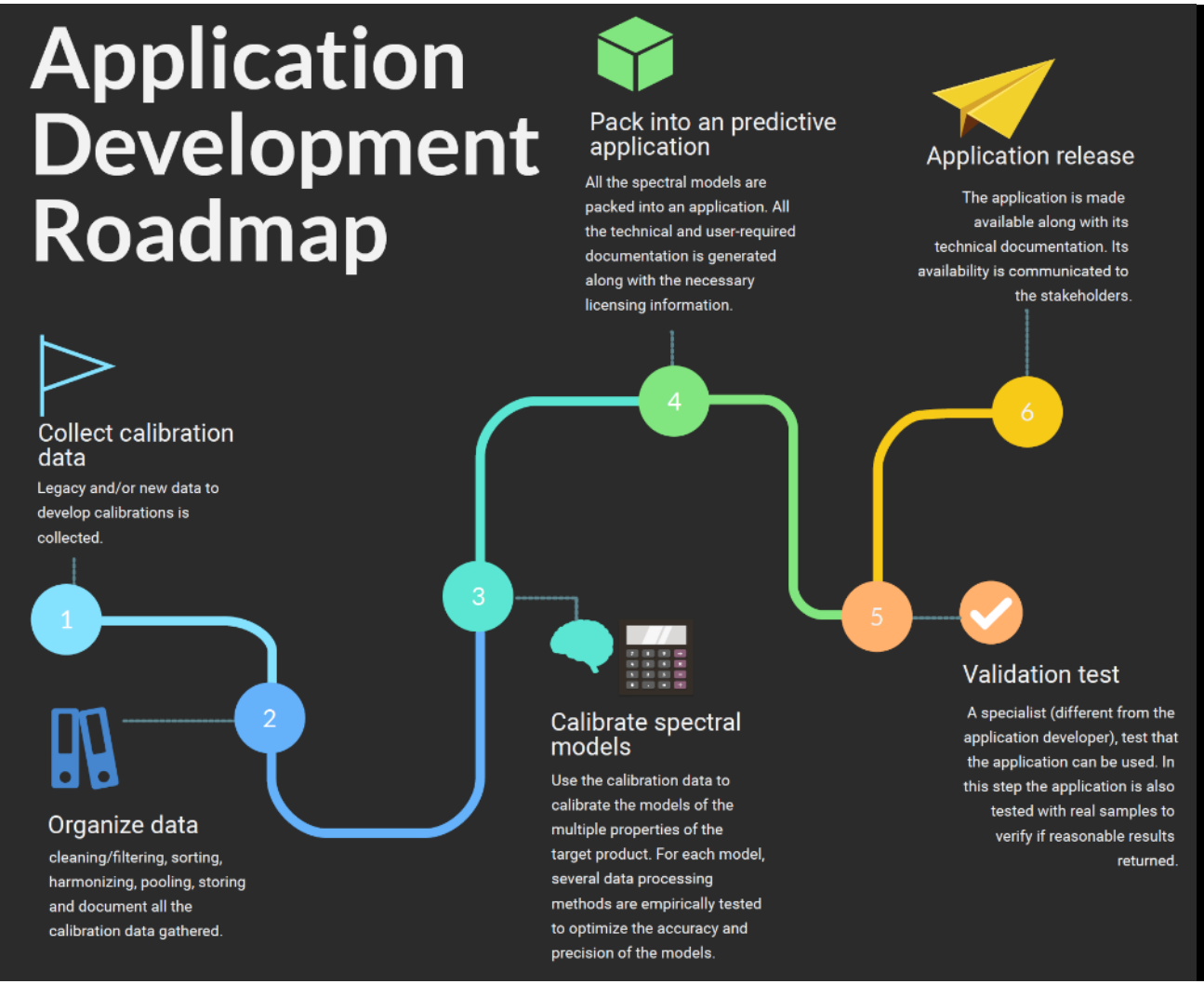
6 Application release

The application is made available along with its technical documentation. Its availability is communicated to the stakeholders.



Challenges

- **It is expensive.**
- **Labs should focus on routine analyses** (not on learning and dealing with chemometrics).
- **For end users/labs,** many time-consuming iterations to get useful applications creates **frustration.**
- **Chemometrics** is a complex subject which **requires time and effort to be learned/taught.**



Challenges

- **It is expensive to calibrate,** although it is extremely cost-efficient if it is released for routine analysis.
- **Labs should be focused on routine analyses** (not on learning and dealing with chemometrics)
- **For end users/labs,** many time-consuming iterations to get useful applications create **frustration**
- **Chemometrics** is a complex subject which **requires time and effort to be learned/taught**

R for spectral data processing

Exercise

- Introduction to R
- Read in spectral data and visualization (1st script)

How to name your samples?

- Material name:
  - `core_[NAMEOFYOURGROUP]`
- Sample names:
  - `[REPLICATE NUMBER]_[DEPTH increment]`
  - eg.: `01_0010`
  - `01_1020`
  - `02_1020`

C:/Users/stevens/Dropbox2/Dropbox/SPECcourse - RStudio

File Edit Code View Project Workspace Plots Tools Help

pres.Rmd | Day1.Rmd

Knit HTML | Run | Chunks

```
67
68  * The expension of __R__ is driven by the increasing number of available functions/packages.
69
70  ![](http://r4stats.files.wordpress.com/2012/04/fig_10_cran.png)
71
72  source: [http://r4stats.com/articles/popularity/](http://r4stats.com/articles/popularity/)
73  ----------------------------------------
74
75  * But, of course, __R__ has also drawbacks:
76   * No GUI (altough solutions exist, such as [Rcmdr](http://socserv.mcmaster.ca/jfox/Misc/Rcmdr/) for data import/export
     and analysis or [DeduceR](http://www.deducer.org/pmwiki/index.php?n=Main.ScreenShots) for graphs)
77   * Steeper learning curve than Excel, SAS or JMP (No GUI...)
78   * Cryptic documentation and error messages
79   * Often, __R__ makes us believe it worked as intended (see Chapter 8 of the [R Inferno](http://www.burns-stat.com/pages
     /Tutor/R_inferno.pdf))
80
81  ```{r}
82  # Exemple:
83  head(iris) # the iris dataset is a data.frame
84  head(iris[,1:2]) # the two first column of the data.frame
85  head(iris[,1]) # subsetting the 1st column returns a vector, not a data.frame!
86  head(iris[,1,drop=F]) # use [,,drop=F] to override the default behavior
87  ```
88
```

111:1 (Top Level) R Markdown

Console C:/Users/stevens/Dropbox2/Dropbox/SPECcourse/

```
11 2005  31 263  32    799        342
12 2006  42 281  47    967        397
13 2007  49 321  60   1220        415
14 2008  45 368 106   1300        431
15 2009  54 371 153   1330        447
16 2010  75 375 187   1620        539
17 2011  74 345 199   1710        556
> save(GS_data,file="GS_hits.Rdata")
>
> ggplot(data=melt(data=GS_data,id="year"),aes(x=year,y=value,colour=variable)) + geom_point() + geom_line() + labs(x="Year",y="Num
Google Scholar") + theme_bw() + scale_color_discrete("Software")
Warning messages:
1: Removed 16 rows containing missing values (geom_point).
2: Removed 16 rows containing missing values (geom_path).
> ggsave("figures/GScholar_spectroscopy.png")
Saving 6.61 x 6.17 in image
Warning messages:
1: Removed 16 rows containing missing values (geom_point).
2: Removed 16 rows containing missing values (geom_path).
> rm() # remove objects
> save() # save in Rdata format
Error in save() : 'file' must be specified
>
```

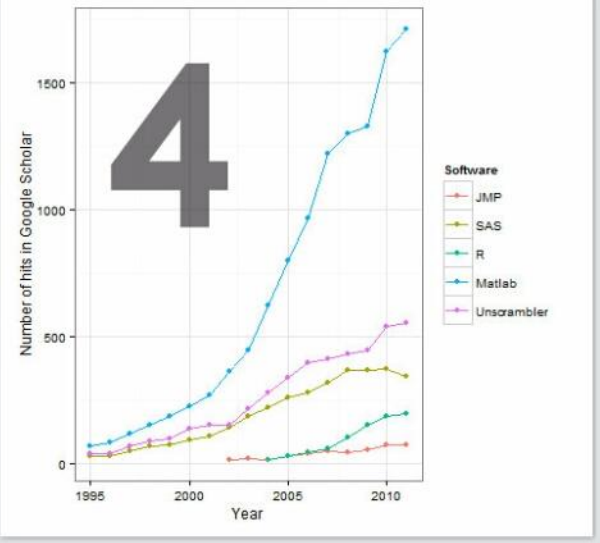
Workspace | History

To Console | To Source

```
h1 <- xpathSApply(doc, "//div[@id='gs_ab_md']", xmlValue)
h2 <- as.numeric(sub(",","",strsplit(h1, " ")[[1]][2]))
h2
}
}
colnames(hits) <- labels
data.frame(year=from:(to-1),hits)
}
GS_data <- GScholar_Scraper_hits(inputs,labels)
GS_data
save(GS_data,file="GS_hits.Rdata")
ggplot(data=melt(data=GS_data,id="year"),aes(x=year,y=value,colou
ggsave("figures/GScholar_spectroscopy.png")
rm() # remove objects
save() # save in Rdata format
```

Files | Plots | Packages | Help

Zoom | Export | Clear All



1 2 3 4

Signal processing

Signal processing aims to improve quality of the spectra before modeling (e.g. by removing undesired spectral variation). In this respect, it improves also the results of quantitative and qualitative spectral models.

The methods must be carefully chosen in order to avoid removing important physical information.

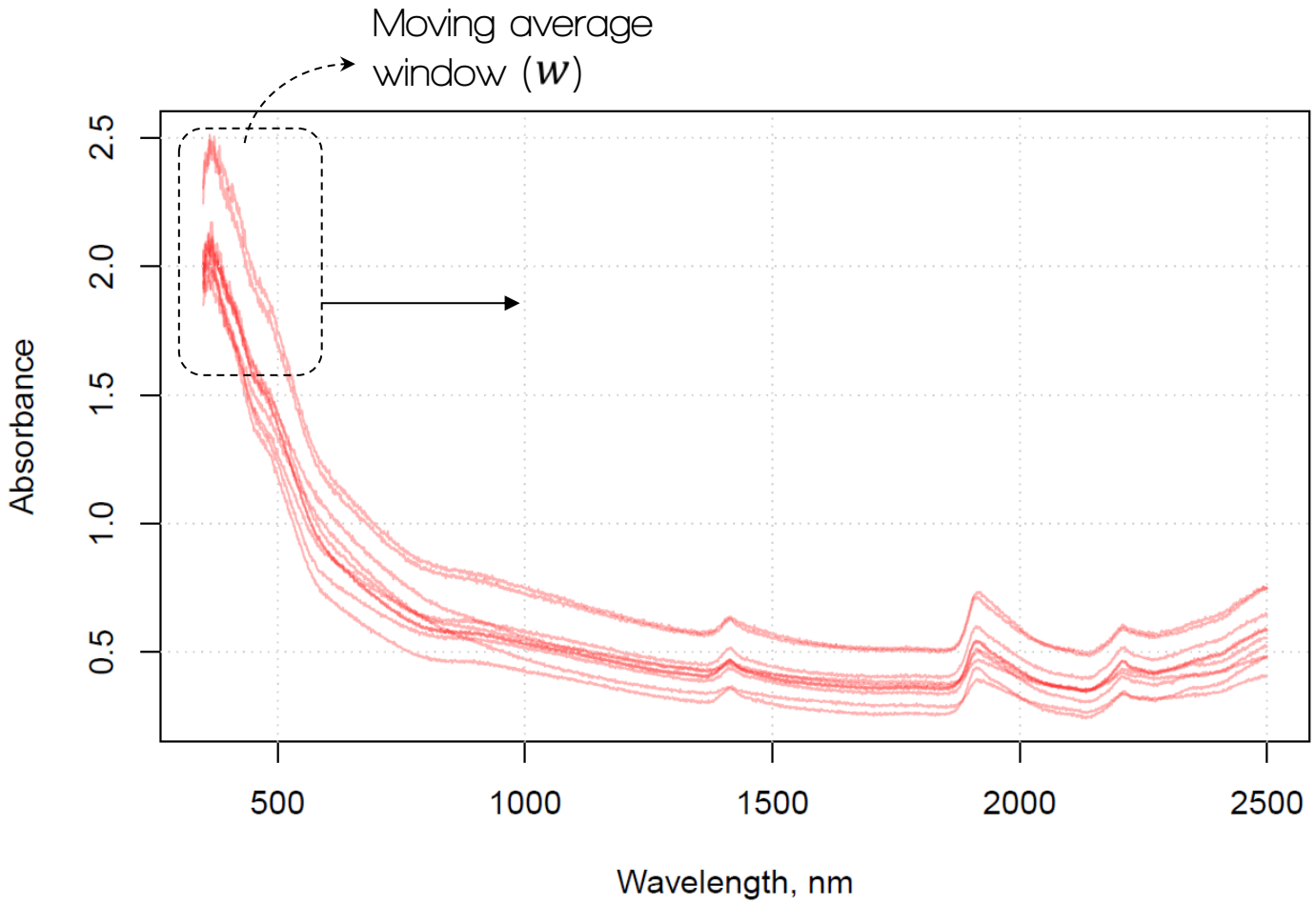
Some of the most common signal processing methods are:

- Splice correction
- Spectra transformation (e.g. reflectance to absorbance)
- Noise removal
- Resampling
- Differentiation
- Scatter correction
- Centering and scaling

Spectra transformation and noise removal

See file: 02_preprocessing_I.R

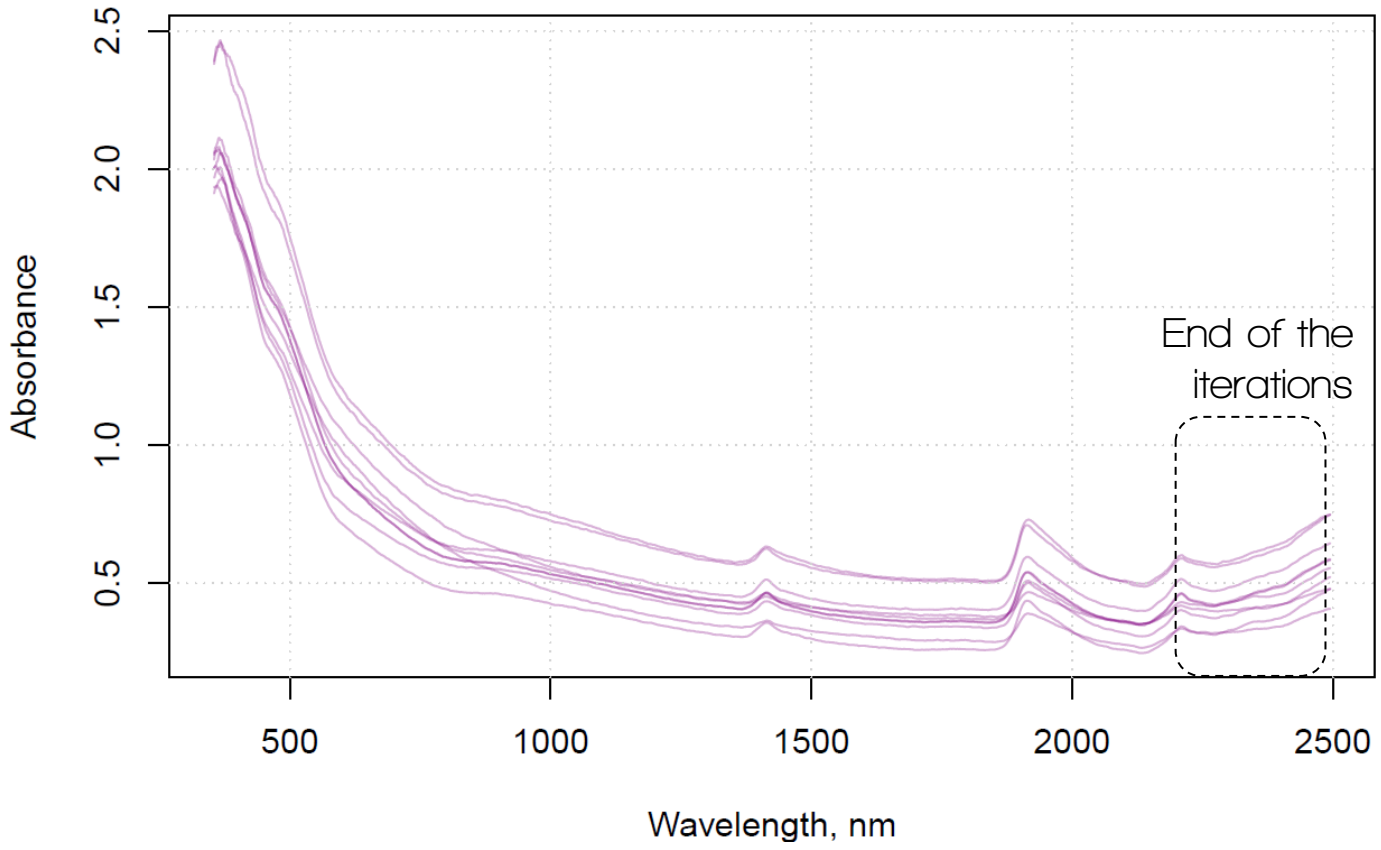
Moving average



Spectra transformation and noise removal

See file: 02_preprocessing_I.R

Moving average



Spectra transformation and noise removal

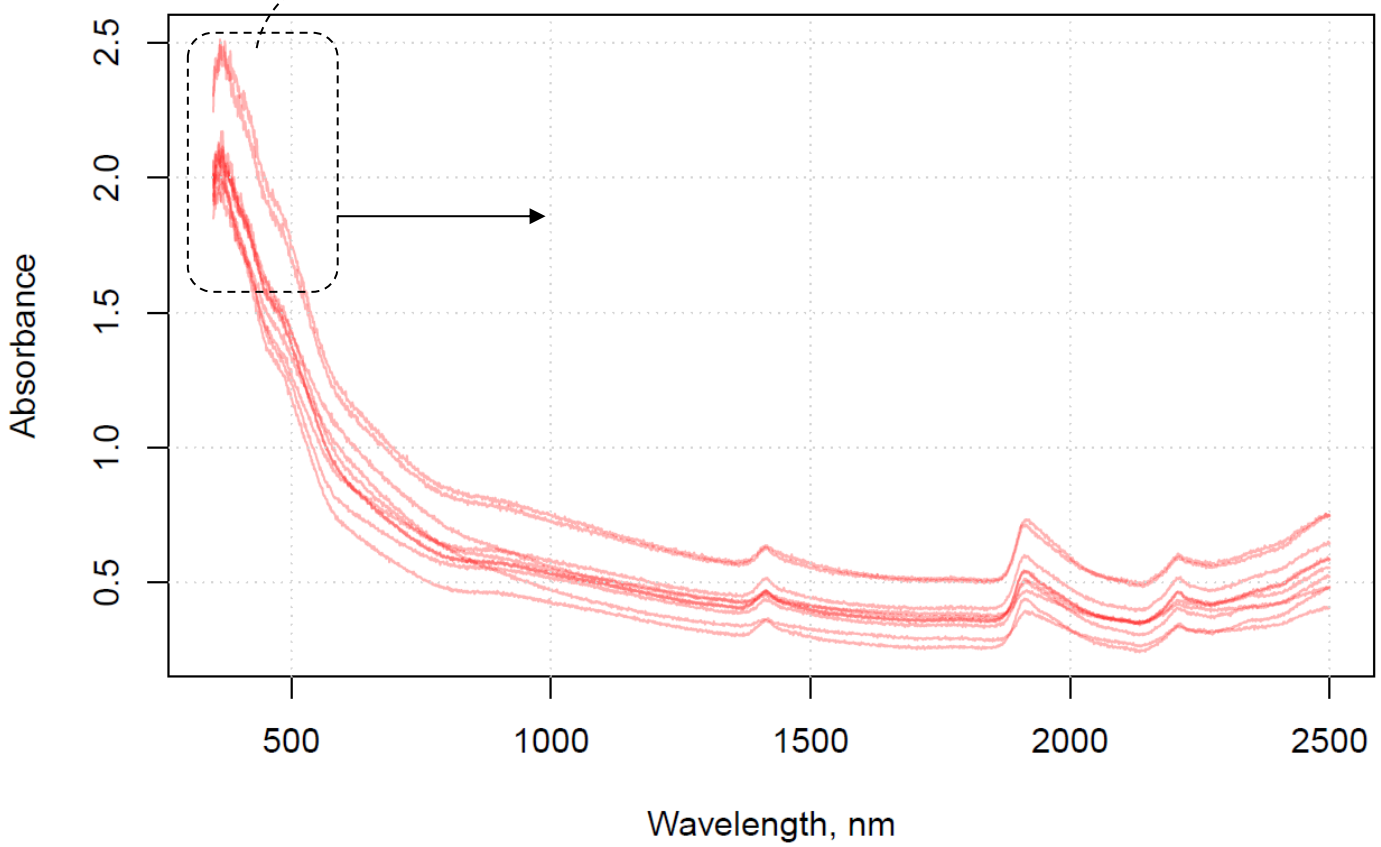
See file: 02_preprocessing_I.R

Savitzky–Golay filter

Polynomial order

Moving Polynomial fit window (w)

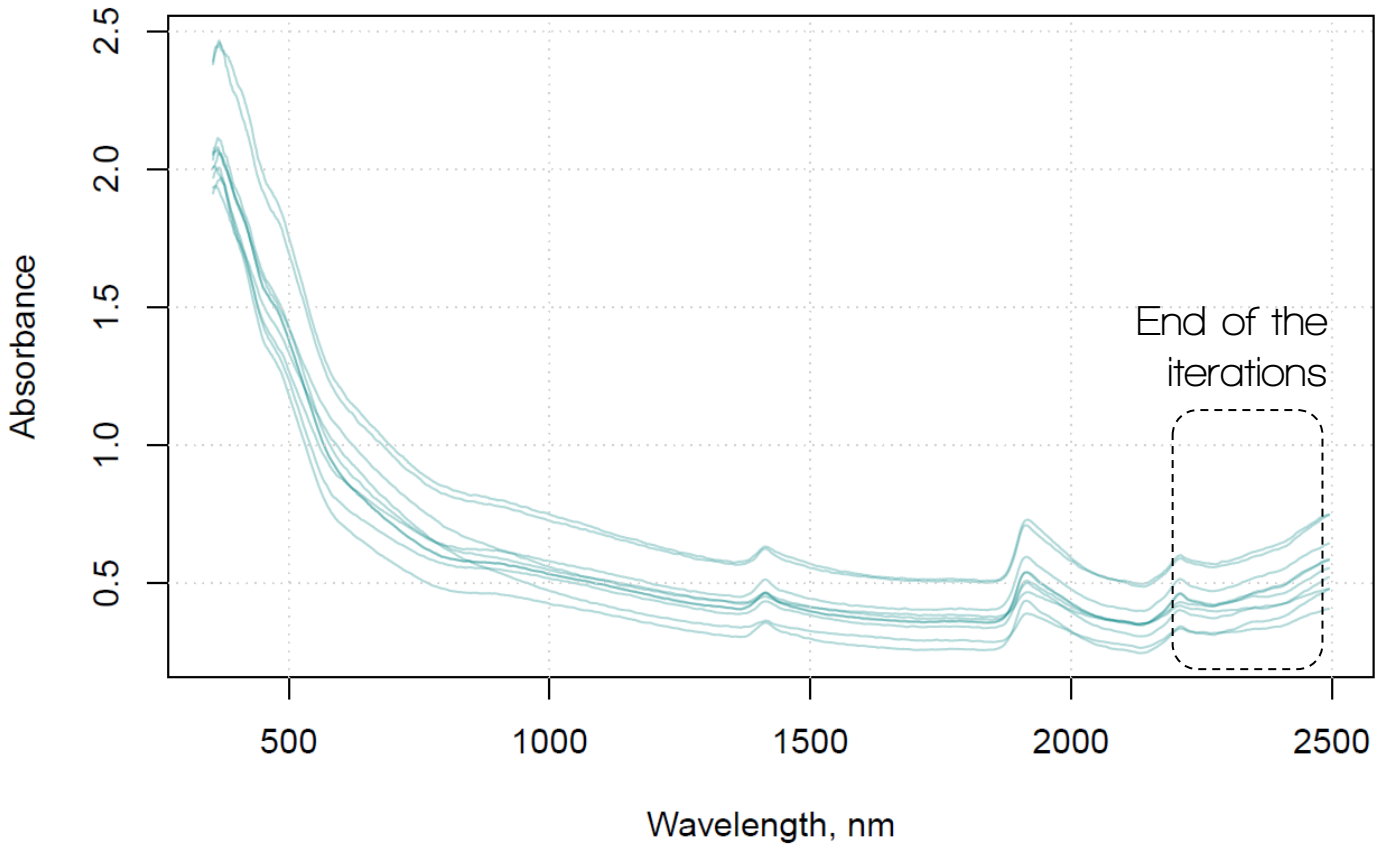
$$x_{sg} = b_p\, x^{p} + \cdots + b_1\, x + b_0$$



Spectra transformation and noise removal

See file: 02_preprocessing_I.R

Savitzky–Golay filter

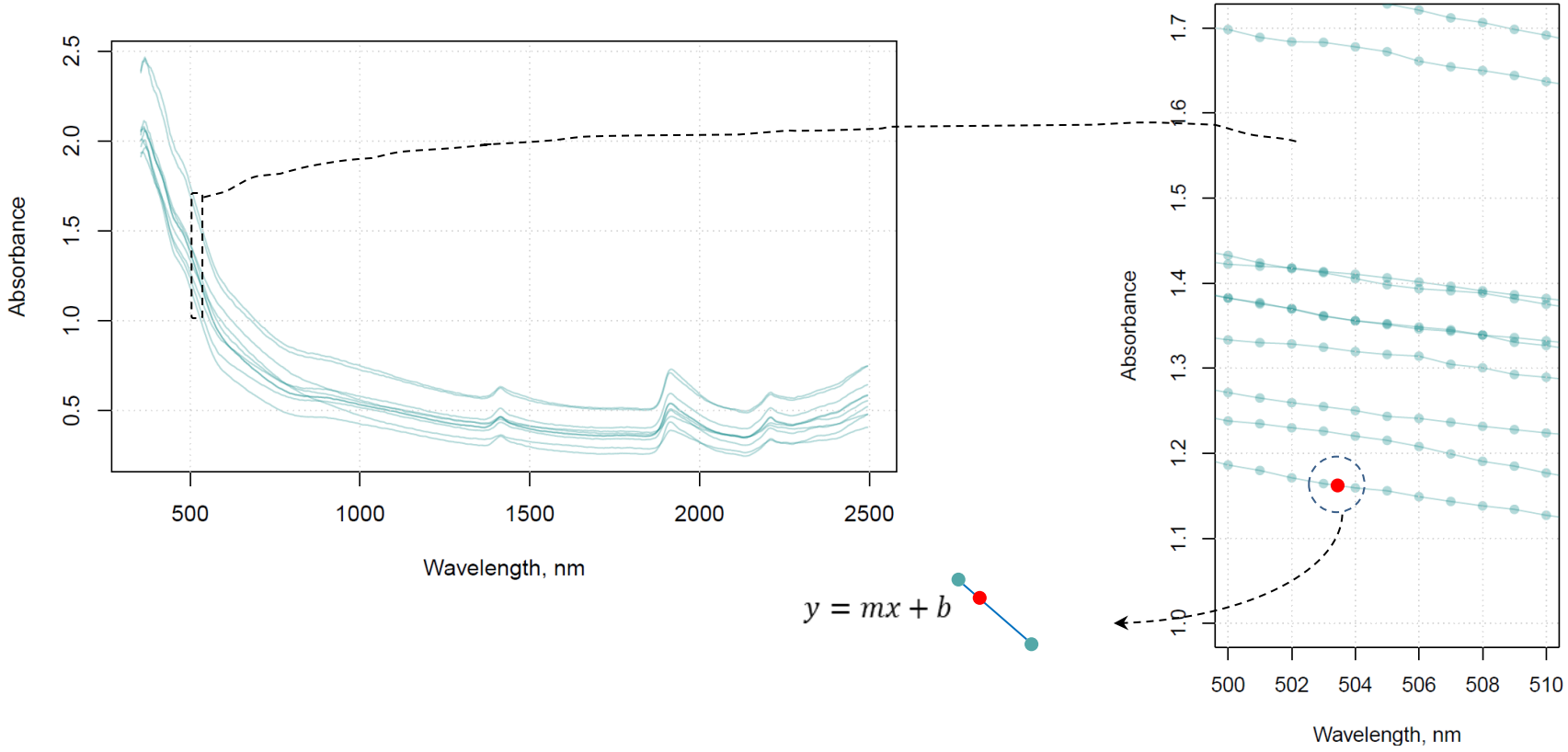


Resampling

See file: 02_preprocessing_I.R

Resampling (also known as interpolation)

Example: if the first wavelength of the new set of wavelengths (at wich the spectra needs to be resampled) is 504.3 nm, the two wavelengths at the right and left sides of the new point are taken. Then a linear model is fitted between these two points and this models is then used to estimate the intensity at the new wavelength



Differentiation

See file: 3.Preprocessing_II.R

Advantages

- Remove additive baseline shifts
- Helps to resolve absorption overlapping
- Compensates for some instrumental drifts
- Enhances small spectral absorption features
- Often increases the predictive accuracy for complex datasets

Drawbacks

- Increased risk of overfitting if not carefully managed
- Amplifies noise, requiring additional smoothing
- Can lead to increased uncertainty in model coefficients
- May complicate spectral interpretation
- Removes baseline information, which may be important in some contexts

First and second derivatives of a spectrum can be computed with the finite difference method (difference between to subsequent data points), assuming that the band width is constant:

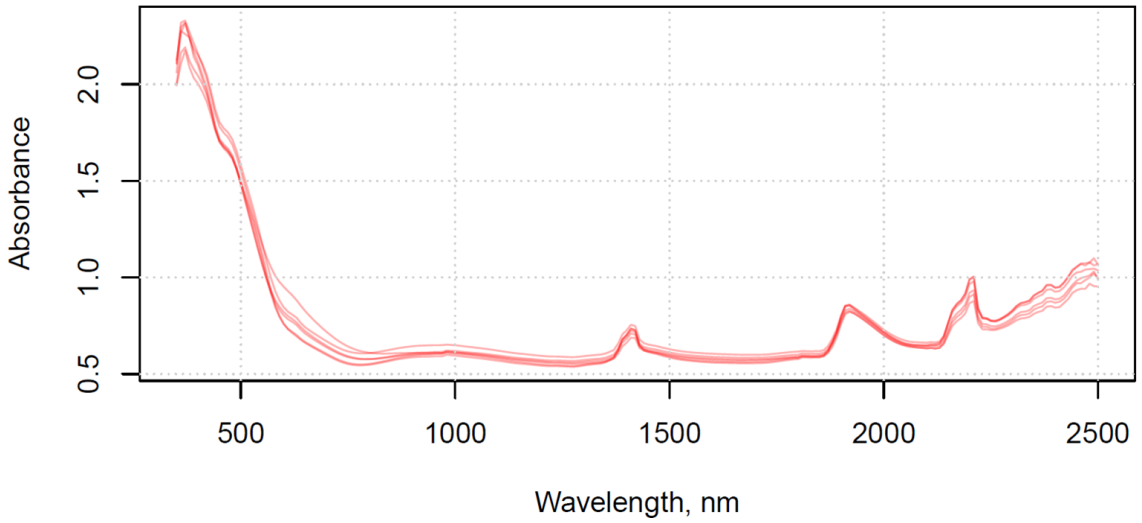
First derivative $x_i' = x_i - x_{i-1}$

Second derivative $x_i'' = x_{i-1} - 2\,x_i + x_{i+1}$

Differentiation

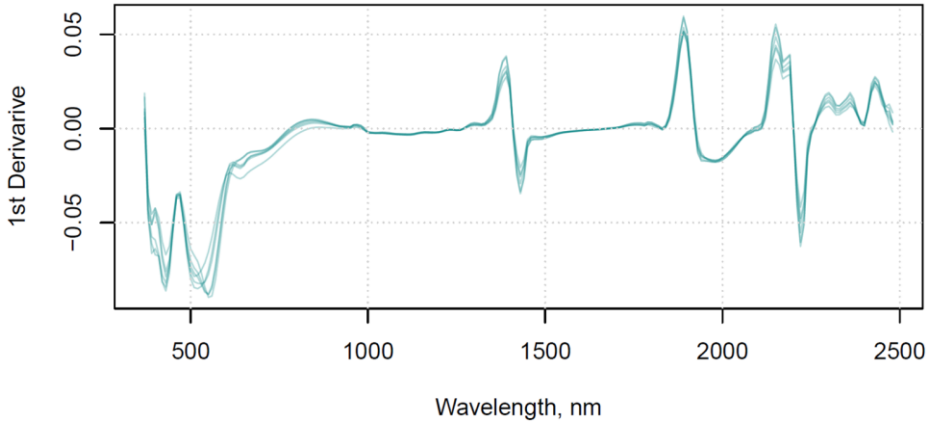
See file: 3.Preprocessing_II.R

Original absorbance spectra of a soil profile

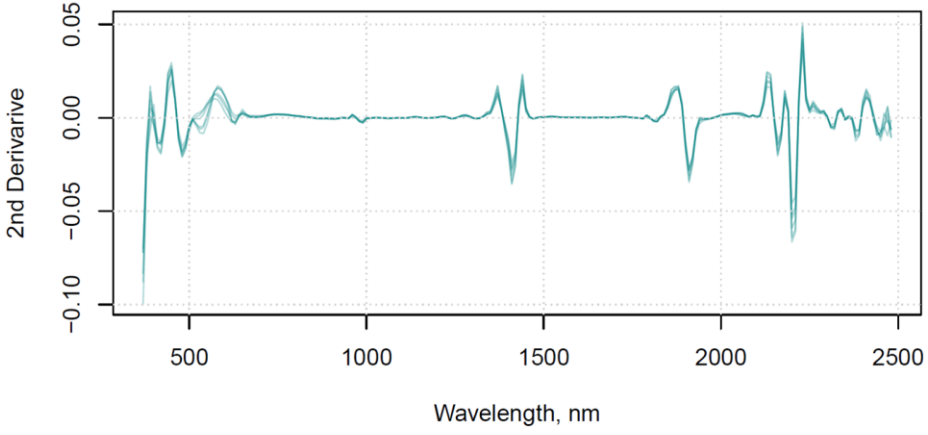


Using the savitzkyGolay function both the first and second derivative spectra, can be computed

First derivative spectra



Second derivative spectra



Standard Normal Variate (SNV)

See file: 04_preprocessing_III.R

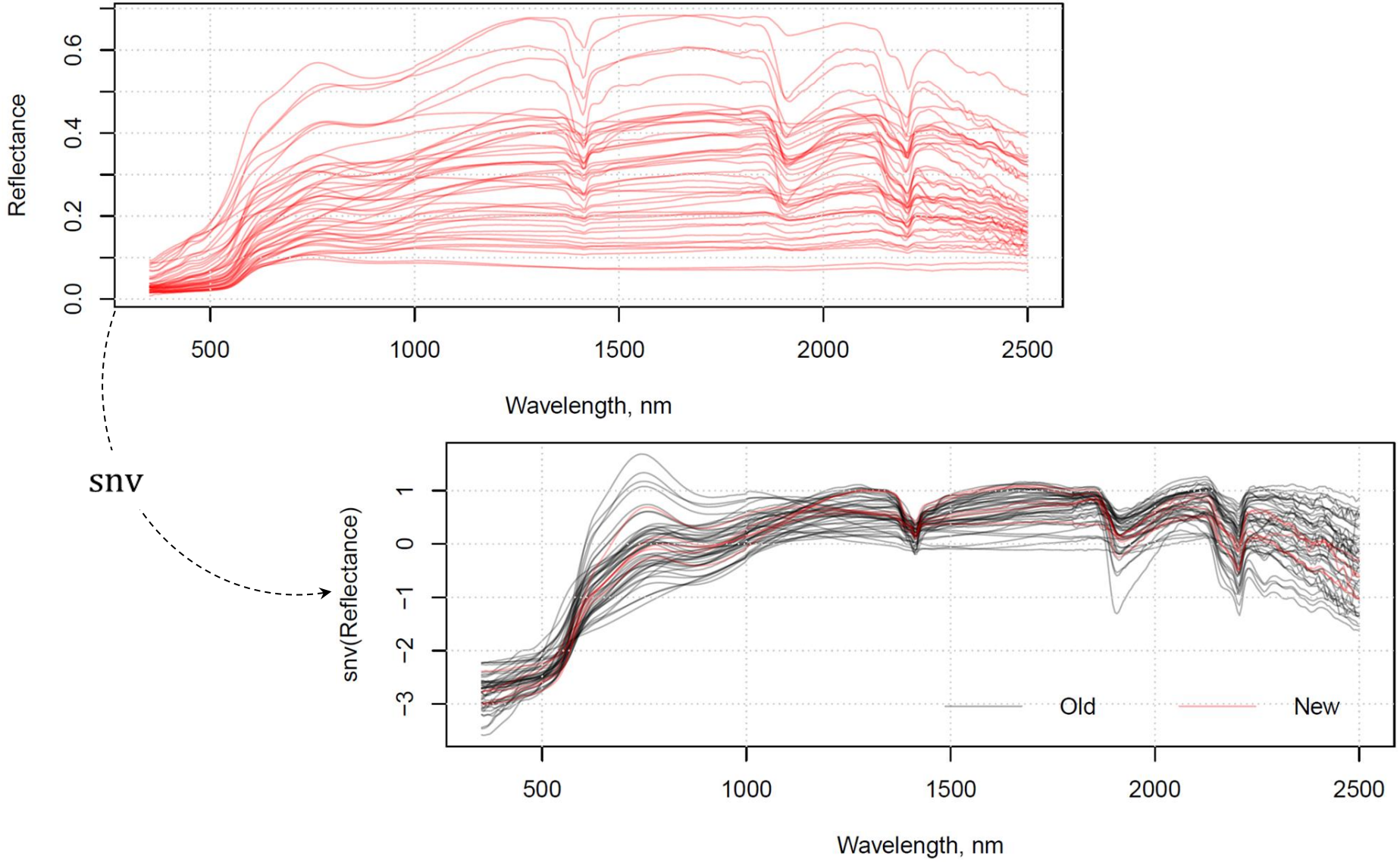
SNV (Standard Normal Variate) is a straightforward method for normalizing spectra, correcting for both multiplicative scatter effects and additive baseline shifts by centering and scaling the data. For a given spectrum x_i, it is applied as follows:

$$\mathrm{snv}(x_i) = \frac{x_i - \bar{x}_i}{s(x_i)}$$

where $\bar{x}_i$and $s(x_i)$ represent the single mean and standard deviation values of the spectrum.

Standard Normal Variate (SNV)

See file: 04_preprocessing_III.R



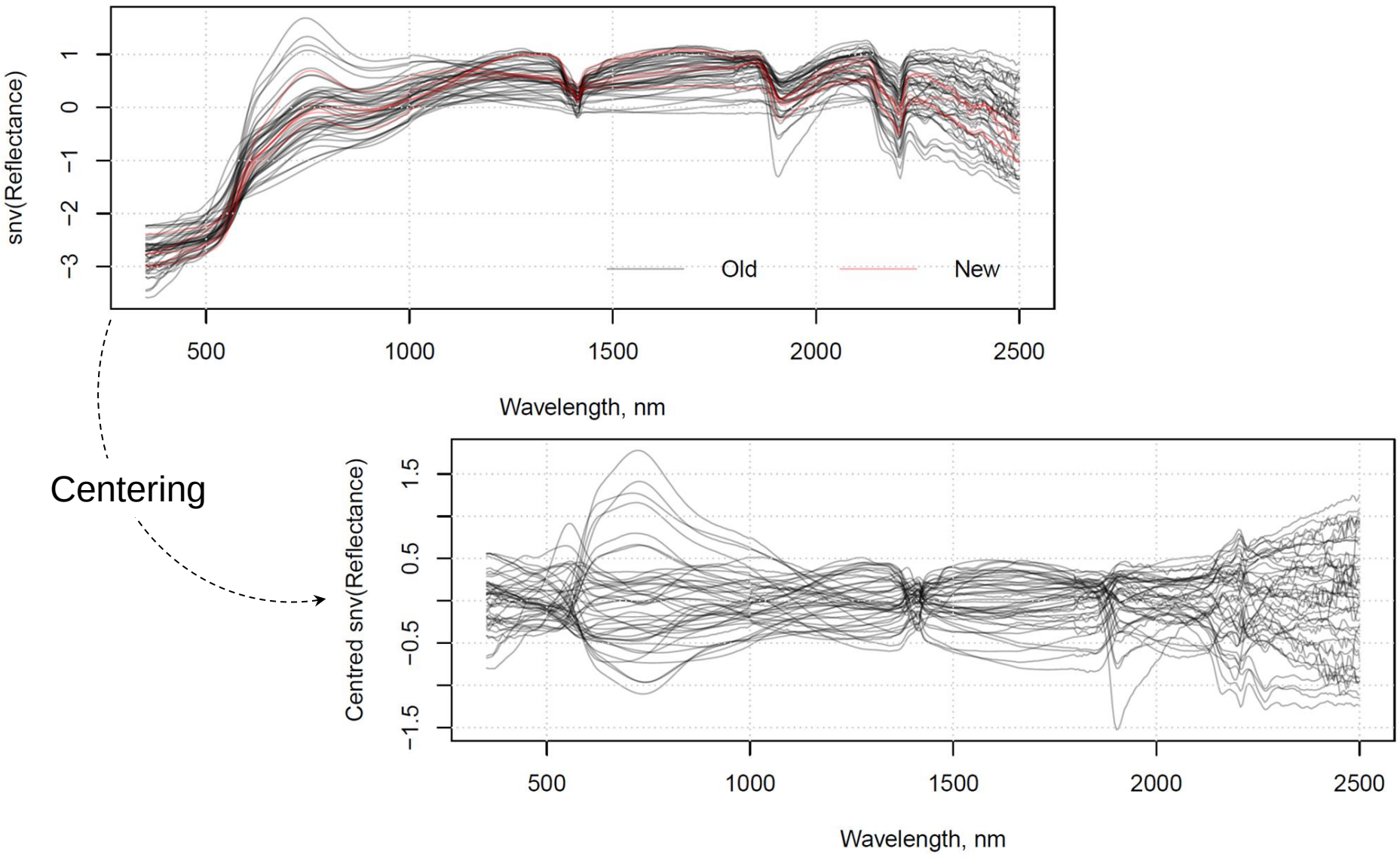
Centering and scaling

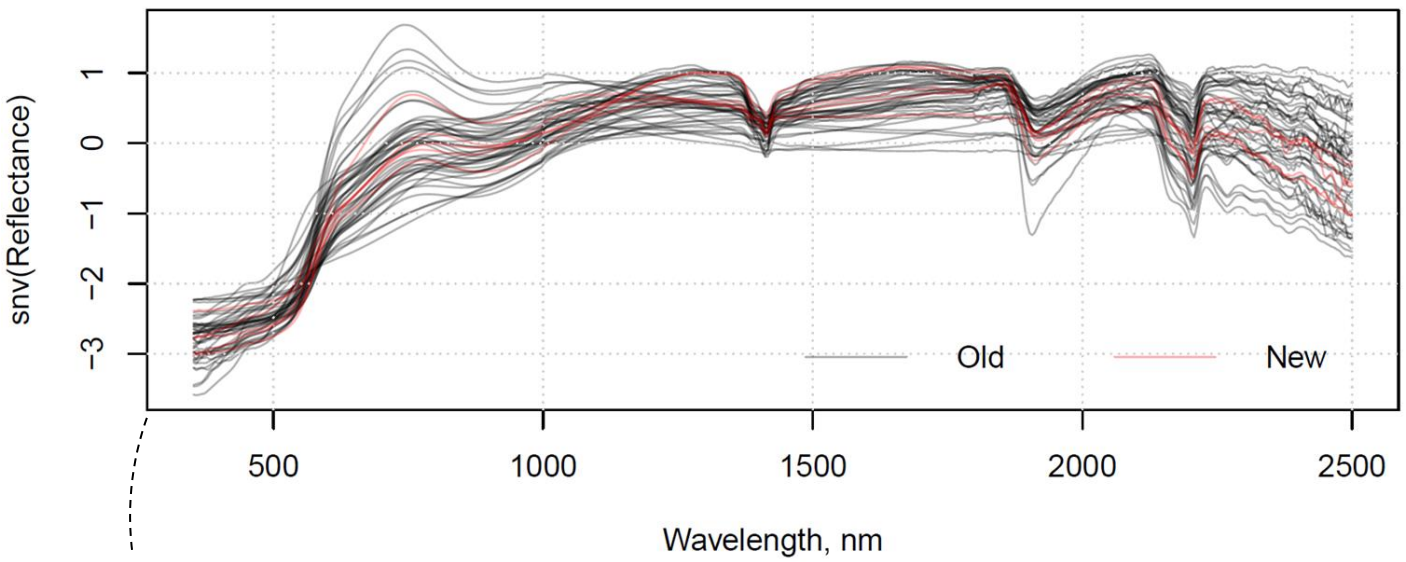
See file: 04_preprocessing_III.R

- Centering involves transforming a matrix so that its columns have a zero mean by subtracting the column mean from each row, simplifying the model by eliminating the need for an intercept.

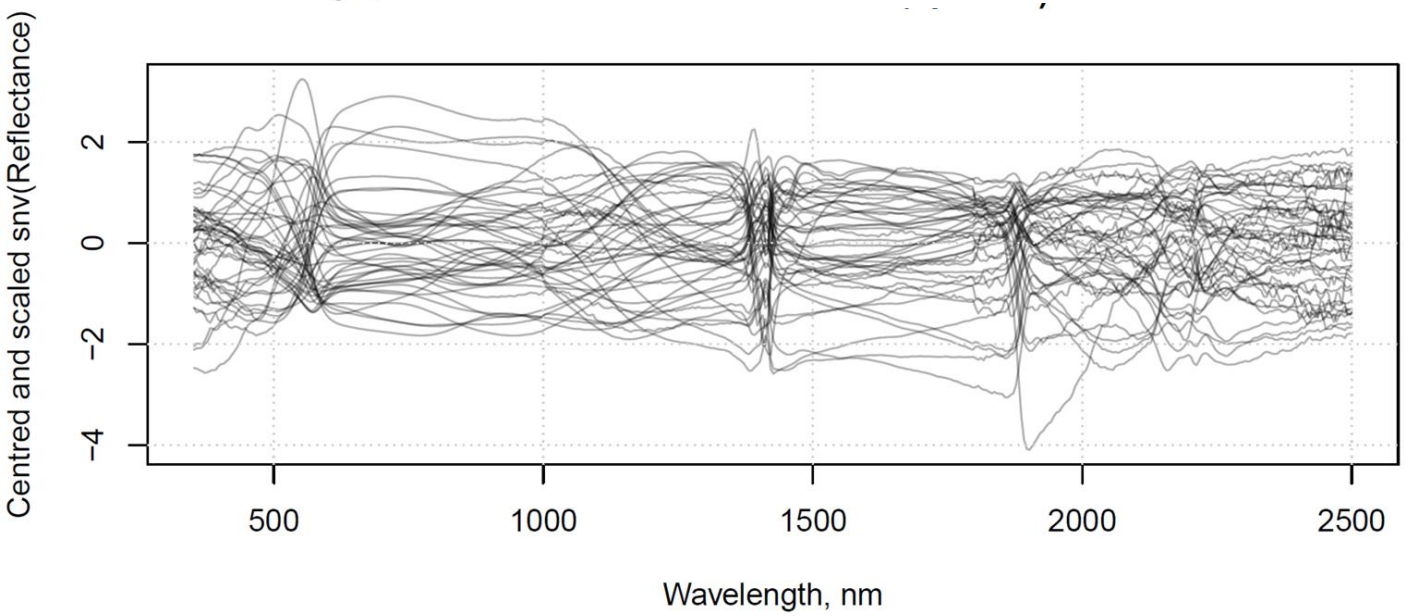
- Scaling adjusts the matrix so that its columns have the same variance by dividing each row by the column's standard deviation, ensuring all variables are on the same scale. Both operations are typically applied after data transformation to enhance model simplicity and comparability, though they don't always guarantee improved model performance.

The `scale()` function in R can be used for applying either centering and scaling or both


snv(Reflectance)
1
0
−1
−2
−3
Old
New
500
1000
1500
2000
2500
Wavelength, nm
Centering
Centred snv(Reflectance)
1.5
0.5
−0.5
−1.5
500
1000
1500
2000
2500
Wavelength, nm



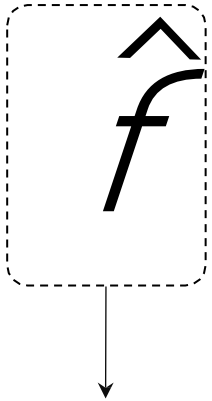
Centering
and
scaling



To *scale* or not to *scale*?

- Scaling will down-scale variables with large variation, but can inflate exaggeratedly variables with small variance (e.g. variables with no variation but small noise).
- Decision depends on the data pre-treatment also: is it meaningful?
- For instance, variation in some variables is greater than in other for good reasons (e.g. absorption features in continuum removed spectra, 1st derivative), so that *scaling* is not appropriate and will reduce model interpretability
- *Centering and scaling* is sensitive to outliers. A robust scaling can be computed using the median instead of the mean and the median absolute deviation (MAD) instead of the standard deviation

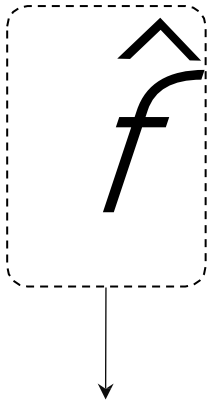
NIR Applications



Function that can be approximated by using chemometrics/machine learning

These functions are device-, product- and property-specific.

NIR Applications

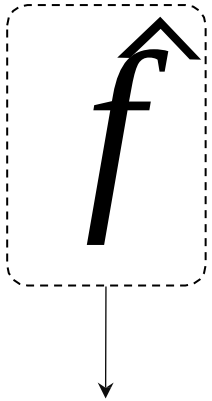


Function that can be approximated by using chemometrics/machine learning

These **functions are device-, product- and property-specific.**

For each product we build and group a set of functions that quantify relevant product properties (e.g. moisture, protein, fat). **This group of functions is called application.**

NIR Applications



Function that can be approximated by using chemometrics/machine learning

We currently use our own BUCHI software for that!

These **functions are device-, product- and property-specific.**

For each product we build and group a set of functions that quantify relevant product properties (e.g. moisture, protein, fat). **This group of functions is called application.**

From a user's perspective, **a NIR device without an application can be perceived as useless.**

We should aim at reducing entry barrier/implementation costs!!!

Implementation

It can be expensive
- Hardware and software costs
- Cost of reference analyses
- Elevated time investments
- People

Routine analysis

It can make boost the efficiency of your lab:
- Reduces need of conventional methods
- A sample is measured in matter of seconds
- Requires periodic validation and model/method updates

We should aim at reducing entry barrier/implementation costs!!!

Time to routine!

Implementation

It can be expensive
- Hardware and software costs
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- Elevated time investments
- People

Routine analysis

It can make boost the efficiency of your lab:
- Reduces need of conventional methods
- A sample is measured in matter of seconds
- Requires periodic validation and model/method updates

Main users

- Big farms (soil, plant tissues, fertilizers, final product, etc)
- Service labs
- Research institutes/Universities

NIR/IR Spectroscopy – An equation for success

Success = f (hardware, software, data, models, people, automation, ...)

debunking myths

1. Could soil spectroscopy eventually **replace** conventional methods?

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Advances in Agronomy

Volume 132, 2015, Pages 139-159

Chapter Four - Soil Spectroscopy: An Alternative to Wet Chemistry for Soil Monitoring

Marco Nocita [*] [§], Antoine Stevens [§], Bas van Wesemael [§], Matt Aitkenhead [¶], Martin Bachmann [‖], Bernard Barthès [#], Eyal Ben Dor [**], David J. Brown [§§], Michael Clairotte [#], Adam Csorba [¶¶], Pierre Dardenne [‖‖], Jose A.M. Demattê [##], Valerie Genot [†], Cesar Guerrero [***], Maria Knadel [§§§], Luca Montanarella [*], Carole Noon [§], Leonardo Ramirez-Lopez [¶¶¶], Jean Robertson [¶], Hiro Sakai [‖‖‖]... Johanna Wetterlind [§§§§]

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Do we really need large spectral libraries for local scale SOC...

Soil and Tillage Research, Volume 155, 2016, p...

César Guerrero, ..., Raphael A. Viscarra Rossel

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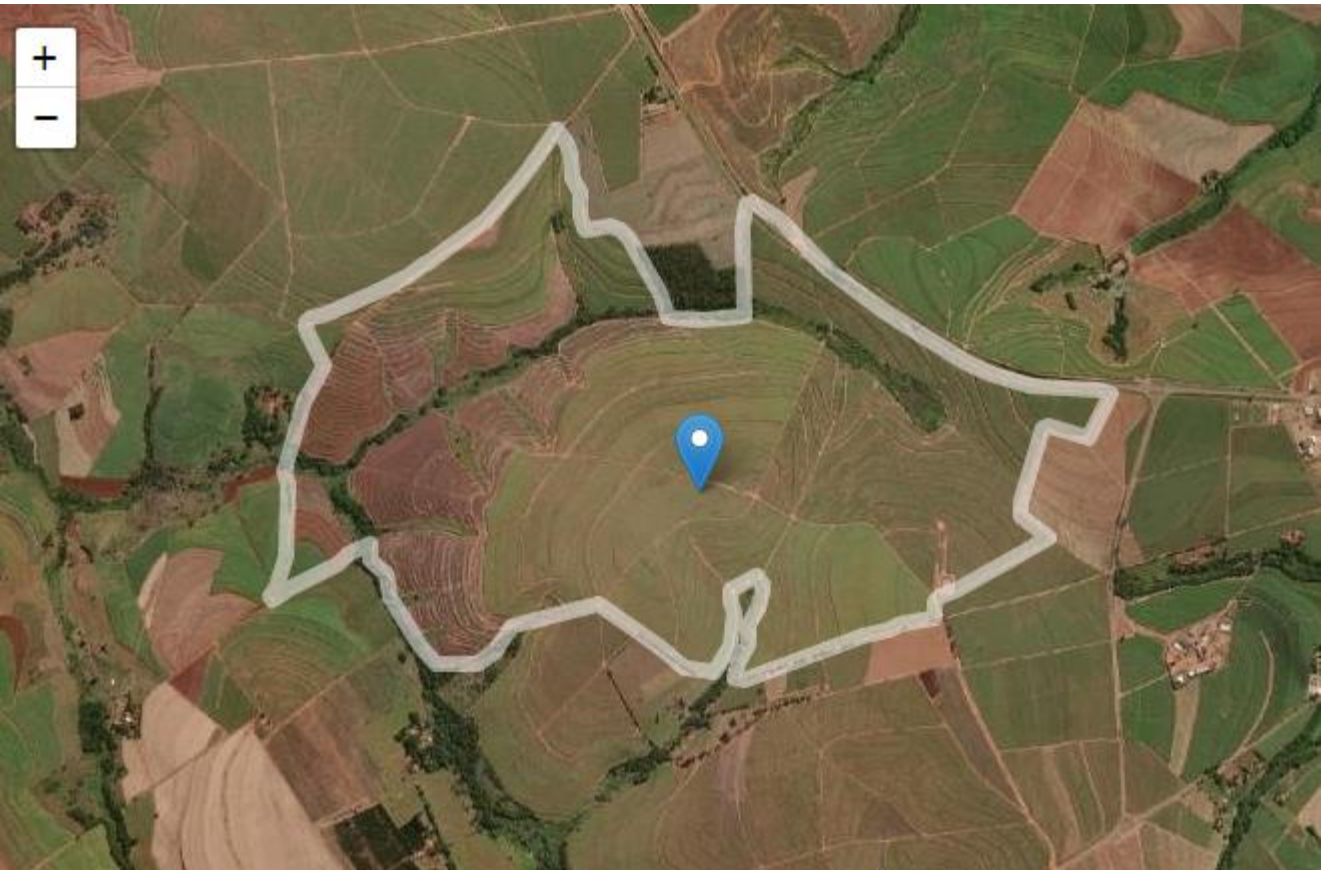
Example: NIR spectroscopy for soil mapping and management

Ramirez-Lopez, Leonardo, et al. "Robust soil mapping at the farm scale with vis–NIR spectroscopy." *European Journal of Soil Science* 70.2 (2019): 378-393.

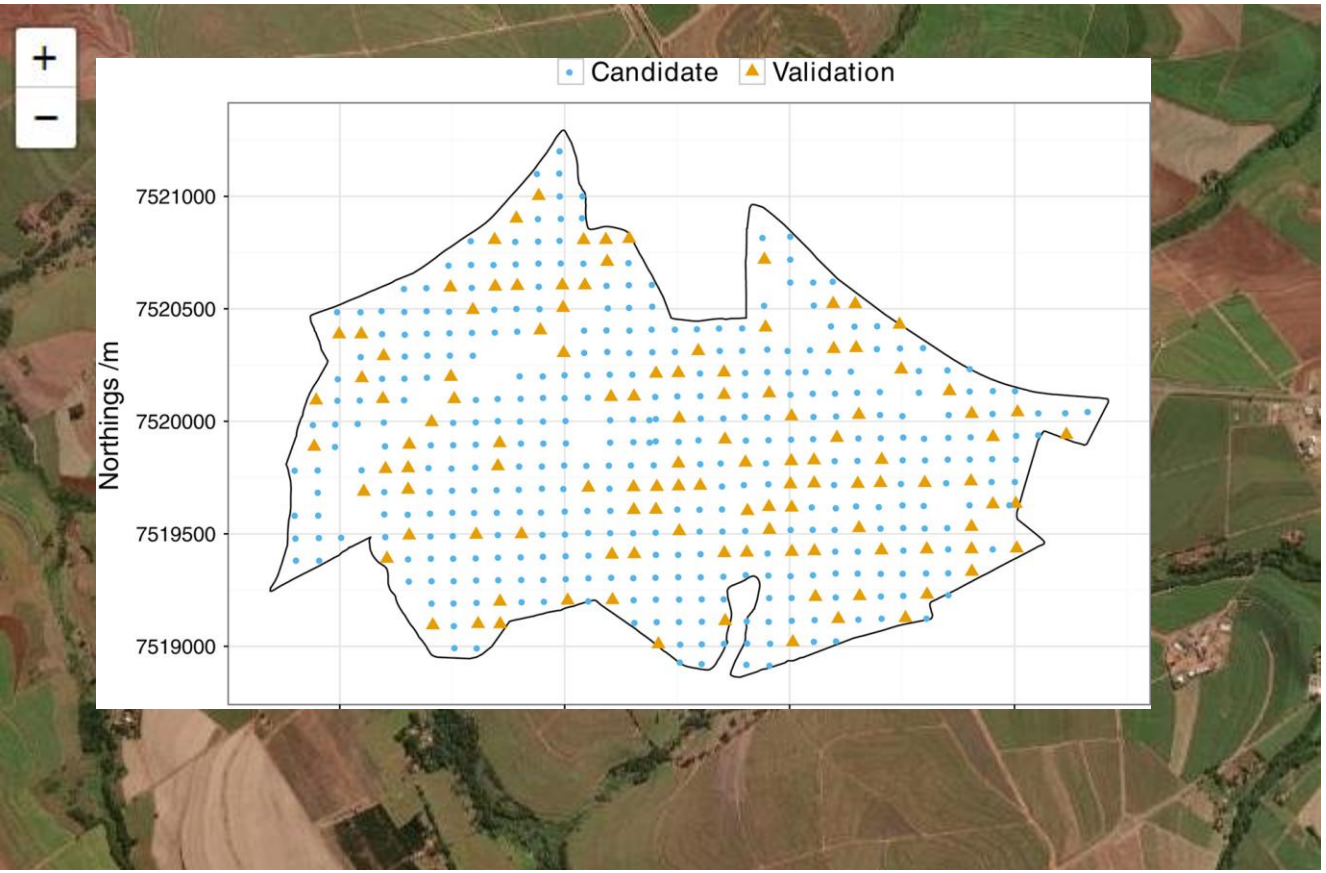
Example:
473 ha in the municipality of Barra Bonita (Brazil)

Sampling at two depths (A: 0 – 20 cm; B: 80 – 100 cm)
Total samples: 910

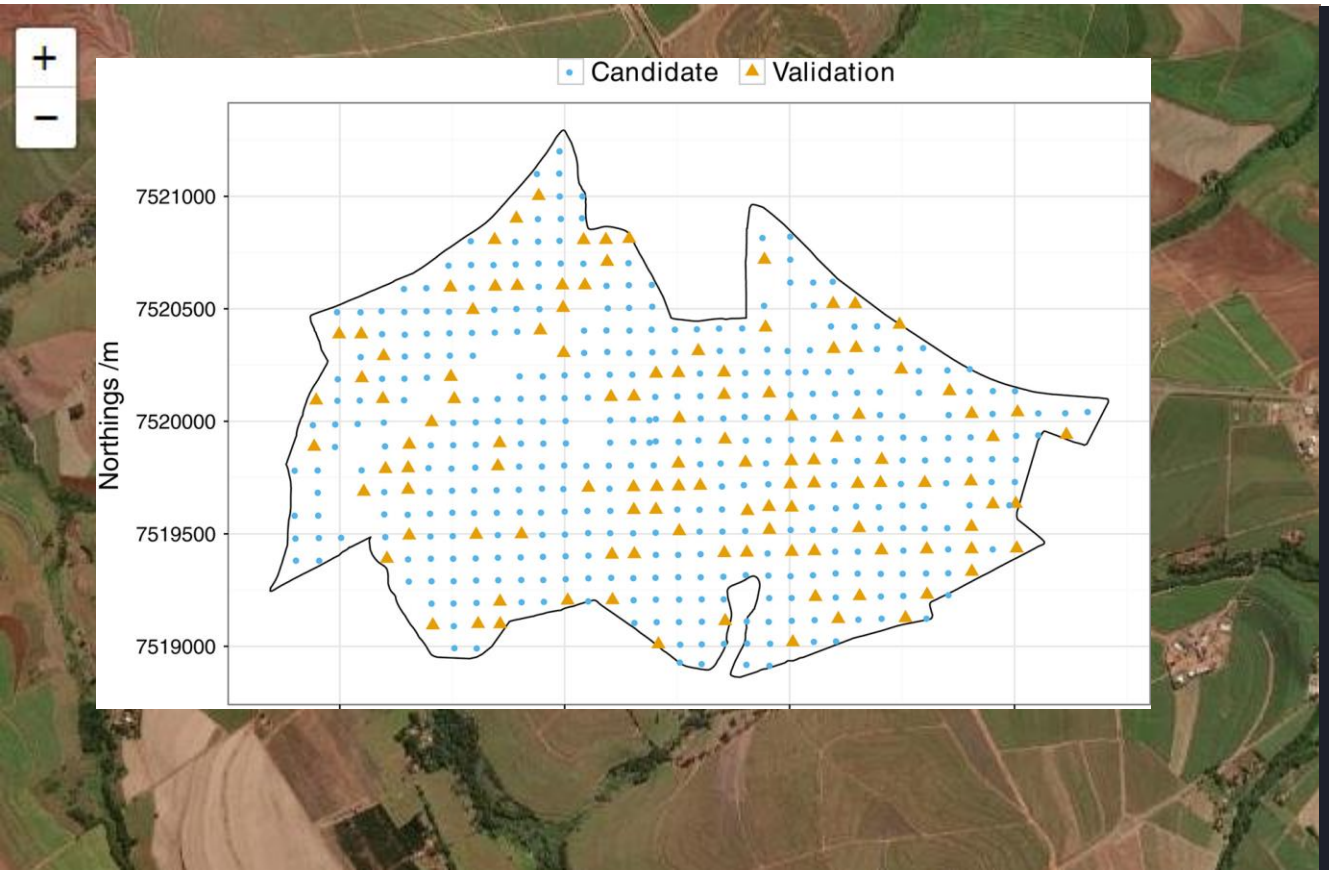


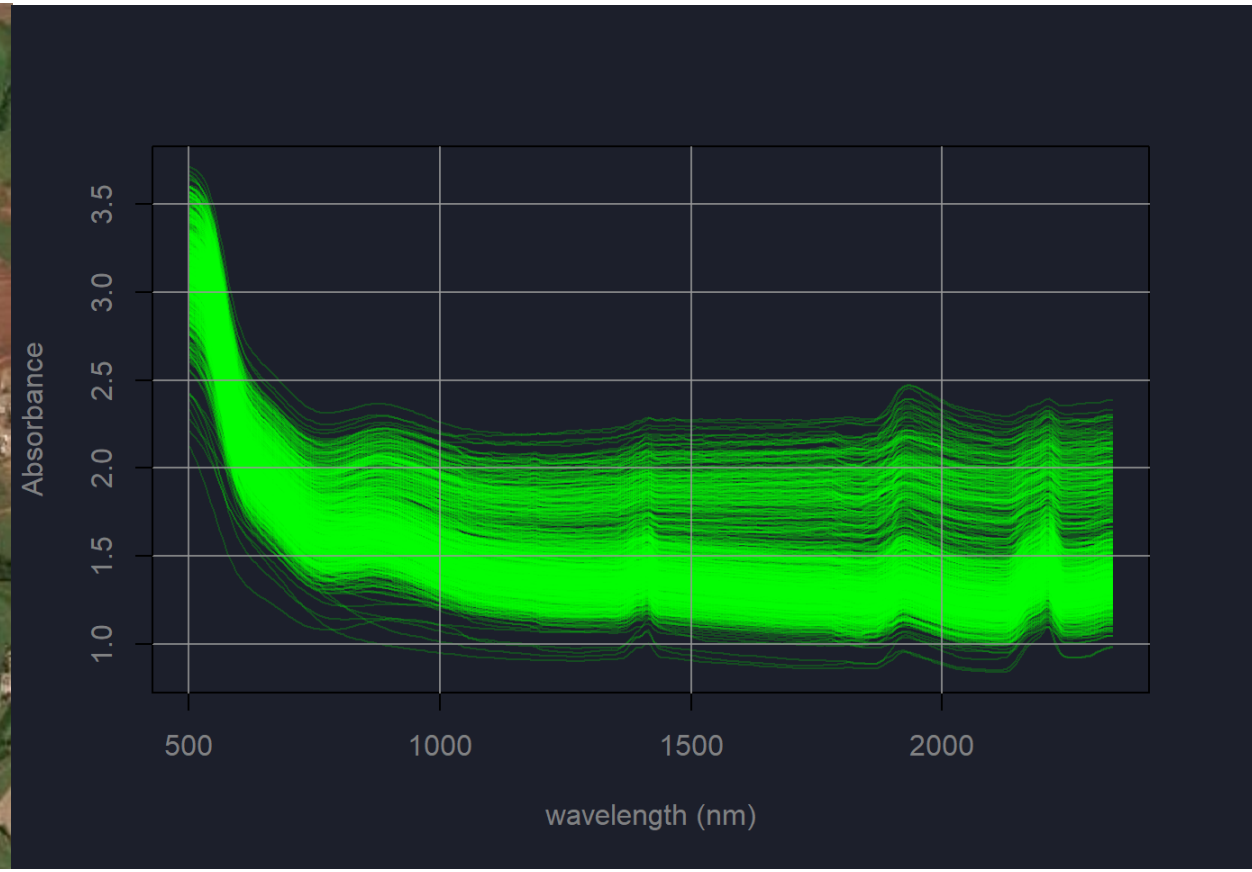
Example:
473 ha in the municipality of Barra Bonita (Brazil)

Sampling at two depths (A: 0 – 20 cm; B: 80 – 100 cm)
Total samples: 910



Sampling at two depths (A: 0 – 20 cm; B: 80 – 100 cm)
Total samples: 910





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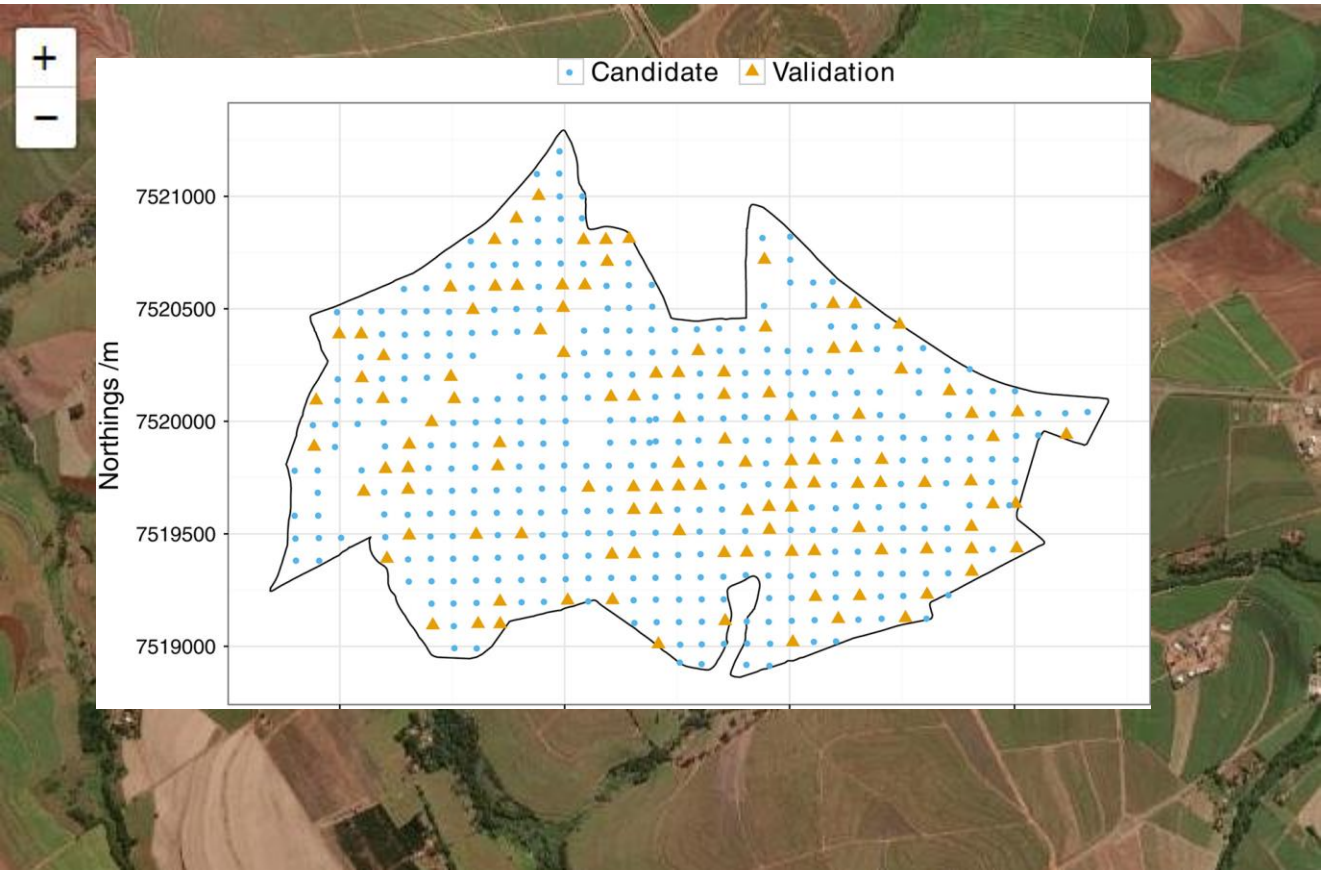
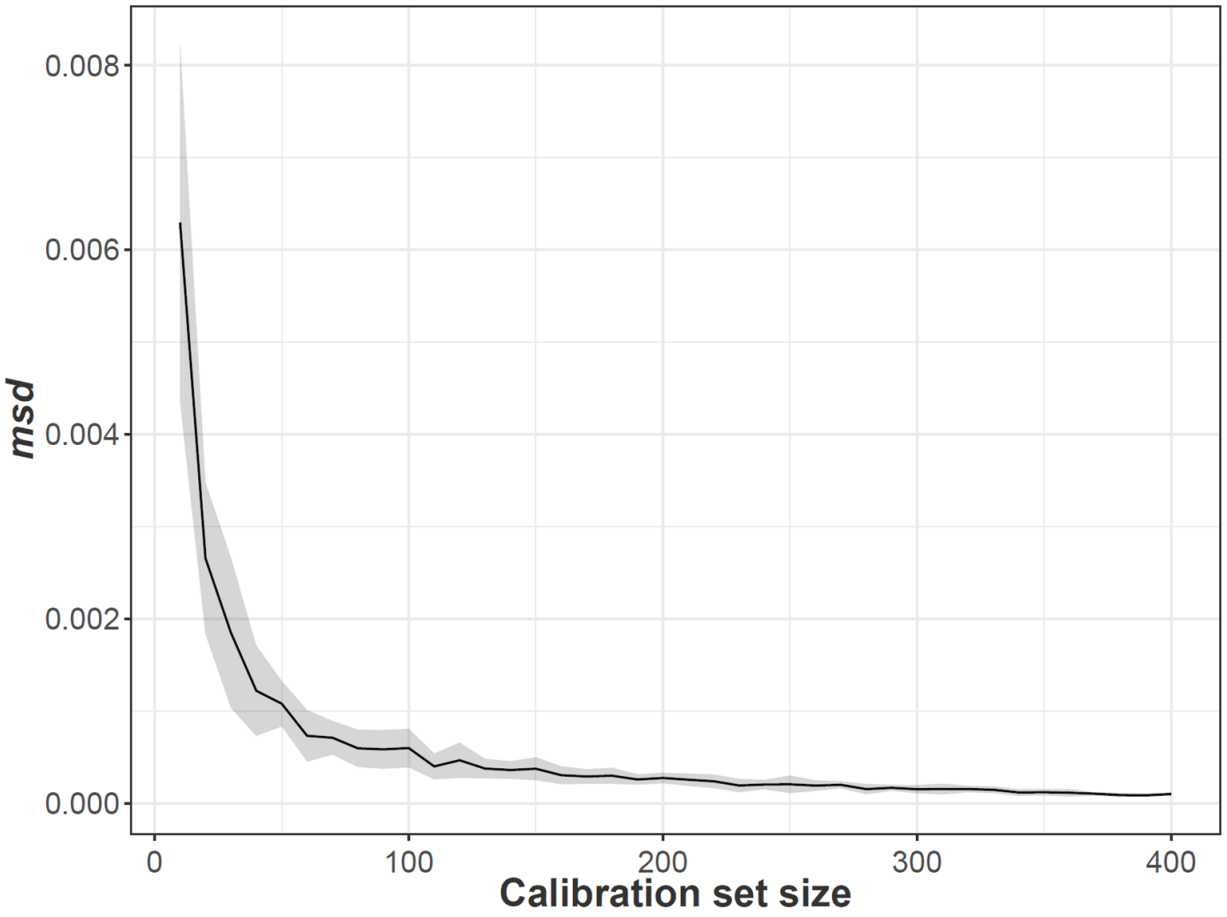
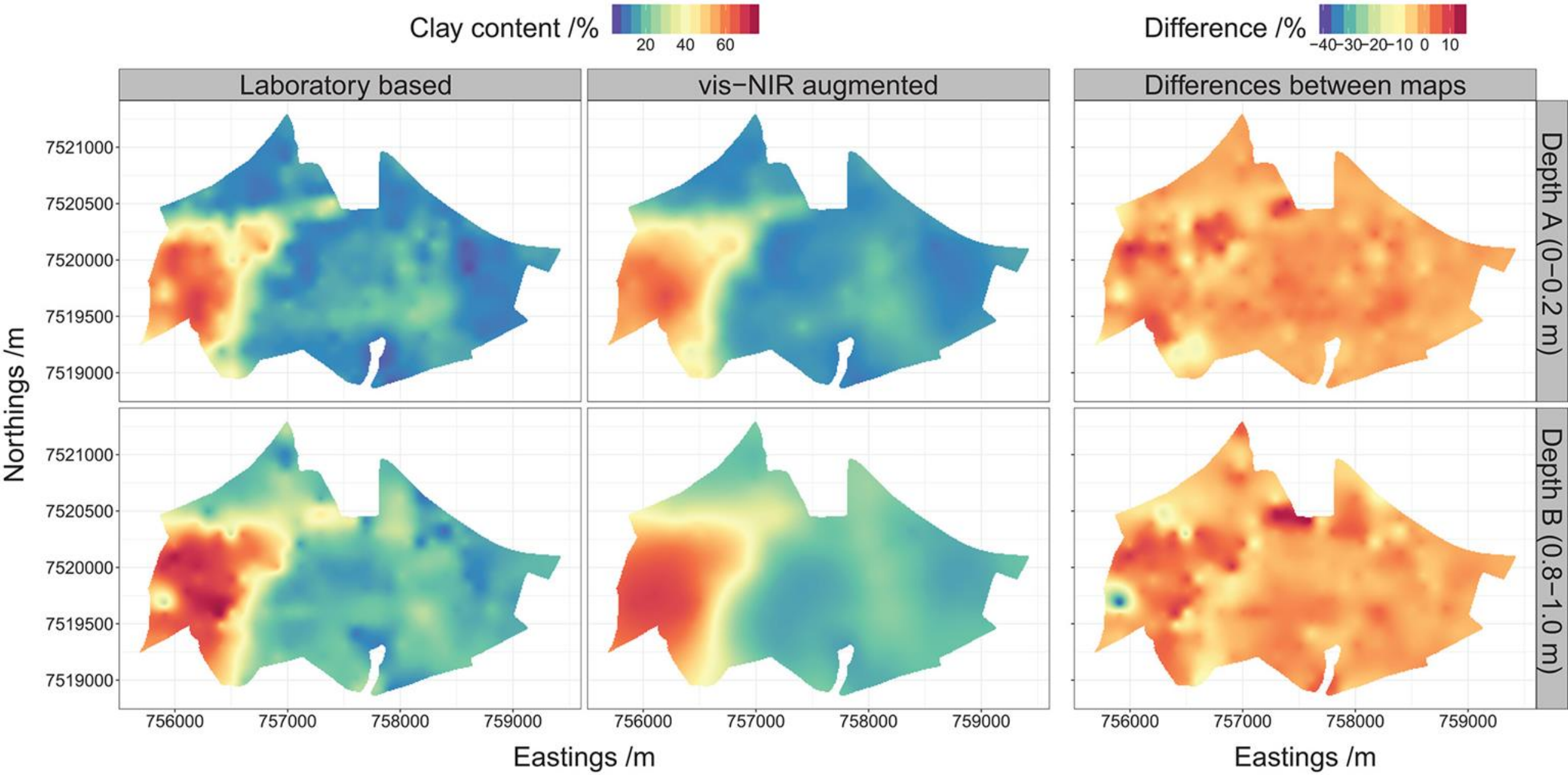
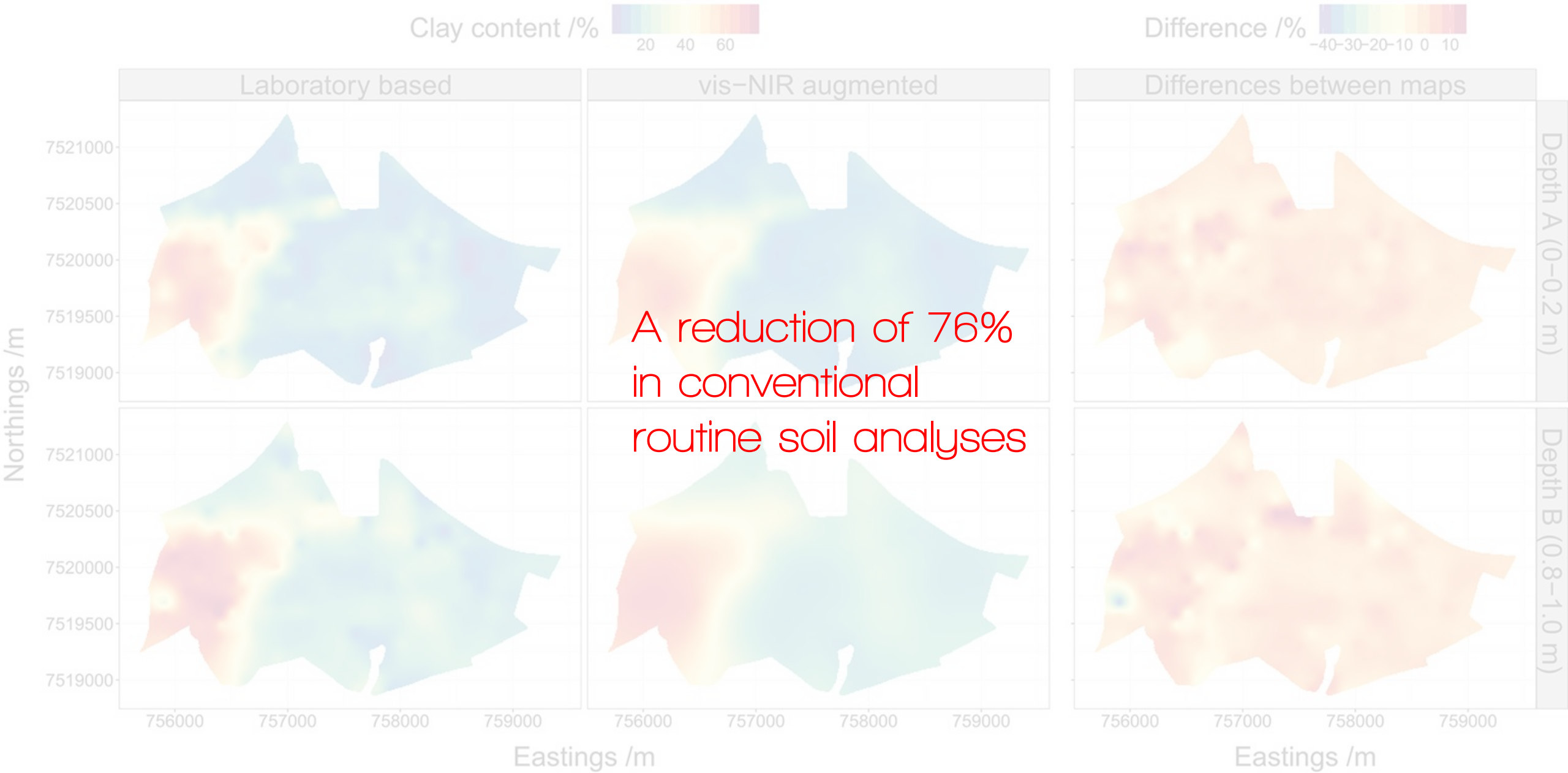


Optimal calibration size: 180 samples




Clay content /%
20
40
60
Difference /%
−40
−30
−20
−10
0
10
Laboratory based
vis−NIR augmented
Differences between maps
Depth A (0−0.2 m)
Depth B (0.8−1.0 m)
Northings /m
7521000
7520500
7520000
7519500
7519000
756000
757000
758000
759000
Eastings /m



A reduction of 76% in conventional routine soil analyses

Scaling soil spectroscopy

Short term

- Learn and adjust

Scaling soil spectroscopy

Short term

Learn and adjust

Mid term

Move to modest amount of samples processed with NIR/IR

Scaling soil spectroscopy

Short term

Learn and adjust

Mid term

Move to modest amount of samples processed with NIR/IR

Long term

Make it fully operational for your properties and move to a significant amount of samples processed with NIR/IR (get all your investments back)

Soil spectroscopy **complements** conventional methods (to different extents)

2. Is soil spectroscopy cheap and fast?

Mmm

Mmmmmmmmmmmmmmm

Mmmmmmmmmmmmmm,
Yeah BUT

Mmmmmmmmmmmmmm,
Yeah BUT not really

Mmmmmmmmmmmmmm,
Yeah BUT not really

Implementation

Routine analysis

Mmmmmmmmmmmmmm,
Yeah BUT not really

Implementation

It can be expensive
- Hardware and software costs
- Cost of reference analyses
- Elevated time investments
- People

Routine analysis

Mmmmmmmmmmmmmm,
Yeah BUT not really

Implementation

It can be expensive
- Hardware and software costs
- Cost of reference analyses
- Elevated time investments
- People

Routine analysis

It can make boost the efficiency of your lab:
- Reduces need of conventional methods
- A sample is measured in matter of seconds
- Requires periodic validation and model/method updates

3. Can **all important soil properties** be quantified?

Let's ask a friend who has read TONS of scientific literature

Sound scientific evidence
[consistently showing good results]

Under research

Sound scientific evidence
[consistently showing good results]

Examples:
- Particle size
- Organic C
- N

Under research

Where do you want go?

Sound scientific evidence
[consistently showing good results]

Under research

4. Are global/universal soil spectroscopy models feasible?

Svalbard, Norway

Svalbard, Norway

Uganda

Mars

Svalbard, Norway

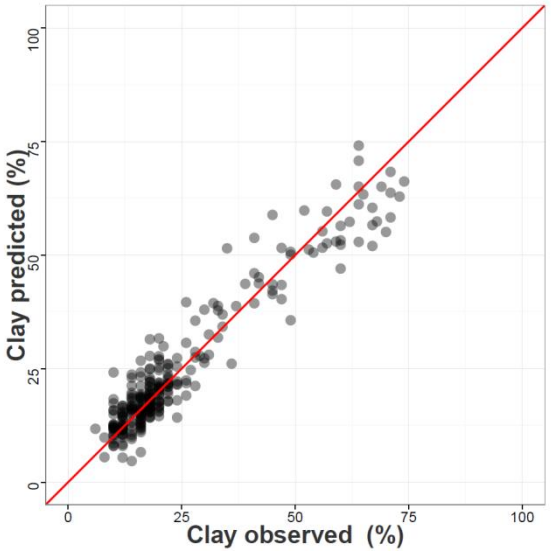
Uganda

Mars

Different soils might require different empirical models

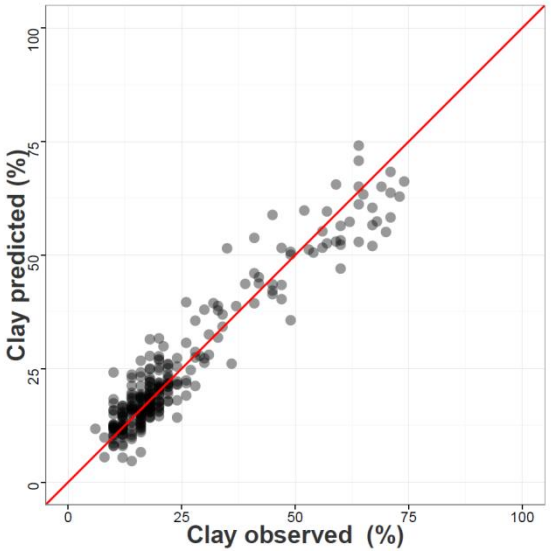
Field scale

R^2 = 0.91; RMSE=5.02%



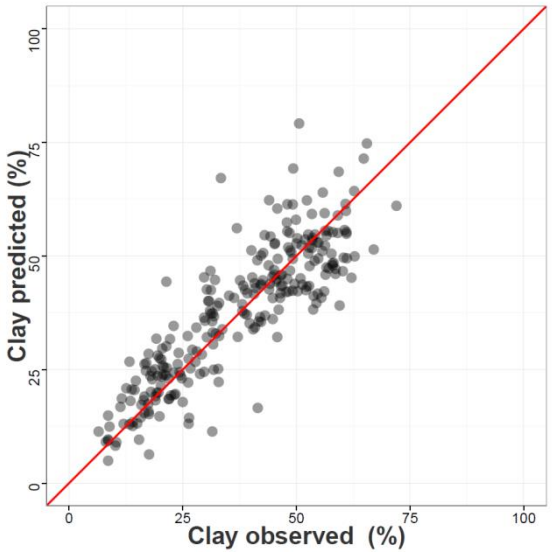
Field scale

R^2 = 0.91; RMSE=5.02%



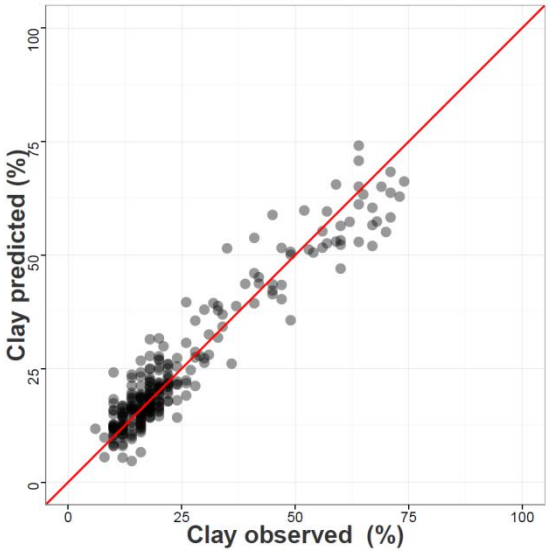
Regional scale

R^2 = 0.75; RMSE=8.03%



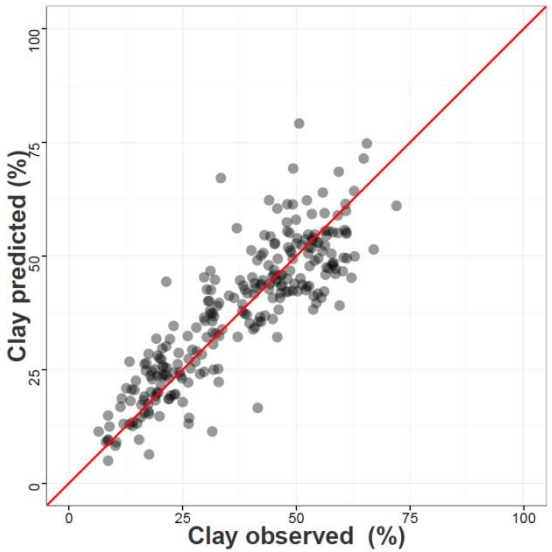
Field scale

R^2 = 0.91; RMSE=5.02%



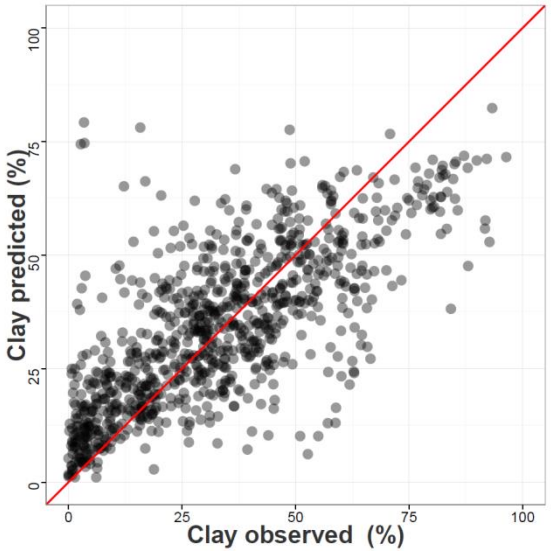
Regional scale

R^2 = 0.75; RMSE=8.03%



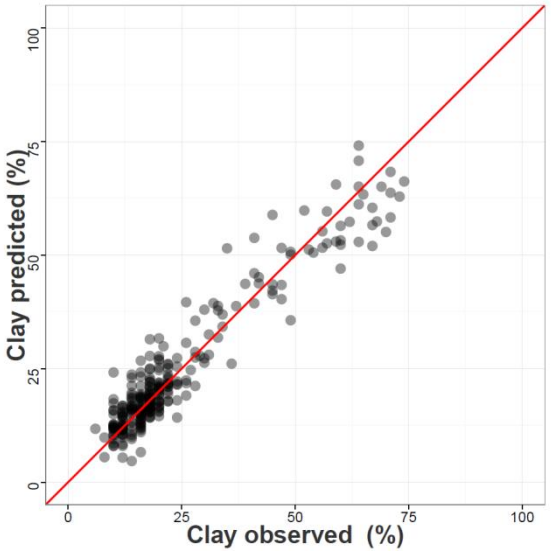
Global scale

R^2 = 0.50; RMSE=15.53%



Field scale

R^2 = 0.91; RMSE=5.02%



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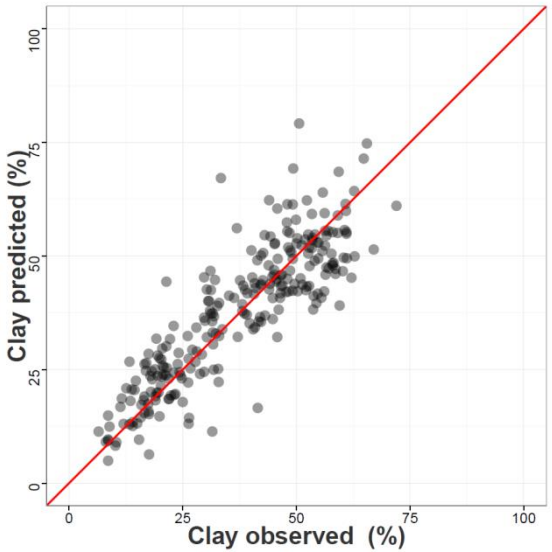

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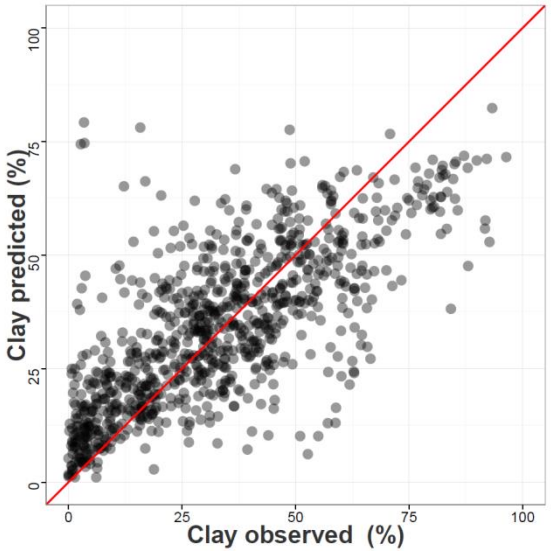
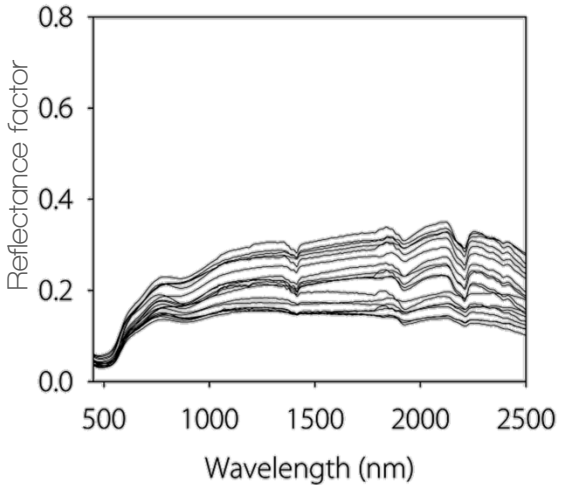


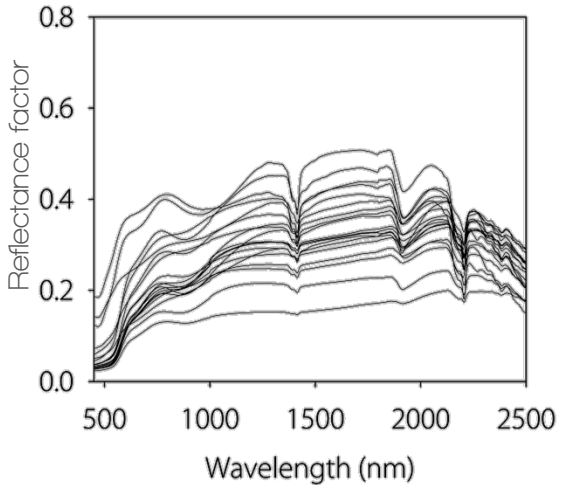
— Data complexity +

Degradation of the accuracy

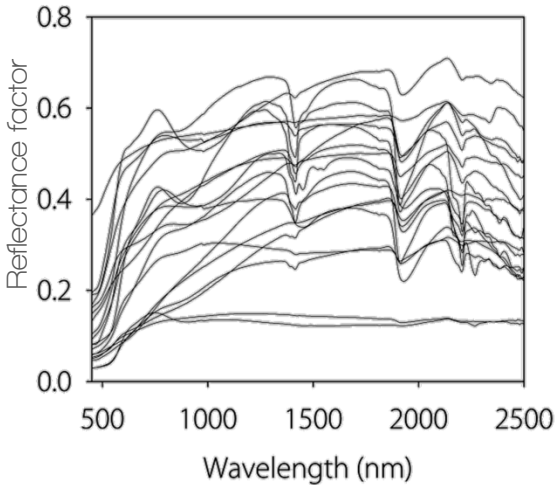
Field scale



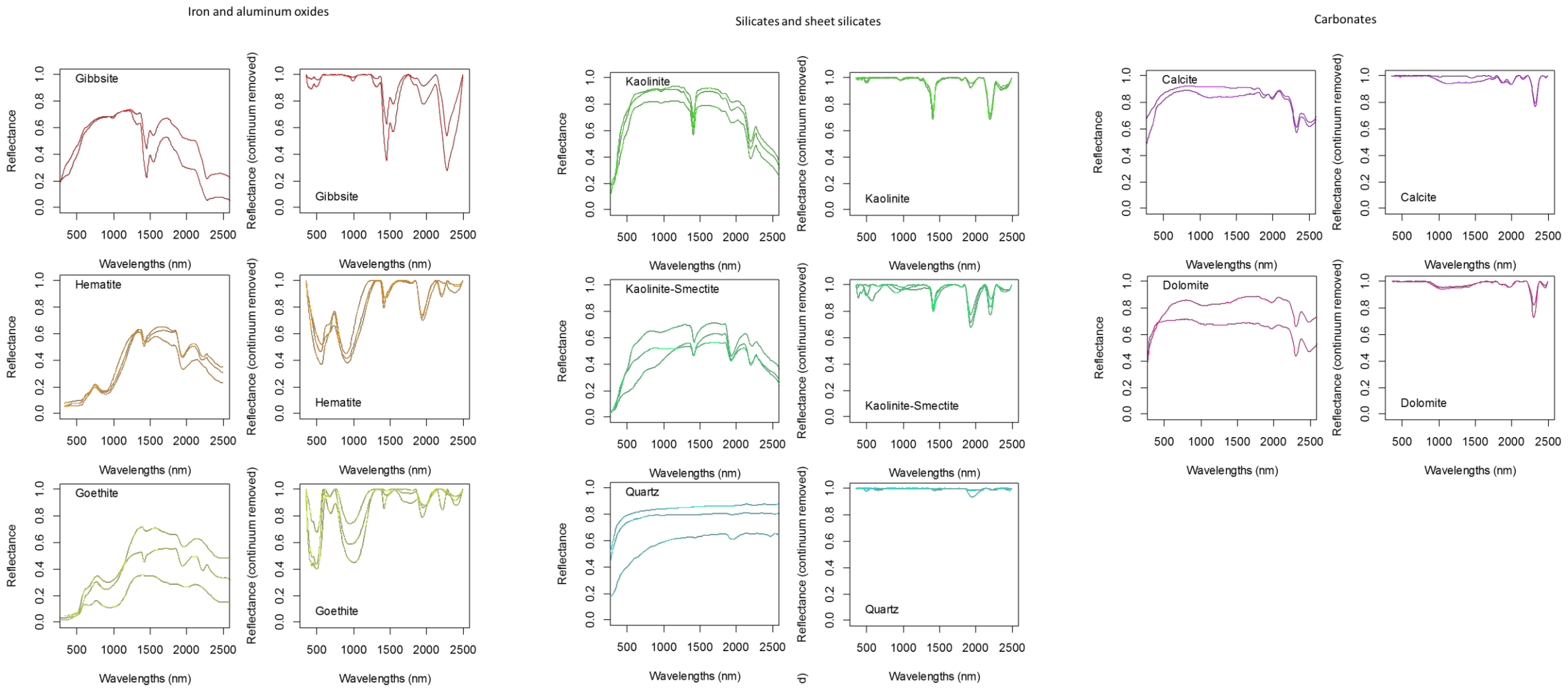
Regional scale

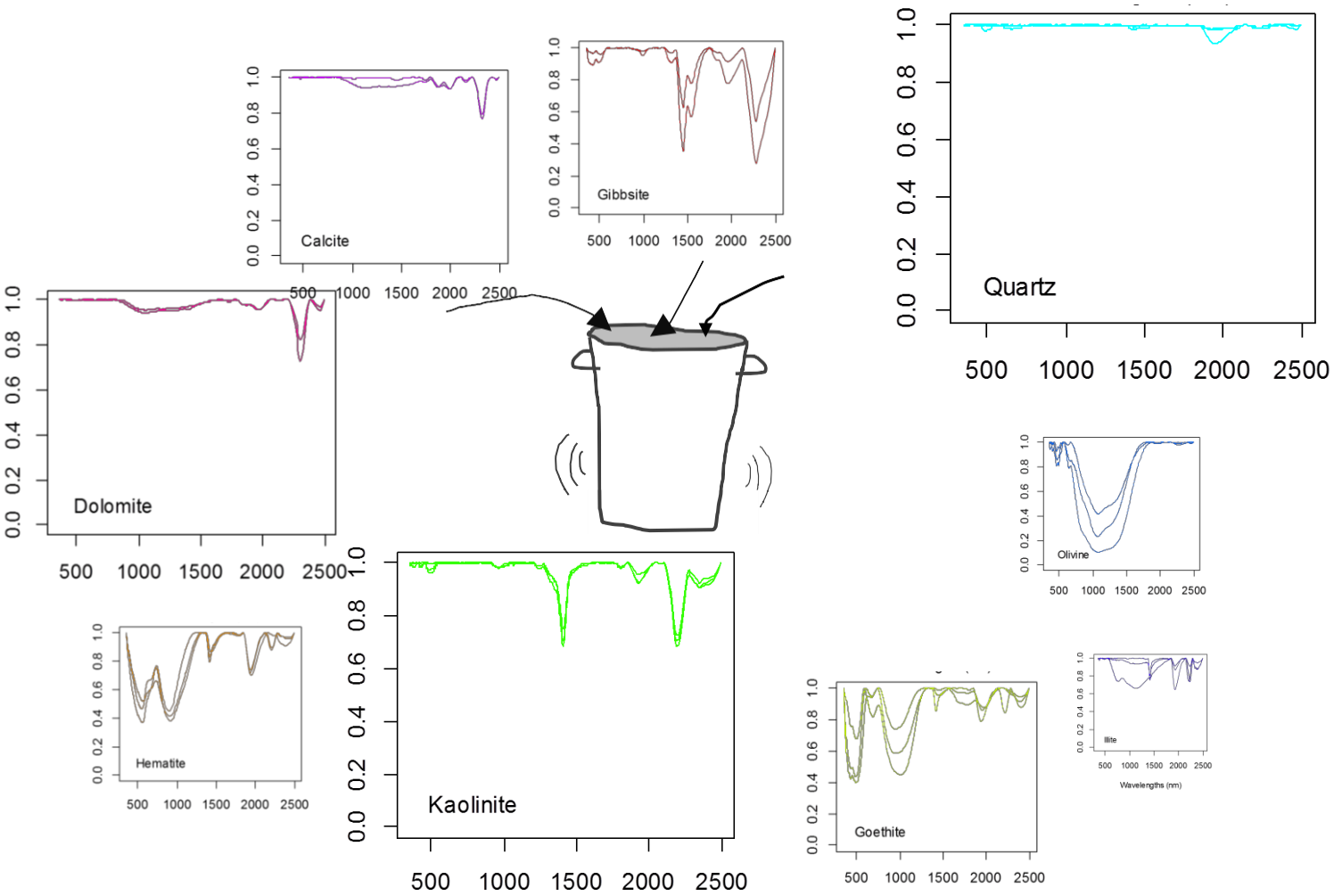


Global scale



20 spectra sampled at random


Iron and aluminum oxides
Silicates and sheet silicates
Carbonates
Gibbsite
Hematite
Goethite
Kaolinite
Kaolinite-Smectite
Quartz
Calcite
Dolomite
Reflectance
Reflectance (continuum removed)
Wavelengths (nm)
0.0 0.2 0.4 0.6 0.8 1.0
500 1000 1500 2000 2500

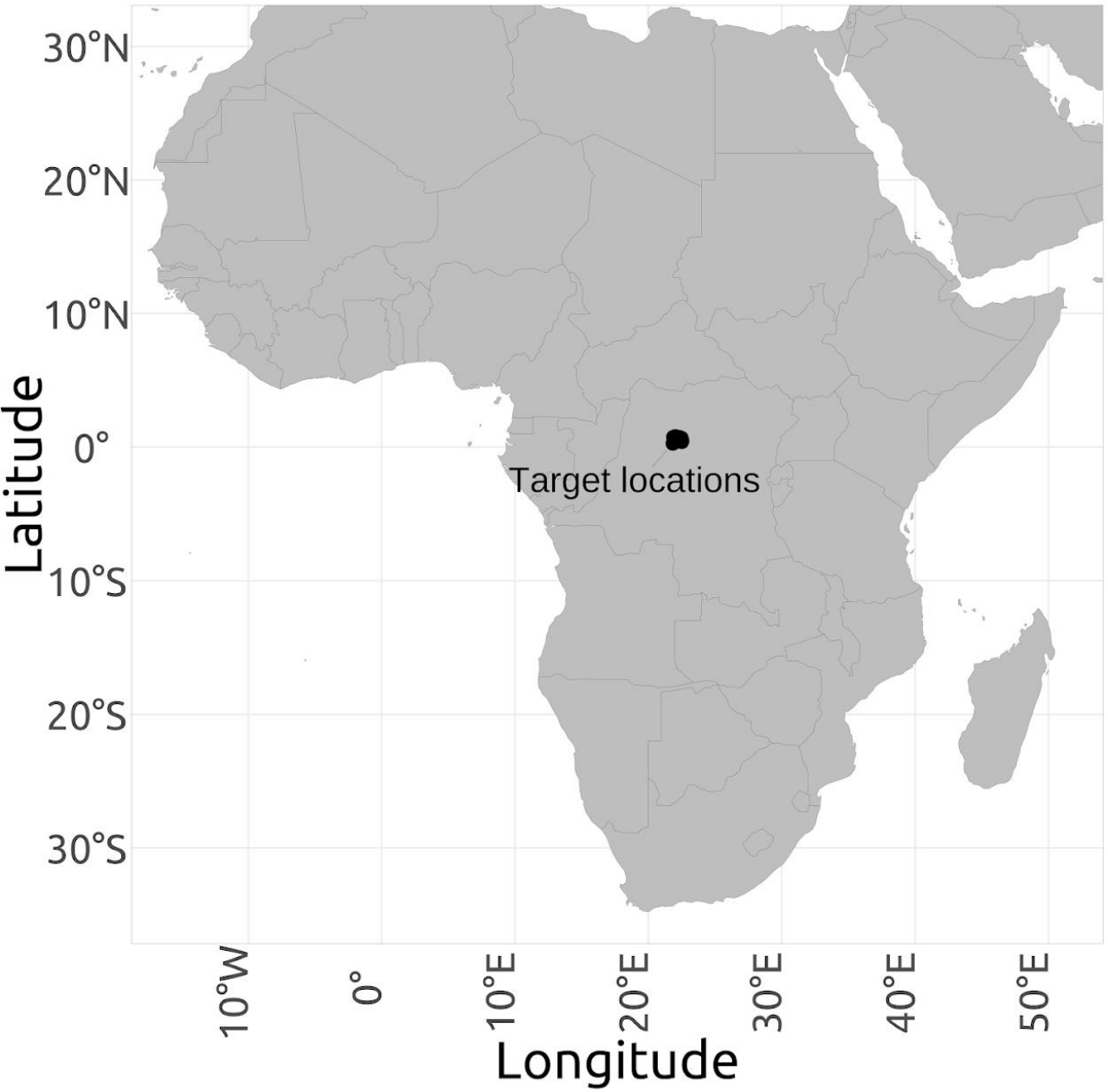

Calcite
Gibbsite
Quartz
Dolomite
Olivine
Hematite
Kaolinite
Goethite
Illite
Wavelengths (nm)

Think globally, fit locally*!

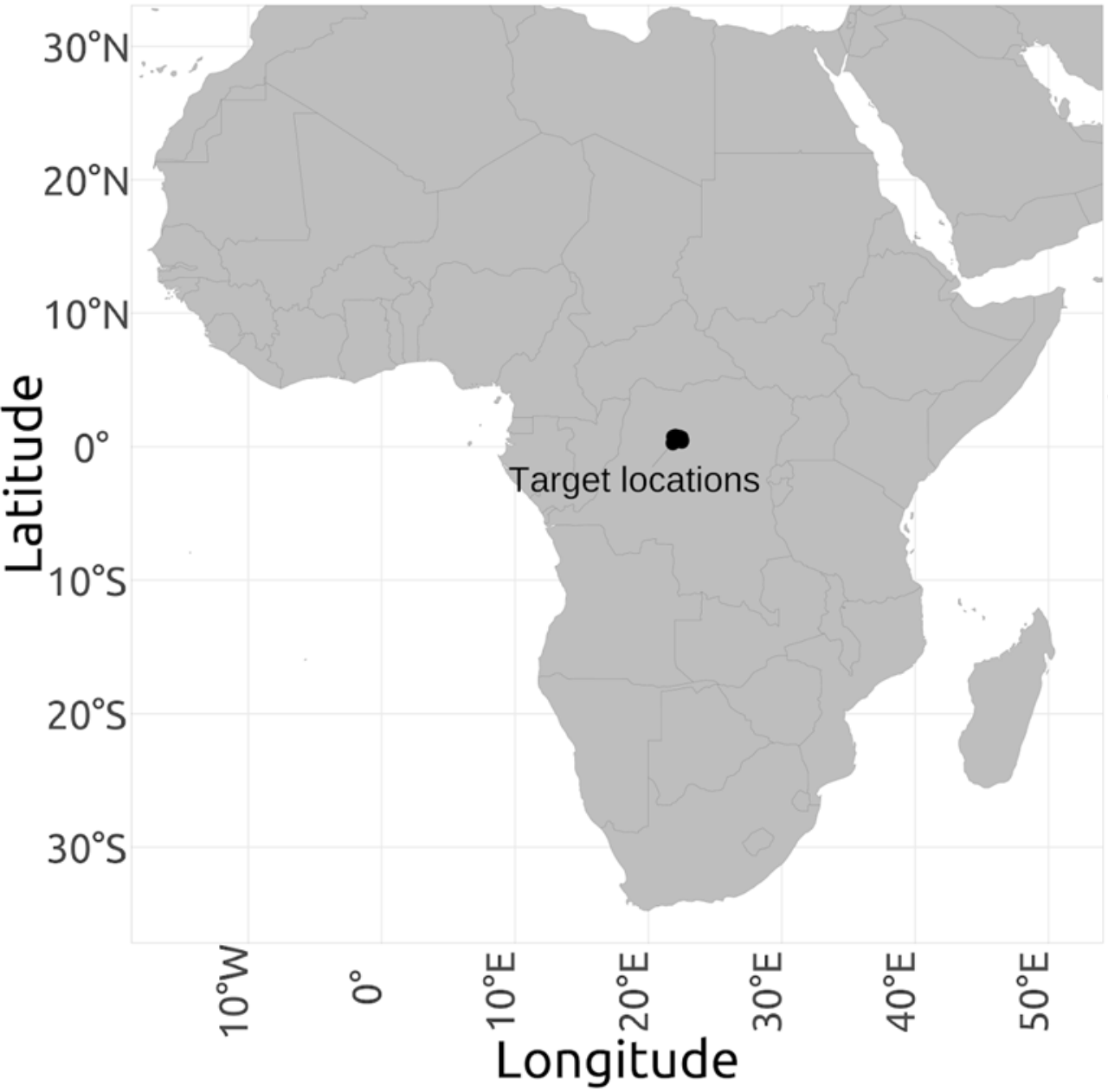
*Saul, L. K., & Roweis, S. T. (2003). Think globally, fit locally: unsupervised learning of low dimensional manifolds. *Journal of machine learning research*, *4*(Jun), 119-155.

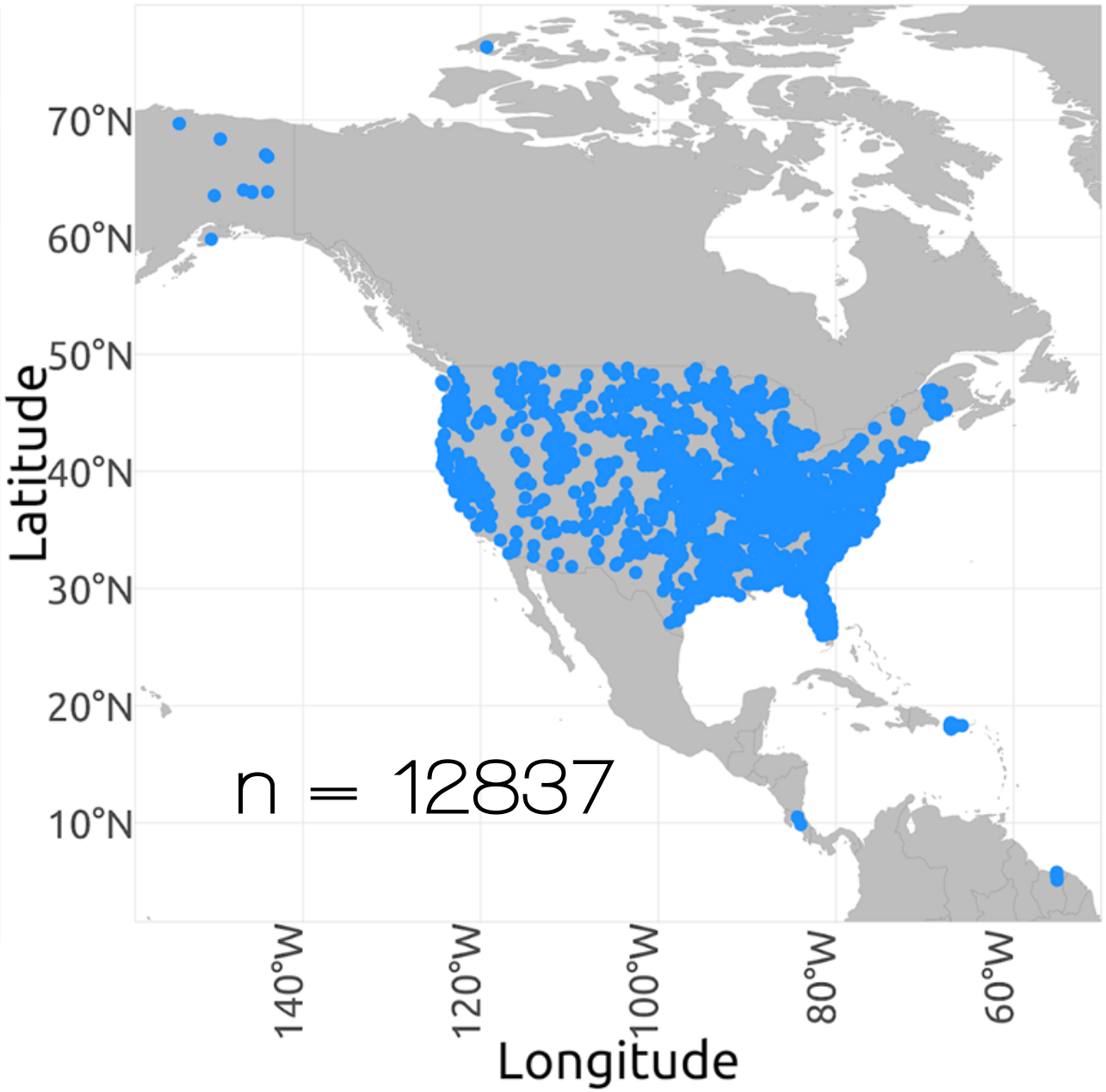
Example

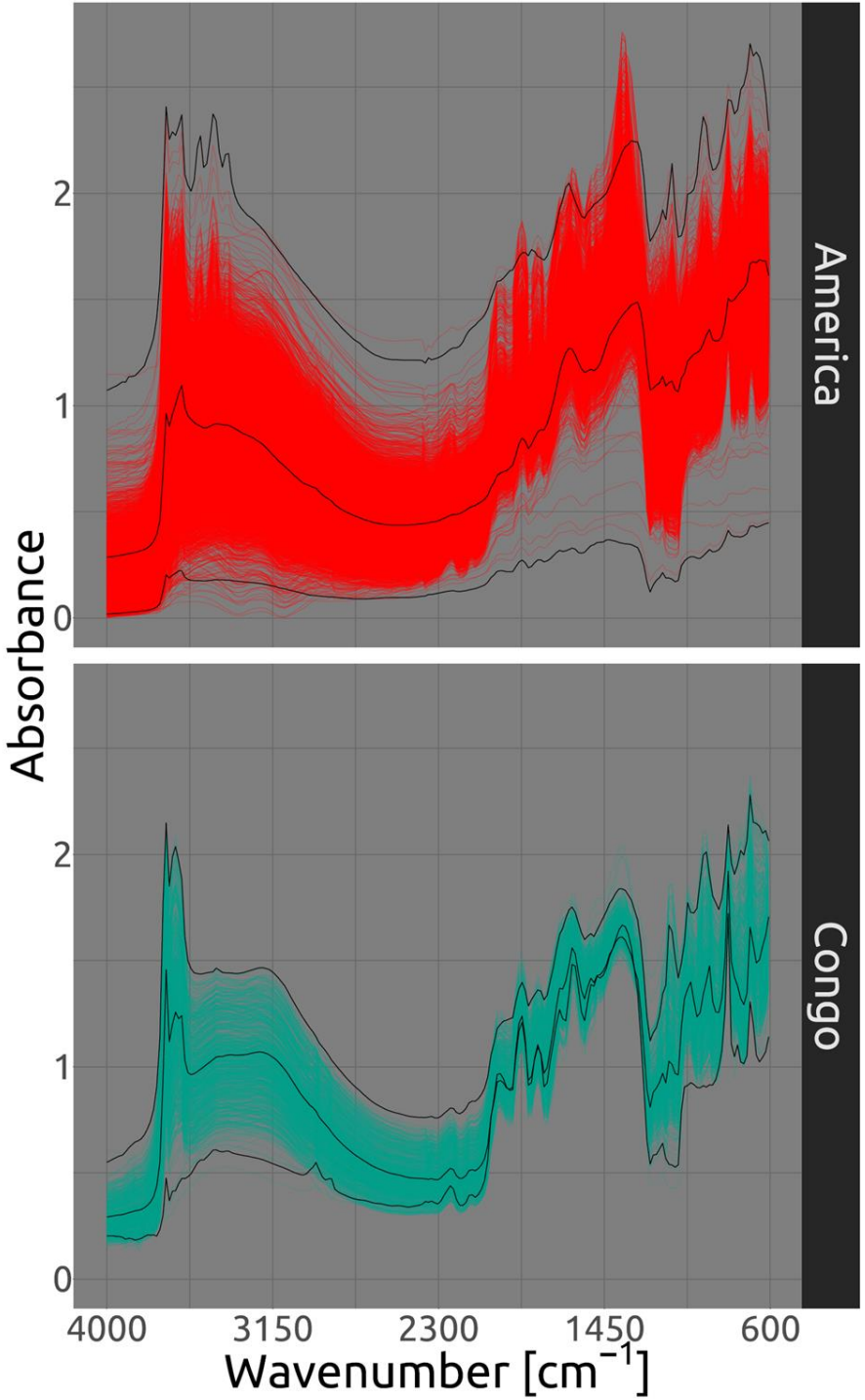
Total Carbon in soils


30°N
20°N
10°N
0°
10°S
20°S
30°S
Latitude
Target locations
10°W
0°
10°E
20°E
30°E
40°E
50°E
Longitude

n: 729


30°N
20°N
10°N
0°
10°S
20°S
30°S
Latitude
Target locations
10°W
0°
10°E
20°E
30°E
40°E
50°E
Longitude


70°N
60°N
50°N
40°N
30°N
20°N
10°N
Latitude
n = 12837
140°W
120°W
100°W
80°W
60°W
Longitude



12837 samples

729 samples

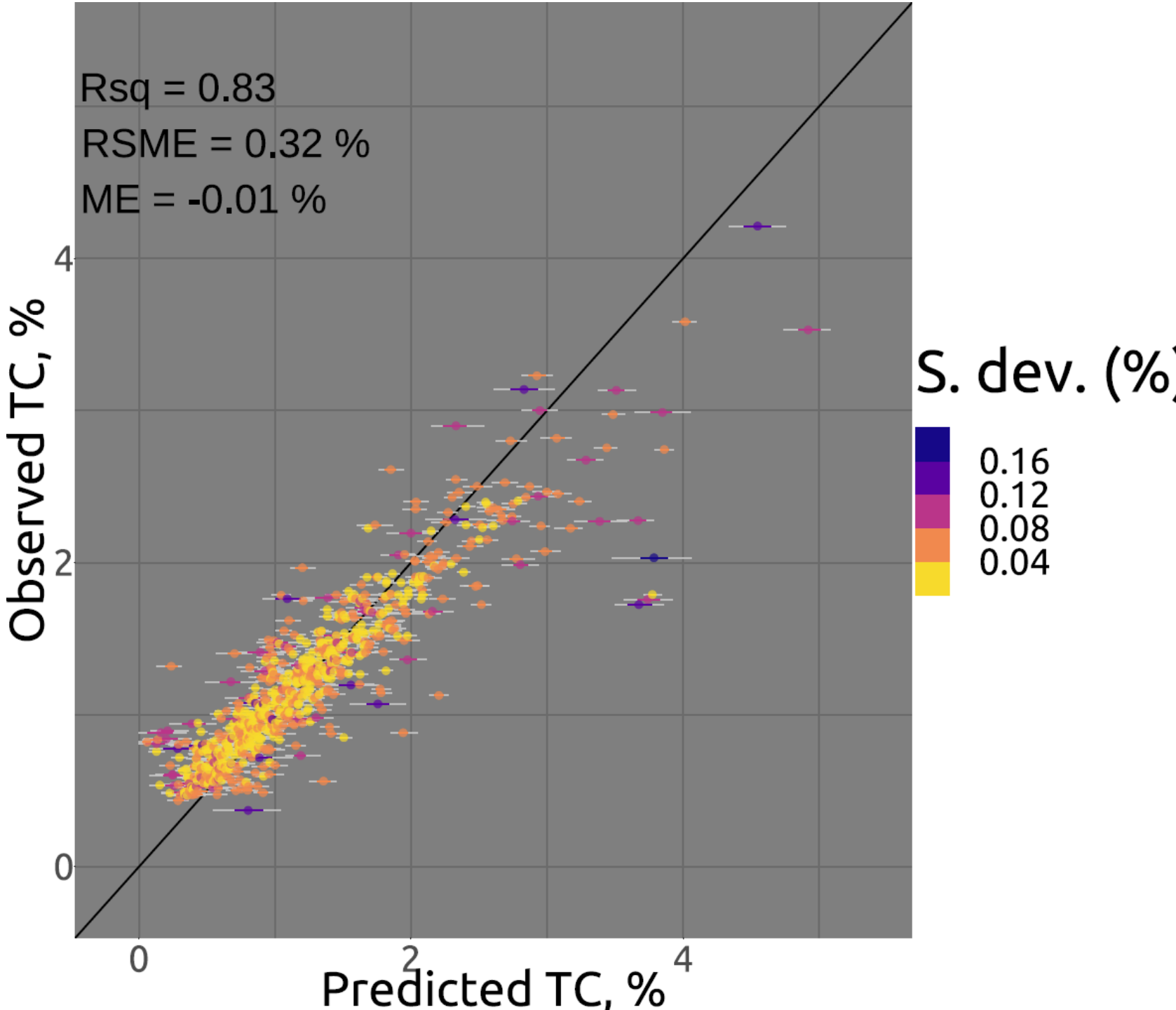
Genetically
derived model

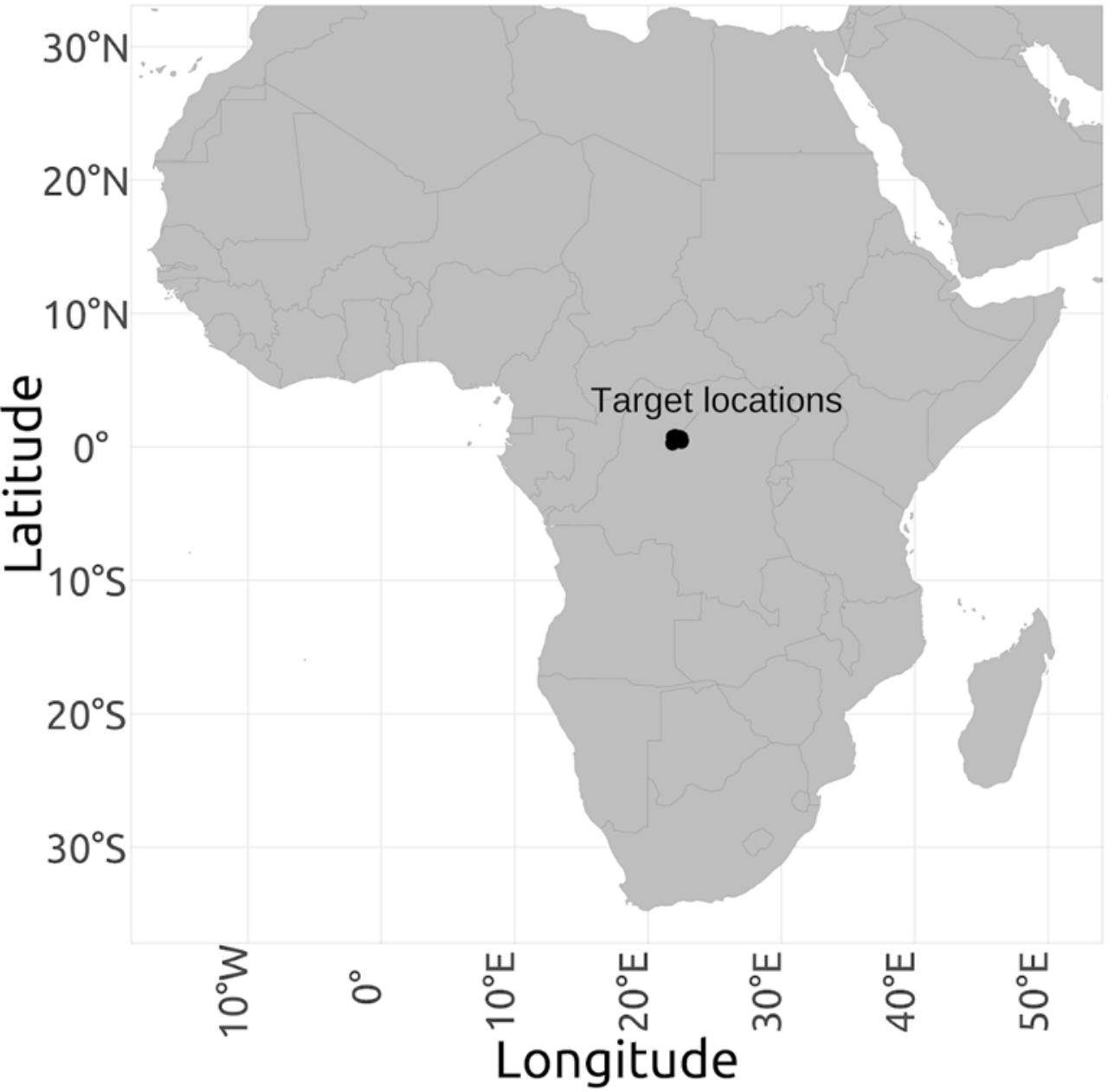
Weakness scores:

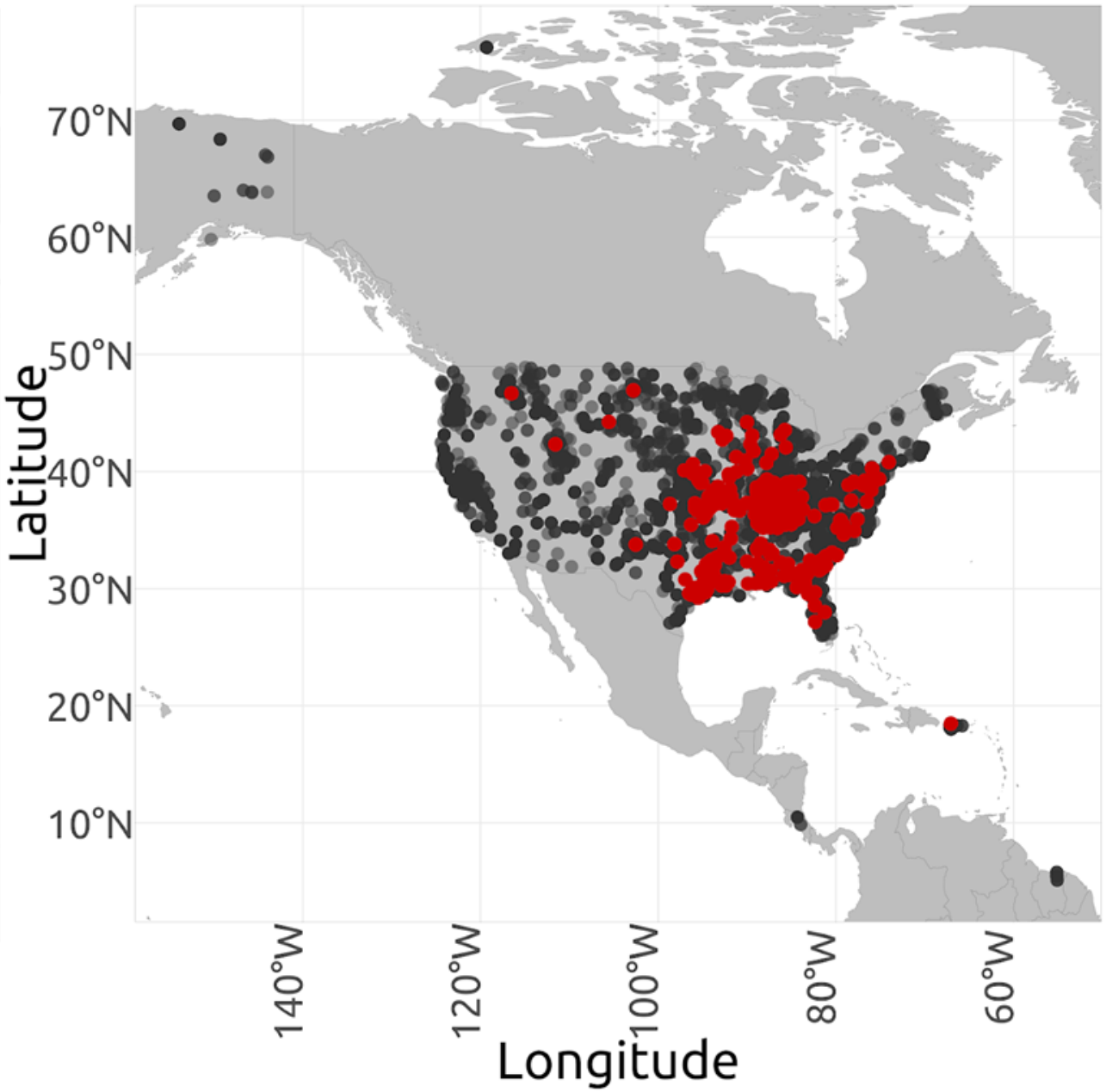
- Spectral reconstruction
- Spectral similarity
- **Response accuracy**

↓

20 samples with response values




Target locations
30°N
20°N
10°N
0°
10°S
20°S
30°S
Latitude
10°W
0°
10°E
20°E
30°E
40°E
50°E
Longitude


70°N
60°N
50°N
40°N
30°N
20°N
10°N
Latitude
140°W
120°W
100°W
80°W
60°W
Longitude

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Field work and prediction of C across a soil profile...