GLOSOLAN
GLOBAL SOIL LABORATORY NETWORK

Ring trial as part of the SoilSpec4GG initiative

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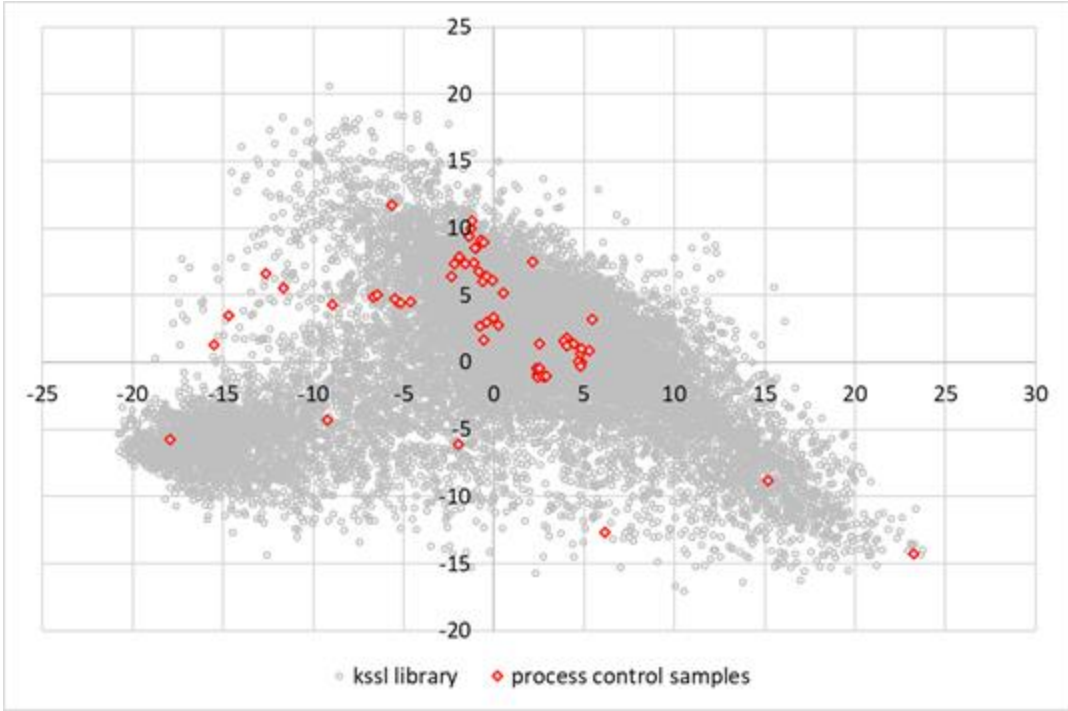
Soil.Spectroscopy

Purpose

- A barrier to routine use of soil spectroscopy with centralized spectral libraries is the variability in spectral response across different instruments.
- We are conducting a ring trial with a set of standard soil samples in order to better understand the lab-to-lab variability in soil spectroscopy.
- How can we overcome this variability when building predictive models?
    - The goal is to develop a systematic study testing different preprocessing, standardization methods, and model types for reducing the variations.
    - Simultaneously, these samples can form the basis of building calibration transfer models with the USDA NRCS KSSL MIR soil spectral library.

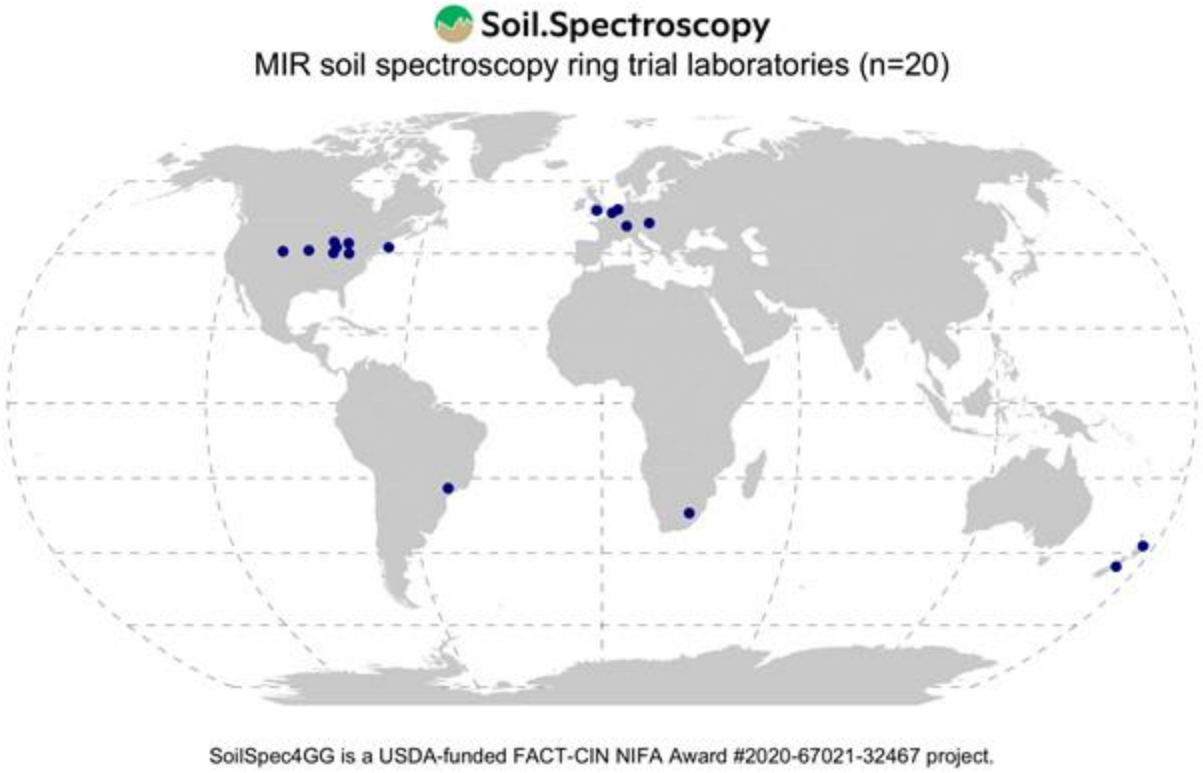
Soil samples/standards

- 60 from KSSL
  - Process control samples
  - Analytical determination at KSSL
  - ~50 cm^3 of fine earth fraction
  - ~10 g of finely milled
- 10 from NAPT
  - ~10 g of finely milled
  - Analytical determination from median NAPT results
  - KSSL vs NAPT (r => 0.99)



VisNIR: IEEE 4005 WG

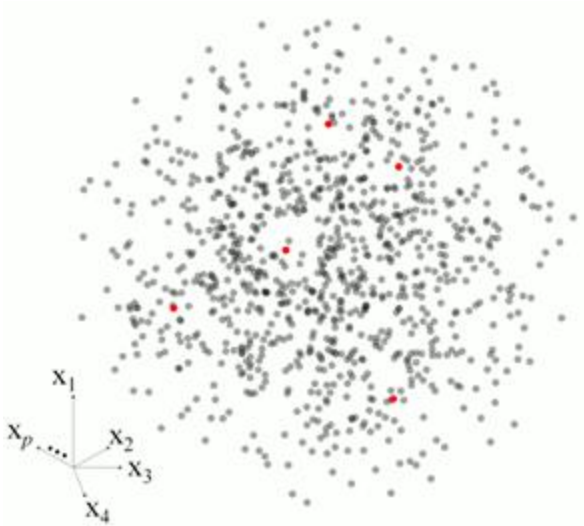
MIR: AgroCares (NLD), Argonne (USA), CSU-SoIL (USA), DAR (LSO), ETHZ-SAE (CHE), IAEA (AUT), KSSL (USA), LandCare (NZL), MSU (USA), OSU (USA), Rothamsted (GBR), Scion (NZL), UGhent (BEL), UIUC (USA), USP (BRA), UWisc (USA), Woodwell (USA)



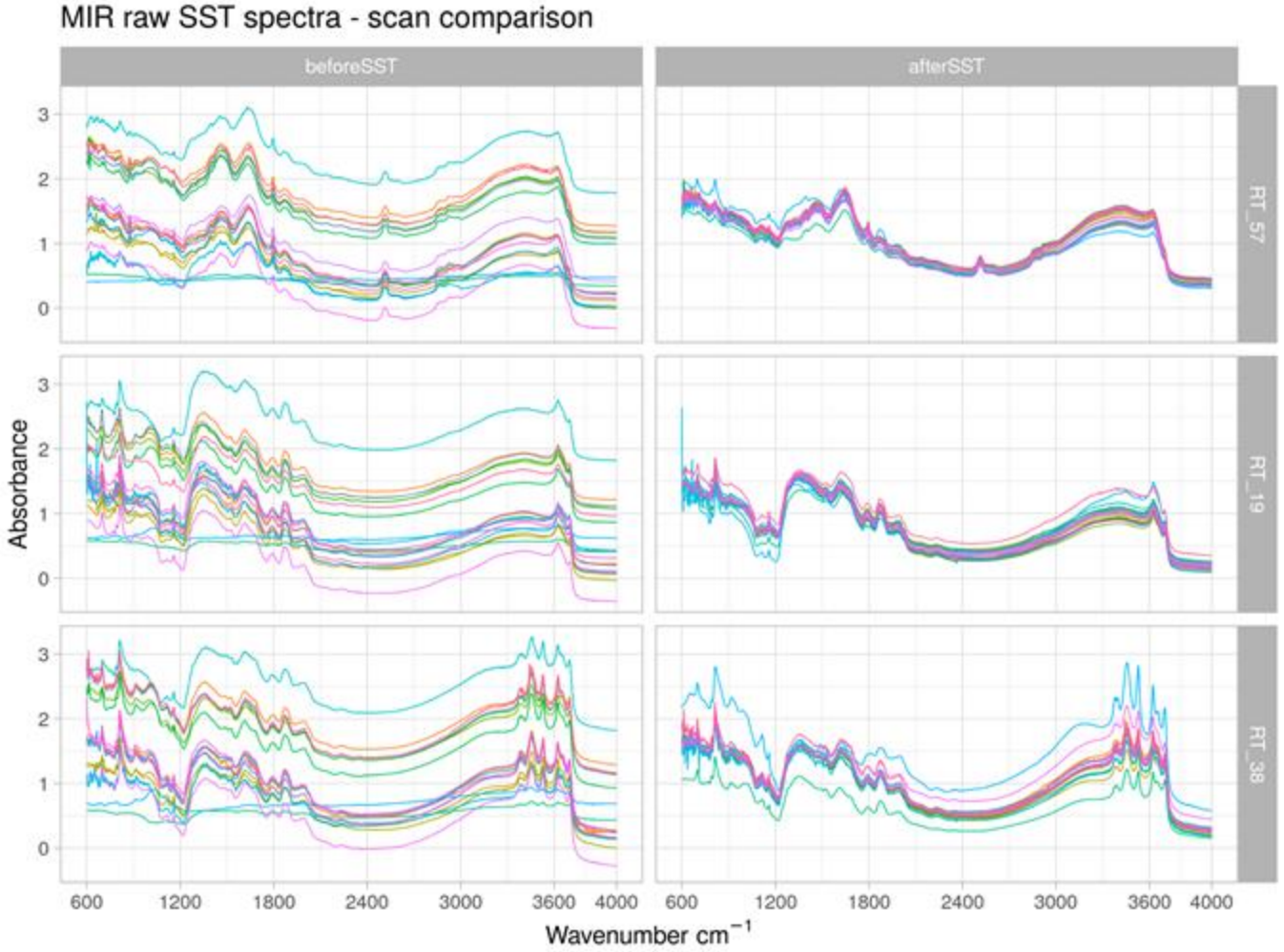
SoilSpec4GG is a USDA-funded FACT-CIN NIFA Award #2020-67021-32467 project.

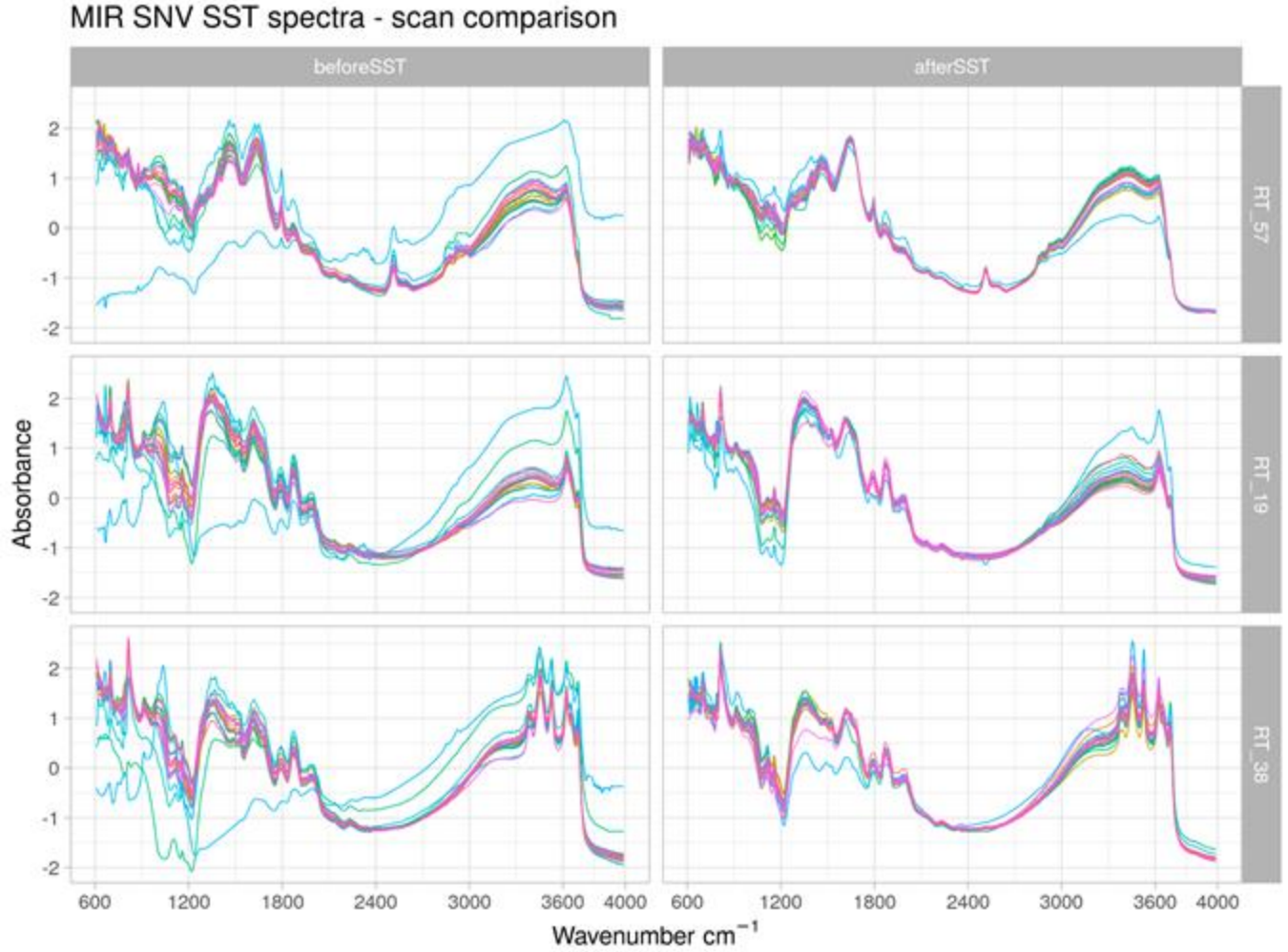
Data analysis

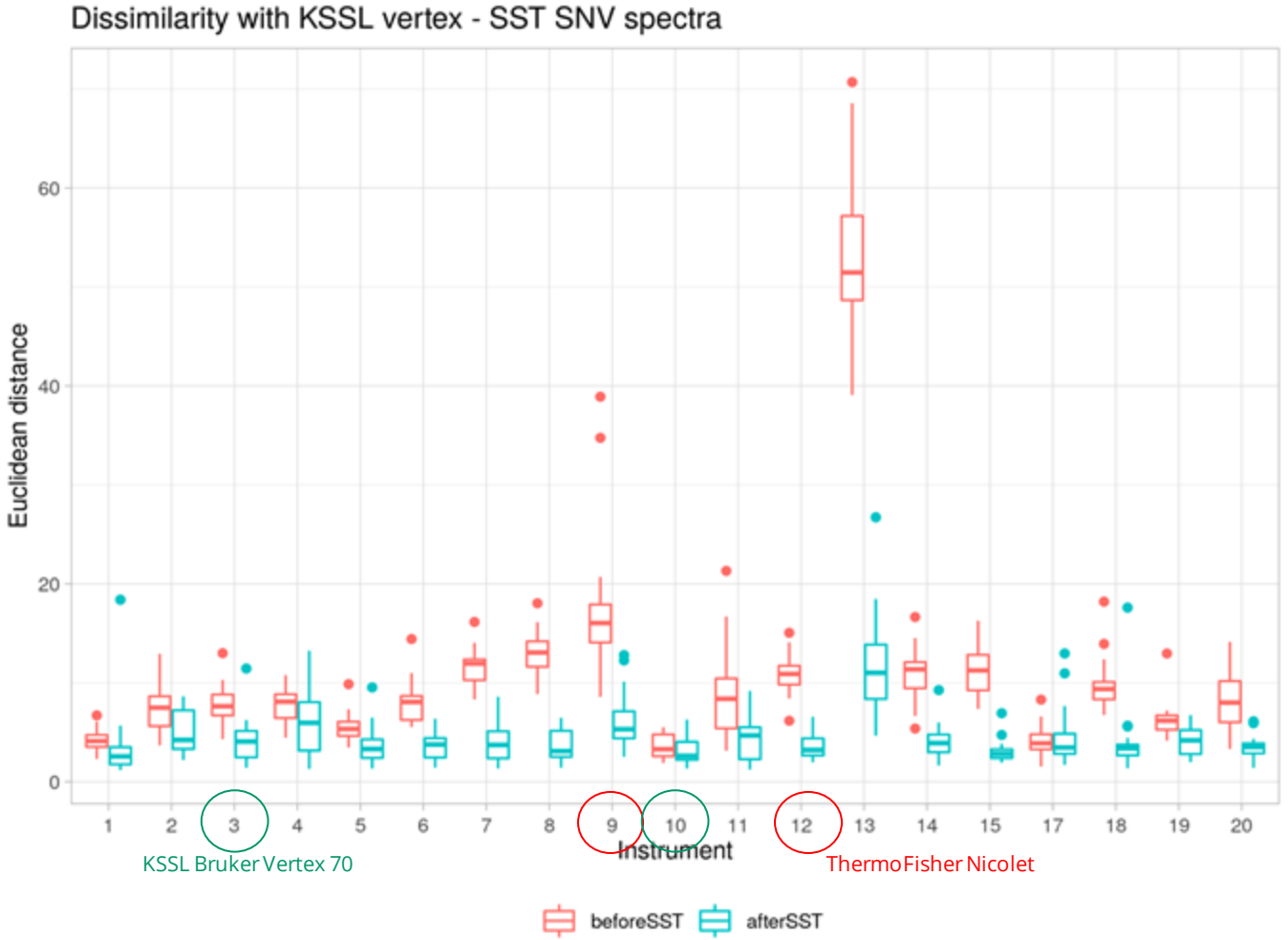
- Preprocessing
  - Raw
  - Baseline offset correction (BOC)
  - Savitzky–Golay 1st derivative (SG1stDer, [s=1, p=2, w=11, delta.wav=2])
  - Standard Normal Variate (SNV)
  - Continuum removal
  - Haar wavelet
- Calibration transfer
  - OC, clay, pH, K
  - Subset of KSSL (n= 15.000)
  - SST (n reference = 50, n test = 20)
- Model types
  - PLSR, MBL and Cubist
- Evaluation metrics:
  - RMSE, bias, R^2, **Lin's CCC**, RPD, RPIQ



https://github.com/l-ramirez-lopez/resemble


MIR raw SST spectra - scan comparison
beforeSST
afterSST
RT_57
RT_19
RT_38
Absorbance
0
1
2
3
600
1200
1800
2400
3000
3600
4000
Wavenumber cm^{-1}


MIR SNV SST spectra - scan comparison
beforeSST
afterSST
RT_57
RT_19
RT_38
Absorbance
2
1
0
-1
-2
600
1200
1800
2400
3000
3600
4000
Wavenumber cm^{-1}


Dissimilarity with KSSL vertex - SST SNV spectra
Euclidean distance
0
20
40
60
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
17
18
19
20
Instrument
KSSL Bruker Vertex 70
ThermoFisher Nicolet
beforeSST
afterSST


SNV preprocessing
carbon_org_perc
clay_perc
Lin's CCC
1.00
0.50
0.00
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
ThermoFisher Nicolet
KSSL Bruker Vertex 70
Internal-PLSR
15K-PLSR
15K-PLSR-SST-KS50
15K-MBL
15K-MBL-SST-KS50

Summary

- All instruments can deliver good predictions when calibrated internally.
- When performing calibration transfer, some huge differences between the primary and secondary instruments are evident, especially for those labs that have contrasting characteristics compared to the KSSL, i.e., instrument manufacturer and SOP.
- Overall, local models deliver better predictions because they are less sensitive to the variations compared to global models.
- SNV preprocessing (normalization) helps to reduce variations but spectral standardization may be necessary especially for contrasting setups.

Thank you

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