Soil Chemistry Dataset

Exploratory analysis

2023-06-15

Table of contents

1.1 Prerequisities and import libraries

- To download data:
  - aws-cli
- To parse and manage datasets:
  - brukeropusreader
  - pandas
  - tqdm

Installation below:

```
#! pip install awscli brukeropusreader tqdm pandas matplotlib folium seaborn pathlib

#commented out after the installation is completed in case you run again the notebook
```

```
#import pyspark
import pandas as pd
import numpy as np
```

```
import matplotlib.pyplot as plt
import seaborn as sns
from IPython.display import Image
import folium
from pathlib import Path
from brukeropusreader import read_file
from collections import Counter

from tqdm import tqdm_notebook as tqdm
```

1.2 Downloading the Soil Chemistry Dataset from AWS

Download s3 bucket content with the `aws-cli` command line tool. Run `aws configure` beforehand to set your credentials.

```
#! aws s3 sync s3://afsis afsis --no-sign-request

# commented out after the download is completed in case you run again the notebook
```

1.3 Loading OPUS spectra

OPUS spectra are created using Bruker instruments Infrared spectrometers To be opened brukeropusreader package is needed.

The function `brukeropusreader.read_file` parses the binaries and returns a data structure containing information about the wave numbers, absorbance spectra, and file metadata.

Here we plot a few of the spectra.

2. Geographical references

The AfSIS Soil Chemistry Dataset contains georeferences for each spectra. It is worth noting that it consists of two datasets, one for the subsaharian Africa and one with additional data recorded only in Tanzania.

2.1 Dataframes exploration

```
GEOREFS_FILE1 = 'afsis/2009-2013/Georeferences/georeferences.csv'
df_geo1 = pd.read_csv(GEOREFS_FILE1)# dataframe for several african countries
df_geo1 = df_geo1.sort_values(by=['Site', 'Cultivated'])
print(df_geo1.shape)
print(df_geo1.isna().sum())
df_geo1.head()
```

```
(1843, 14)
SSN                0
Public             0
Latitude           0
Longitude          0
Cluster            0
Plot               0
Depth              0
Soil material     94
Scientist          0
Site               0
Country            0
Region           232
Cultivated       798
Gid                0
dtype: int64
```

	SSN	Public	Latitude	Longitude	Cluster	Plot	Depth	Soil material	Scie
460	icr016032	True	5.423182	-0.709083	15	1	top	Aju.15.1.Topsoil.Std fine soil	Jero
500	icr016033	True	5.423182	-0.709083	15	1	sub	Aju.15.1.Subsoil.Std fine soil	Jero
666	icr015913	True	5.377035	-0.726425	9	1	sub	Aju.9.1.Subsoil.Std fine soil	Jero
732	icr016053	True	5.447667	-0.717422	16	1	sub	Aju.16.1.Subsoil.Std fine soil	Jero
957	icr015973	True	5.434675	-0.728883	12	1	sub	Aju.12.1.Subsoil.Std fine soil	Jero

```
GEOREFS_FILE2 = 'afsis/tansis/Georeferences/georeferences.csv'
df_geo2 = pd.read_csv(GEOREFS_FILE2)# dataframe with additional data for Tanzania
df_geo2 = df_geo2.sort_values(by=['Site', 'Cultivated'])
print(df_geo2.shape)

df_geo2.head()
```

```
(18819, 14)
```

	Cluster	Country	Cultivated	Depth	Gid	Latitude	Longitude	Plot	Region	SSN
29	2.0	Tanzania	False	top	46.0	-3.029698	33.015202	2.0	East Africa	icr011843
31	4.0	Tanzania	False	top	48.0	-2.992815	33.016113	1.0	East Africa	icr011881
32	5.0	Tanzania	False	top	49.0	-3.060982	33.030663	1.0	East Africa	icr011901
35	8.0	Tanzania	False	top	52.0	-2.987467	33.033264	1.0	East Africa	icr011960
36	9.0	Tanzania	False	top	53.0	-3.058480	33.065014	3.0	East Africa	icr011978

The tansis folder contains measurements for Tanzania only. FTIR spectra in this folder are not readable and make it unusable

```
todrop = ['Soil material','Scientist', 'Site', 'Region', 'Gid','Plot','Public'] #irrelevan
df_geo = df_geo1.drop(todrop, axis = 1)
```

3. Dry Chemistry

The AfSIS Soil Chemistry dataset contains dry and wet chemistry data taken at each sampling location.

3.1 X-ray fluorescence (XRF) elemental analysis

with XRF we get the concentration of various chemical elements in the sample

Units are parts per million (ppm)

https://www.elementalanalysis.com/xrf.html

```
file1path = "afsis/2009-2013/Dry_Chemistry/ICRAF/Bruker_TXRF/TXRF.csv"
file2path = "afsis/tansis/Dry_Chemistry/ICRAF/Bruker_TXRF/TXRF.csv"
xrf_africa = pd.read_csv(file1path)
xrf_tanzania = pd.read_csv(file2path)

print('measurements 2009-13',xrf_africa.shape,'measurements  2014', xrf_tanzania.shape)

print("the table below shows the concentration in ppm for each element detected")
xrf_africa.head()
```

```
measurements 2009-13 (1904, 42) measurements  2014 (224, 42)
the table below shows the concentration in ppm for each element detected
```

	SSN	Public	Na	Mg	Al	P	S	Cl	K	Ca	...	Pr	Nd	S
0	icr005965	True	16023.3	4433.5	37618.6	84.4	45.7	268.1	12412.2	30705.6	...	0.9	14.7	
1	icr005966	True	20524.6	5832.2	40248.2	72.1	45.7	229.6	12892.2	23234.5	...	1.1	15.8	
2	icr005985	True	19350.4	5085.8	36766.3	50.6	45.7	157.3	16839.7	16746.2	...	1.2	19.2	
3	icr005986	True	17410.2	5271.2	37912.2	50.6	45.7	285.2	16818.0	31939.6	...	1.1	16.7	
4	icr005998	True	19092.5	9169.8	37359.8	50.6	45.7	251.4	17577.9	25298.2	...	1.1	16.7	

```
mask_diff_xrf = xrf_africa[xrf_africa['SSN'].isin(diff_list )]
df_xrf = pd.concat([xrf_tanzania, mask_diff_xrf])
```

```
print(df_xrf.shape, len(df_xrf.SSN.unique()))
```

```
(1838, 42) 1838
```

```
print('important elements for agriculture')
# https://www.qld.gov.au/environment/land/management/soil/soil-properties/fertility

important_elements = ['P','K', 'S','Ca','Mg','Cu','Cl','Zn','Fe', 'Mn','Mo' ]
df_xrf_reduced = df_xrf[important_elements]#/10000# express in %
df_xrf_reduced['SSN'] = df_xrf['SSN']
df_xrf_reduced.head()
```

```
important elements for agriculture

SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide
  df_xrf_reduced['SSN'] = df_xrf['SSN']
```

	P	K	S	Ca	Mg	Cu	Cl	Zn	Fe	Mn	Mo	SSN
0	84.4	12412.2	45.7	30705.6	4433.5	10.1	268.1	25.3	22263.2	356.1	184.5	icr005965
1	72.1	12892.2	45.7	23234.5	5832.2	11.8	229.6	29.4	26269.6	379.7	184.5	icr005966
2	50.6	16839.7	45.7	16746.2	5085.8	22.1	157.3	32.4	22790.2	323.4	184.5	icr005985
3	50.6	16818.0	45.7	31939.6	5271.2	24.9	285.2	34.4	22939.1	332.5	184.5	icr005986
4	50.6	17577.9	45.7	25298.2	9169.8	13.1	251.4	35.4	24985.2	408.3	184.5	icr005998

```
# how disperse are the XRF data?
print(df_xrf_reduced.shape)
df_xrf_reduced.describe()
```

```
(1838, 12)
```

	P	K	S	Ca	Mg	Cu	Cl	Z
count	1838.000000	1838.000000	1838.000000	1838.000000	1838.000000	1838.000000	1838.000000	1
mean	0.011513	1.126107	0.007641	0.758606	0.730171	0.001519	0.026368	0
std	0.046650	1.268460	0.040276	2.284191	0.733123	0.001496	0.222005	0
min	0.002950	0.009040	0.003320	0.004400	0.402890	0.000050	0.000600	0
25%	0.005060	0.240008	0.004570	0.046742	0.557500	0.000450	0.005687	0
50%	0.005060	0.696950	0.004570	0.141455	0.557500	0.001125	0.010050	0
75%	0.005060	1.624108	0.004570	0.518190	0.557500	0.002050	0.016350	0
max	1.246380	10.627340	0.970400	42.643090	13.689340	0.012840	7.438340	0

3.2 Fourier transform infrared spectroscopy (FTIR)

A word about units. Most spectra using electromagnetic radiation are presented with wavelength as the X-axis in nm or m. Originally, IR spectra were presented in units of micrometers. Later (1953) a different measure, the wavenumber given the unit cm-1, was adopted.

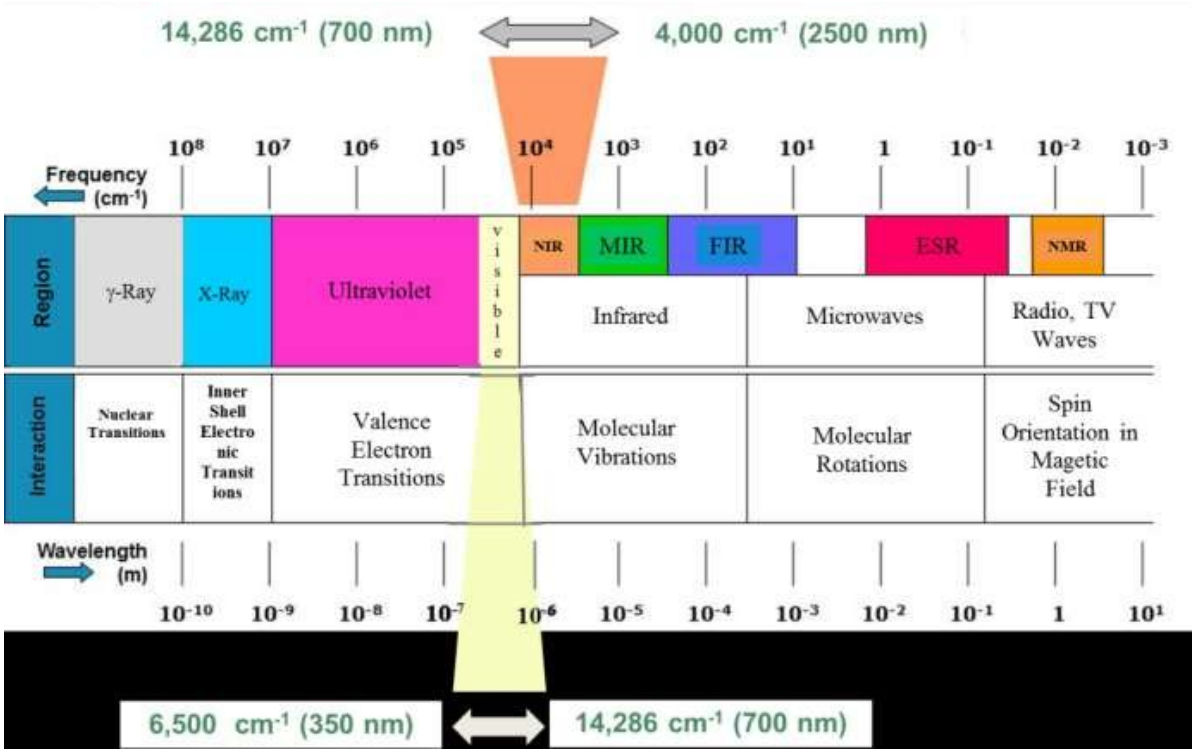
(cm-1)= 10,000/ (m)

The spectra may appear to be "backward" (large wavenumber values on the left, running to low values on the right); this is a consequence of the m to cm-1 conversion

3.2.1 NIR (near infrared range) FTIR

spectral range: 12500 - 4000 cm-1 or 700 - 2500 nm for near infrared (NIR)

```
Image(filename='img/NIR.jpeg')
```




```
NIR_SPECTRA_DIR = 'Bruker_MPA/*'
AFSIS_PATH = Path('afsis/2009-2013/Dry_Chemistry/ICRAF')
names = []
spectra = []

for path in tqdm(AFSIS_PATH.glob(NIR_SPECTRA_DIR )):
    if path.is_file():
        spect_data = read_file(path)
        spectra.append(spect_data["AB"])
        names.append(path.stem)
wave_nums = spect_data.get_range()

column_names = ['{:.0f}'.format(x) for x in wave_nums]
near_infrared_df = pd.DataFrame(spectra, index=names, columns=column_names)
near_infrared_df.head()
```

```
TqdmDeprecationWarning: This function will be removed in tqdm==5.0.0
```

```
Please use `tqdm.notebook.tqdm` instead of `tqdm.tqdm_notebook`
  for path in tqdm(AFSIS_PATH.glob(NIR_SPECTRA_DIR )):
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', max=1.0), HTML(value='')))
```

	12493	12489	12485	12482	12478	12474	12470	12466	12462
icr033603	0.744053	0.744943	0.737978	0.734149	0.738894	0.741579	0.738796	0.740573	0.745435
icr042897	0.553651	0.549628	0.549979	0.555073	0.561452	0.566700	0.571925	0.578335	0.582339
icr049675	0.533260	0.531480	0.535772	0.545087	0.551631	0.550375	0.546267	0.545179	0.545328
icr034693	0.568058	0.566100	0.563312	0.560136	0.556757	0.558751	0.566576	0.575022	0.580073
icr033950	0.555743	0.550596	0.548068	0.554348	0.559019	0.554218	0.551323	0.556638	0.561071

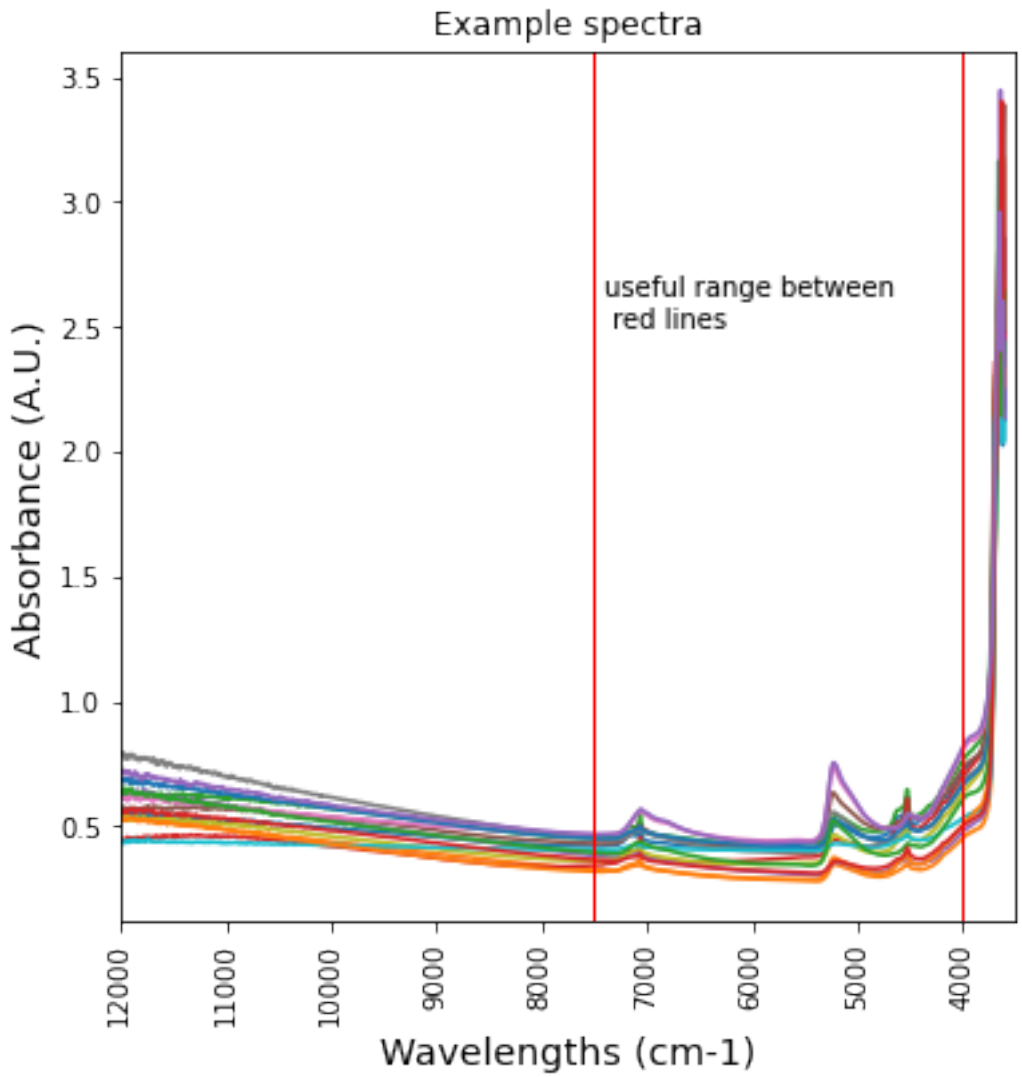
```
# table with FTIR spectra for each sample

df_NIR_FTIRspectra = near_infrared_df.T.reset_index()

df_NIR_FTIRspectra = df_NIR_FTIRspectra.rename(columns={'index': 'labda'})
df_NIR_FTIRspectra.labda = pd.to_numeric(df_NIR_FTIRspectra.labda)

df_NIR_FTIRspectra.head()
```

	labda	icr033603	icr042897	icr049675	icr034693	icr033950	icr034794	icr015953	icr050394	icr0
0	12493	0.744053	0.553651	0.533260	0.568058	0.555743	0.643860	0.431300	0.684270	0.56
1	12489	0.744943	0.549628	0.531480	0.566100	0.550596	0.648193	0.434562	0.684778	0.56
2	12485	0.737978	0.549979	0.535772	0.563312	0.548068	0.648293	0.435362	0.677241	0.56
3	12482	0.734149	0.555073	0.545087	0.560136	0.554348	0.642154	0.436202	0.676640	0.56
4	12478	0.738894	0.561452	0.551631	0.556757	0.559019	0.641057	0.436053	0.683005	0.56

```
plt.figure(figsize= (6,6))

plt.plot(df_NIR_FTIRspectra['labda'],df_NIR_FTIRspectra.iloc[:, [4,5,6,7,8,9,10,11,12,13,1

plt.title('Example spectra')


plt.xticks(rotation=90)
```

```
plt.xlim(12000,3500)
plt.ylabel('Absorbance (A.U.)', fontsize=14)
plt.xlabel('Wavelengths (cm-1)', fontsize = 14)

plt.axvline(x=7500 , ymin=0, ymax=1, color='r', linewidth = 1)
plt.axvline(x=4000, ymin=0, ymax=1, color='r', linewidth = 1)
plt.text(7400, 2.5, 'useful range between \n red lines')
```

```
Text(7400, 2.5, 'useful range between \n red lines')
```



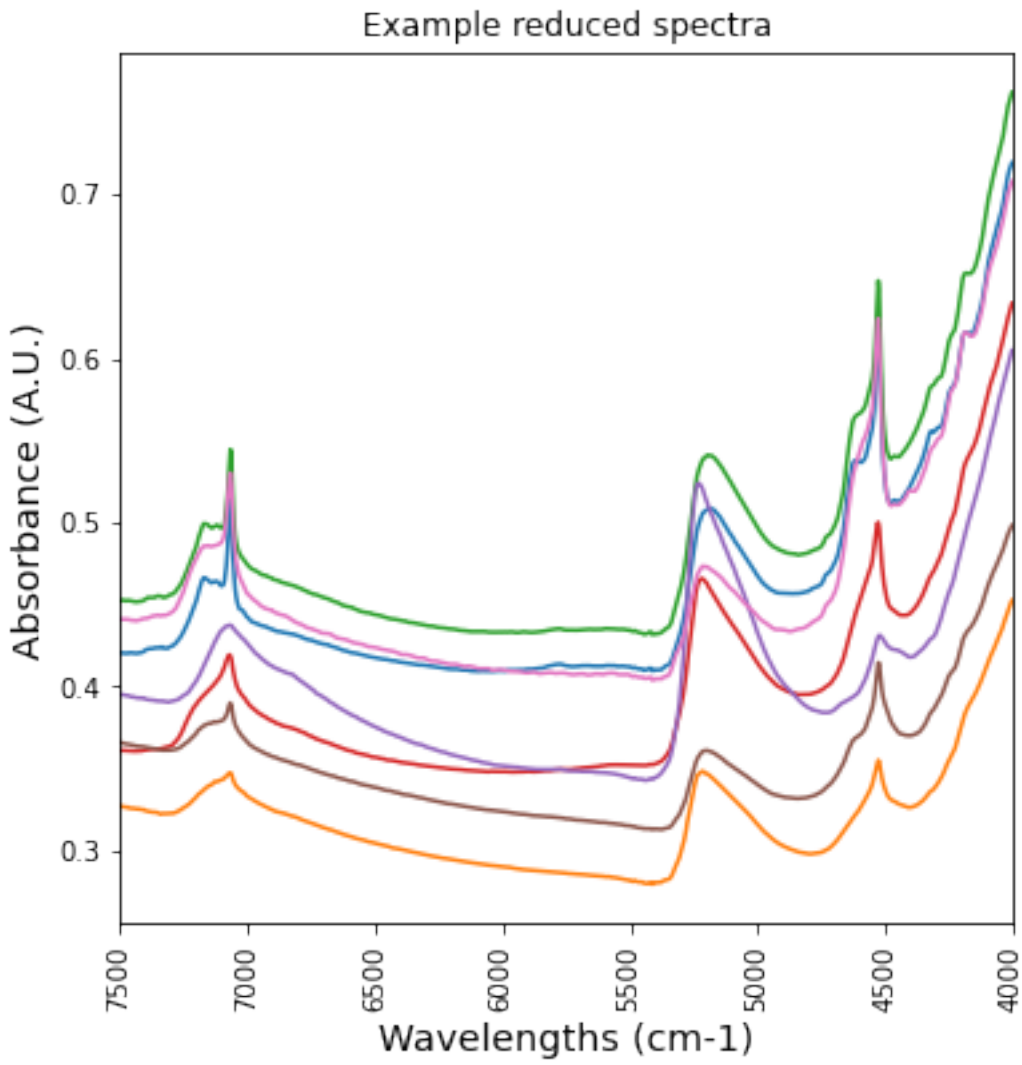
In the region 12000 - 7500 cm-1 there are no peaks, this part of the spectrum can be ignored below 4000 cm-1 the signal is unrealistic. It is an experimental artifact and this part of the spectrum should be cut off.

Absorbance in this range is analized with mid-range FTIR spectrometers (see section 3.2.2 below)

```
df_NIR_FTIRspectra =  df_NIR_FTIRspectra[df_NIR_FTIRspectra['labda'] < 7500]
df_NIR_FTIRspectra = df_NIR_FTIRspectra[df_NIR_FTIRspectra['labda'] > 4000]
```

```
plt.figure(figsize= (6,6))

plt.plot(df_NIR_FTIRspectra['labda'],df_NIR_FTIRspectra.iloc[:, [4,5,6,12,16,17,48]])

plt.title('Example reduced spectra')

plt.xticks(rotation=90)
plt.xlim(7500,4000)
plt.ylabel('Absorbance (A.U.)', fontsize=14)
plt.xlabel('Wavelengths (cm-1)', fontsize = 14)
```

```
Text(0.5, 0, 'Wavelengths (cm-1)')
```




```
# change original dataset accordingly

df_NIR_reindexed = df_NIR_FTIRspectra.set_index('labda')
near_infrared_df = df_NIR_reindexed.T
near_infrared_df.head()
```

labda	7498	7494	7491	7487	7483	7479	7475	7471	7467
icr033603	0.469107	0.469056	0.469180	0.469344	0.469312	0.469145	0.469012	0.469019	0.469138
icr042897	0.453903	0.453874	0.453821	0.453781	0.453818	0.453874	0.453957	0.454082	0.454211
icr049675	0.311495	0.311474	0.311484	0.311448	0.311298	0.311103	0.310900	0.310745	0.310745

labda	7498	7494	7491	7487	7483	7479	7475	7471	7467
icr034693	0.420559	0.420480	0.420528	0.420549	0.420534	0.420425	0.420276	0.420284	0.420467
icr033950	0.327227	0.327036	0.326880	0.326711	0.326502	0.326389	0.326441	0.326477	0.326314

3.2.2 MIR (middle infrared range) FTIR

spectral range 400 - 4000 cm-1

data recorded with three spectrometers that differ for the method for collecting data.

- ALPHA Kbr spectrometer: transmission, using samples pressed into a Kbr pellet
- ALPHA ZnSe spectrometer: reflection over a diamond window and ZnSe filter / beam splitter
- Tensor27 Kbr spectrometer further reading about experimental details can be found at afsis/2009-2013/Dry_Chemistry/ICRAF/SOP/METH07V01 ALPHA.pdf

and a general introduction can be found here: https://www.shimadzu.com/an/service-support/technical-support/analysis-basics/ftirtalk/talk8.html

- 2014-2018 Most FTIR spectra could not be opened using the Bruker open files library, in this kernel only those obtained with the Tensor27 spectrometer are analyzed

- ALPHA spectrometer - KBr window

```
KBR_SPECTRA_DIR = 'Bruker_Alpha_KBr/*'
AFSIS_PATH = Path('afsis/2009-2013/Dry_Chemistry/ICRAF')
TANSIS_PATH = Path('afsis/tansis/Dry_Chemistry/ICRAF')
names = []
spectra = []

for path in tqdm(AFSIS_PATH.glob(KBR_SPECTRA_DIR )):
    if path.is_file():
        spect_data = read_file(path)
        spectra.append(spect_data["AB"])
        names.append(path.stem)
wave_nums = spect_data.get_range()

column_names = ['{:.0f}'.format(x) for x in wave_nums]
kbr_df = pd.DataFrame(spectra, index=names, columns=column_names)
kbr_df.head()
```

```
TqdmDeprecationWarning: This function will be removed in tqdm==5.0.0
Please use `tqdm.notebook.tqdm` instead of `tqdm.tqdm_notebook`
  for path in tqdm(AFSIS_PATH.glob(KBR_SPECTRA_DIR )):

HBox(children=(FloatProgress(value=1.0, bar_style='info', max=1.0), HTML(value='')))
```

	3998	3997	3996	3994	3993	3991	3990	3988	3987
icr033603	0.908592	0.908981	0.909435	0.909956	0.910562	0.911266	0.912069	0.912953	0.913888
icr042897	0.810133	0.809940	0.809745	0.809616	0.809566	0.809563	0.809558	0.809516	0.809437
icr049675	0.711836	0.712355	0.713021	0.713747	0.714438	0.715037	0.715535	0.715951	0.716298
icr034693	0.788686	0.789201	0.789494	0.789611	0.789634	0.789656	0.789744	0.789912	0.790109
icr033950	0.752478	0.753251	0.753915	0.754423	0.754733	0.754816	0.754683	0.754402	0.754084

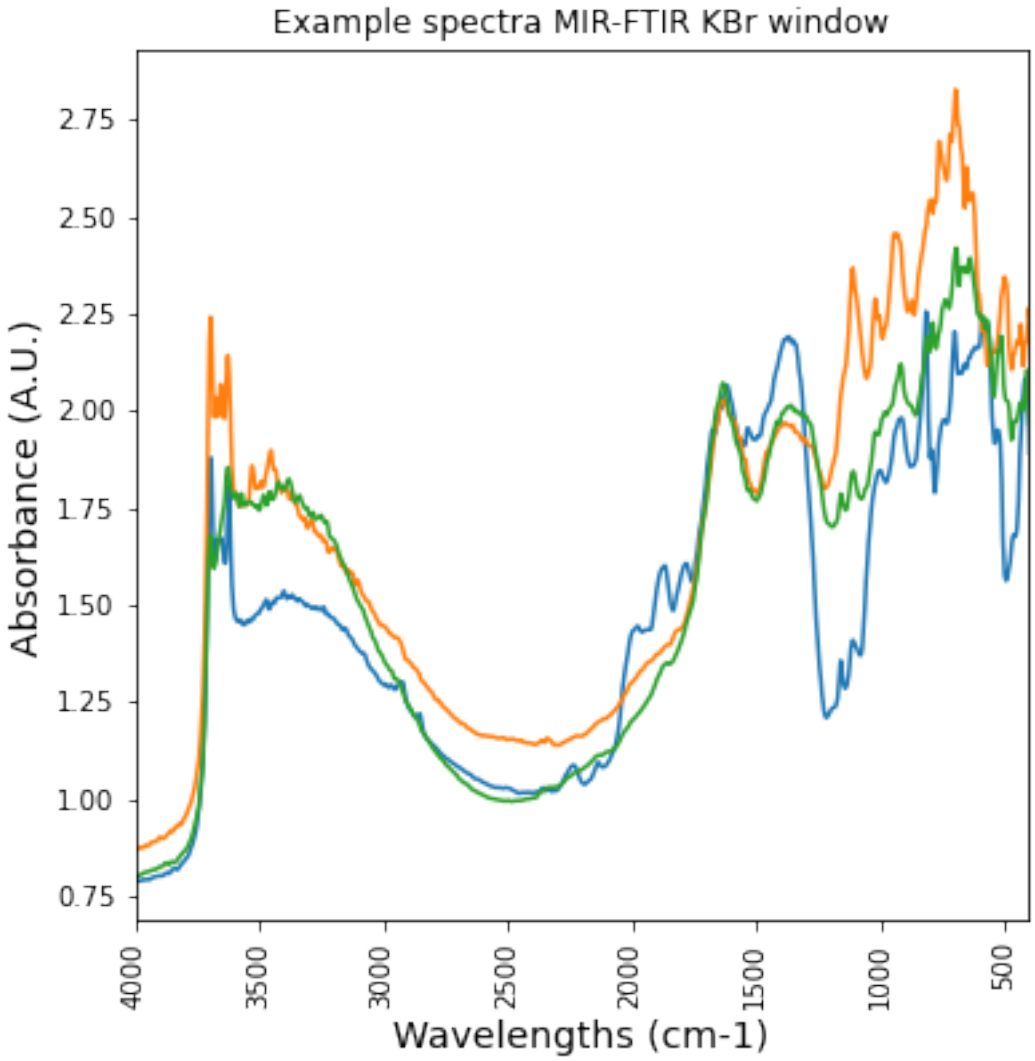
```
# table with FTIR spectra for each sample
df_KBR_FTIRspectra = kbr_df.T.reset_index()

df_KBR_FTIRspectra = df_KBR_FTIRspectra.rename(columns={'index': 'labda'})
df_KBR_FTIRspectra.labda = pd.to_numeric(df_KBR_FTIRspectra.labda)

df_KBR_FTIRspectra.head()
```

	labda	icr033603	icr042897	icr049675	icr034693	icr033950	icr034794	icr015953	icr050394	icr0
0	3998	0.908592	0.810133	0.711836	0.788686	0.752478	0.799947	0.819920	0.701762	0.85
1	3997	0.908981	0.809940	0.712355	0.789201	0.753251	0.801083	0.819910	0.702142	0.85
2	3996	0.909435	0.809745	0.713021	0.789494	0.753915	0.802259	0.820077	0.702510	0.85
3	3994	0.909956	0.809616	0.713747	0.789611	0.754423	0.803318	0.820496	0.702824	0.85
4	3993	0.910562	0.809566	0.714438	0.789634	0.754733	0.804114	0.821235	0.703081	0.85

```
plt.figure(figsize= (6,6))

plt.plot(df_KBR_FTIRspectra['labda'],df_KBR_FTIRspectra.iloc[:, [4,257,100]])

plt.title('Example spectra MIR-FTIR KBr window')

plt.xticks(rotation=90)
plt.xlim(4000,400)
```

```
  plt.ylabel('Absorbance (A.U.)', fontsize=14)
  plt.xlabel('Wavelengths (cm-1)', fontsize = 14)
```

```
Text(0.5, 0, 'Wavelengths (cm-1)')
```



- **Alpha spectrometer - ZnSe window**

```
ZnSe_SPECTRA_DIR = 'Bruker_Alpha_ZnSe/*'
AFSIS_PATH = Path('afsis/2009-2013/Dry_Chemistry/ICRAF')

names = []
spectra = []

for path in tqdm(AFSIS_PATH.glob(ZnSe_SPECTRA_DIR )):
    if path.is_file():
        spect_data = read_file(path)
        spectra.append(spect_data["AB"])
        names.append(path.stem)
wave_nums = spect_data.get_range()

column_names1 = ['{:.0f}'.format(x) for x in wave_nums]
ZnSe_df = pd.DataFrame(spectra, index=names, columns=column_names1)
```

```
TqdmDeprecationWarning: This function will be removed in tqdm==5.0.0
Please use `tqdm.notebook.tqdm` instead of `tqdm.tqdm_notebook`
  for path in tqdm(AFSIS_PATH.glob(ZnSe_SPECTRA_DIR )):
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', max=1.0), HTML(value='')))
```

```
ZnSe_df.head()
```

	3996	3994	3992	3990	3988	3986	3984	3982	3980
icr033603	1.336817	1.337777	1.338591	1.339180	1.339602	1.339999	1.340485	1.341091	1.341770
icr042897	1.217690	1.218229	1.218768	1.219244	1.219670	1.220118	1.220660	1.221307	1.221991
icr049675	1.155588	1.155937	1.156262	1.156588	1.156925	1.157270	1.157606	1.157913	1.158161
icr034693	1.215348	1.215774	1.216170	1.216544	1.216940	1.217407	1.217960	1.218564	1.219142
icr033950	1.163011	1.163466	1.163930	1.164330	1.164612	1.164770	1.164867	1.165003	1.165248

```
# - table with FTIR spectra for each sample

df_ZnSe_FTIRspectra = ZnSe_df.T.reset_index()

df_ZnSe_FTIRspectra = df_ZnSe_FTIRspectra.rename(columns={'index': 'labda'})
```

```
df_ZnSe_FTIRspectra.labda = pd.to_numeric(df_ZnSe_FTIRspectra.labda)
```

```
print("spectral range:", df_ZnSe_FTIRspectra.labda.min(), "cm-1 - ",df_ZnSe_FTIRspectra.la
```

```
spectral range: 500 cm-1 -  3996 cm-1
```

- Tensor 27 HTS-XT spectrometer

KBr window and wider range: both MID and Near IR

```
HTSXT_SPECTRA_DIR = 'Bruker_HTSXT/*'
AFSIS_PATH = Path('afsis/2009-2013/Dry_Chemistry/ICRAF')

names = []
spectra = []

for path in tqdm(AFSIS_PATH.glob(HTSXT_SPECTRA_DIR )):
    if path.is_file():
        spect_data = read_file(path)
        spectra.append(spect_data["AB"])
        names.append(path.stem)
wave_nums = spect_data.get_range()

column_names = ['{:.0f}'.format(x) for x in wave_nums]
htsxt_df = pd.DataFrame(spectra, index=names, columns=column_names)
```

```
TqdmDeprecationWarning: This function will be removed in tqdm==5.0.0
Please use `tqdm.notebook.tqdm` instead of `tqdm.tqdm_notebook`
  for path in tqdm(AFSIS_PATH.glob(HTSXT_SPECTRA_DIR )):
```

```
HBox(children=(FloatProgress(value=1.0, bar_style='info', max=1.0), HTML(value='')))
```

```
print('Total measurements',len(htsxt_df.index),', unique samples', len(htsxt_df.index.uniq
```

```
Total measurements 7346 , unique samples 1839
```

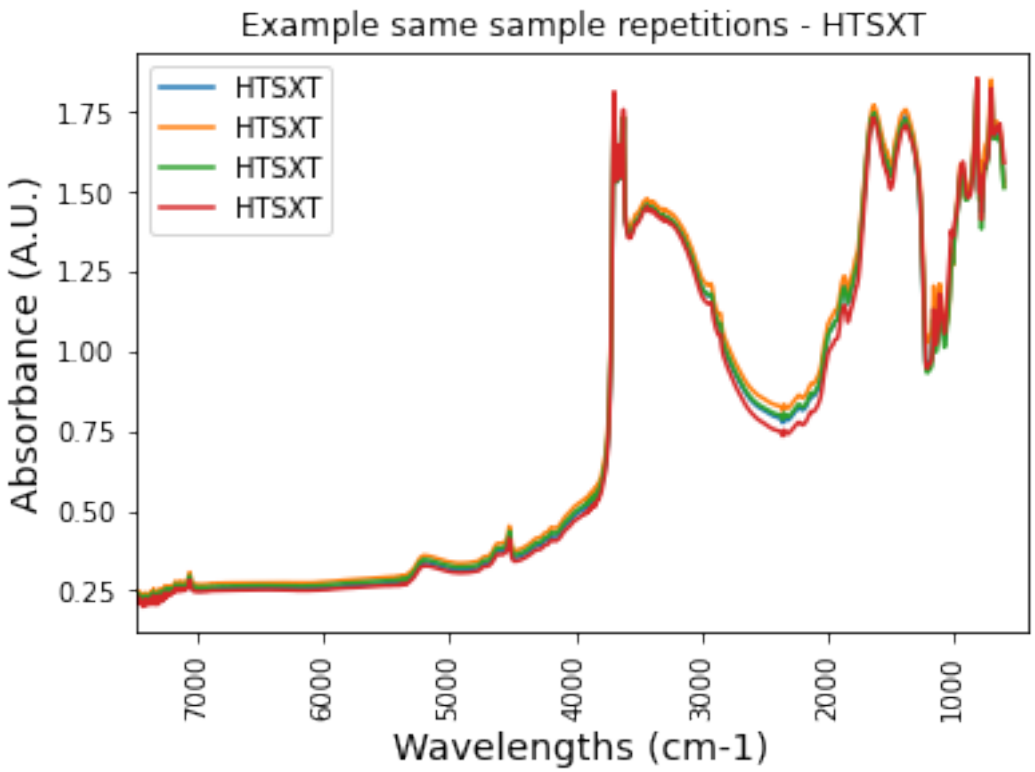
```
# table with FTIR spectra for each sample

df_htsxt_FTIRspectra = htsxt_df.T.reset_index()

df_htsxt_FTIRspectra = df_htsxt_FTIRspectra.rename(columns={'index': 'labda'})
df_htsxt_FTIRspectra.labda = pd.to_numeric(df_htsxt_FTIRspectra.labda)
print("spectral range:", df_htsxt_FTIRspectra.labda.min(), "cm-1 - ",df_htsxt_FTIRspectra.
```

```
spectral range: 600 cm-1 -  7498 cm-1
```

Are Tensor 27 HTS-XT spectrometer measurements reproducible?

```
plt.plot(df_htsxt_FTIRspectra['labda'],df_htsxt_FTIRspectra['icr034794'], label = 'HTSXT')

plt.title('Example same sample repetitions - HTSXT')
plt.legend()

plt.xticks(rotation=90)
plt.xlim(7500,400)
plt.ylabel('Absorbance (A.U.)', fontsize=14)
plt.xlabel('Wavelengths (cm-1)', fontsize = 14)

print('4 repetitions, identical result')
```

```
4 repetitions, identical result
```



let's average the repetitions

```
htsxt_df = htsxt_df.reset_index()
htsxt_df.head()
```

	index	7498	7496	7494	7492	7490	7488	7486	7485	7483
0	icr033603	0.363767	0.358597	0.352962	0.355229	0.364906	0.370382	0.363909	0.354324	0.3504
1	icr010356	0.138930	0.132892	0.136494	0.148280	0.153970	0.145607	0.134926	0.131624	0.1309
2	icr055782	0.198082	0.193039	0.187723	0.190430	0.200350	0.205885	0.199621	0.190752	0.1880
3	icr011264	0.327606	0.321836	0.325163	0.336058	0.341134	0.332636	0.321906	0.318676	0.3177
4	icr034402	0.339334	0.334438	0.329383	0.331227	0.339271	0.343485	0.337471	0.329251	0.3266

```
htsxt_df = htsxt_df.rename(columns={'index': 'SSN'})
```

```
gb_htsxt = htsxt_df.groupby(['SSN']).mean().reset_index()
print(gb_htsxt.shape)
```

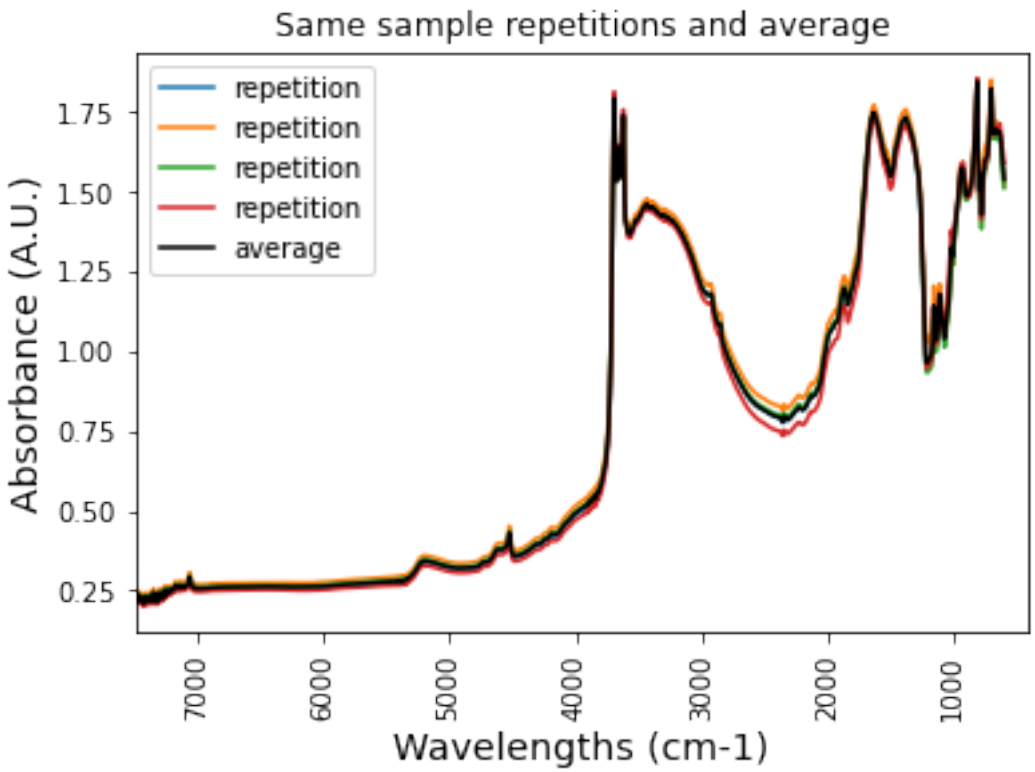
```
(1839, 3579)
```

```
gb_htsxt = gb_htsxt.set_index('SSN')
```

```
gb_htsxt_FTIRspectra = gb_htsxt.T.reset_index()

gb_htsxt_FTIRspectra = gb_htsxt_FTIRspectra.rename(columns={'index': 'labda'})
gb_htsxt_FTIRspectra.labda = pd.to_numeric(gb_htsxt_FTIRspectra.labda)
```

```
plt.plot(df_htsxt_FTIRspectra['labda'],df_htsxt_FTIRspectra['icr034794'], label = 'repetit
plt.plot(gb_htsxt_FTIRspectra['labda'],gb_htsxt_FTIRspectra['icr034794'],color = 'k', labe
plt.title('Same sample repetitions and average')
plt.legend()

plt.xticks(rotation=90)
plt.xlim(7500,400)
plt.ylabel('Absorbance (A.U.)', fontsize=14)
plt.xlabel('Wavelengths (cm-1)', fontsize = 14)

print('4 repetitions, identical result')
```

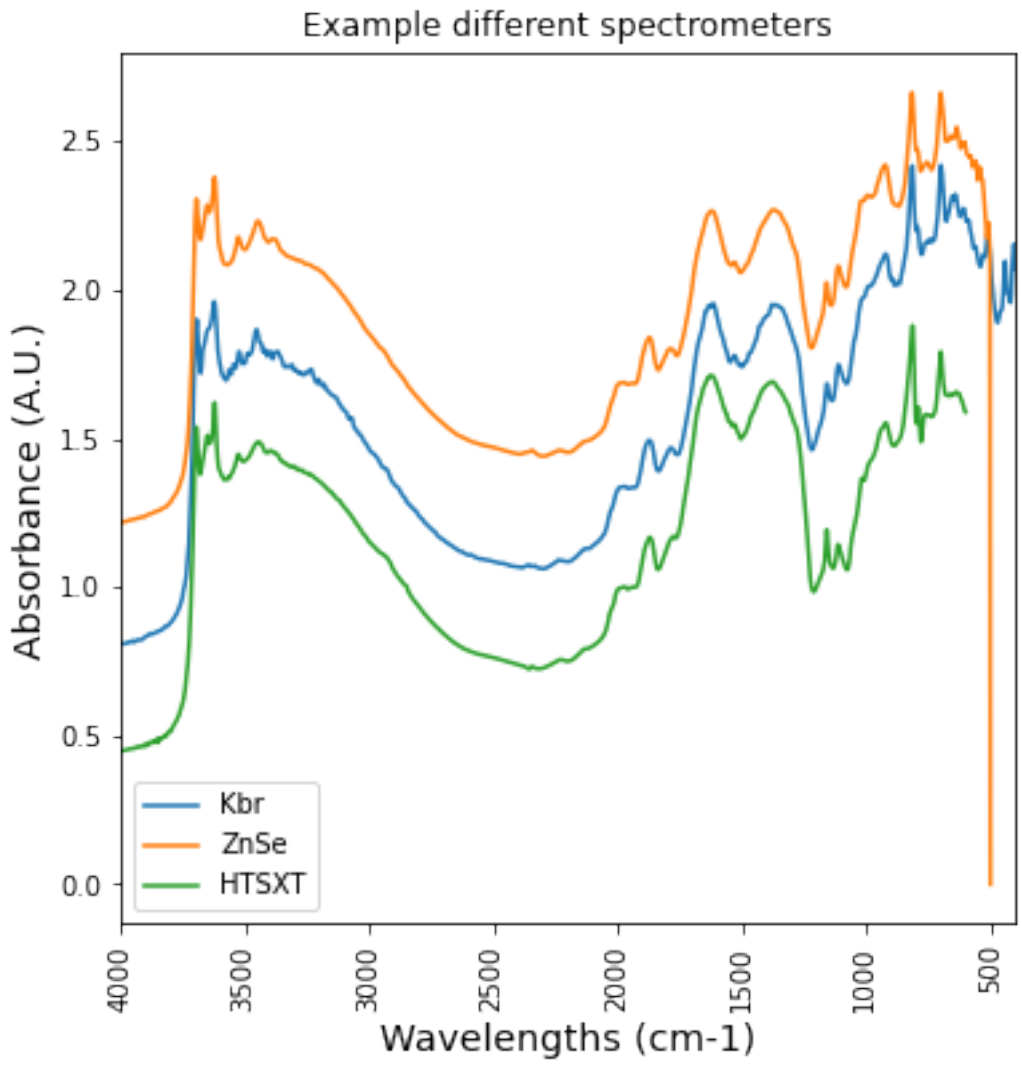
```
4 repetitions, identical result
```




```
print('what is the difference between different spectrometers measurements?')
plt.figure(figsize= (6,6))

plt.plot(df_KBR_FTIRspectra['labda'],df_KBR_FTIRspectra['icr042897'], label = 'Kbr')
plt.plot(df_ZnSe_FTIRspectra['labda'],df_ZnSe_FTIRspectra['icr042897'], label = 'ZnSe')
plt.plot(gb_htsxt_FTIRspectra['labda'],gb_htsxt_FTIRspectra['icr042897'], label = 'HTSXT')

plt.title('Example different spectrometers')
plt.legend()

plt.xticks(rotation=90)
plt.xlim(4000,400)
plt.ylabel('Absorbance (A.U.)', fontsize=14)
plt.xlabel('Wavelengths (cm-1)', fontsize = 14)
```

```
what is the difference between different spectrometers measurements?
```

```
Text(0.5, 0, 'Wavelengths (cm-1)')
```




```
print(df_KBR_FTIRspectra.shape)
df_KBR_FTIRspectra.head()
```

```
(2542, 1889)
```

	labda	icr033603	icr042897	icr049675	icr034693	icr033950	icr034794	icr015953	icr050394	icr0
0	3998	0.908592	0.810133	0.711836	0.788686	0.752478	0.799947	0.819920	0.701762	0.85
1	3997	0.908981	0.809940	0.712355	0.789201	0.753251	0.801083	0.819910	0.702142	0.85
2	3996	0.909435	0.809745	0.713021	0.789494	0.753915	0.802259	0.820077	0.702510	0.85

	labda	icr033603	icr042897	icr049675	icr034693	icr033950	icr034794	icr015953	icr050394	icr0
3	3994	0.909956	0.809616	0.713747	0.789611	0.754423	0.803318	0.820496	0.702824	0.85
4	3993	0.910562	0.809566	0.714438	0.789634	0.754733	0.804114	0.821235	0.703081	0.85

- build unique dataset for FTIR

```
KBr_list = kbr_df.index.tolist()
ZnSe_list = ZnSe_df.index.tolist()
HTSXT_list = gb_htsxt.index.tolist()
print('samples tested with alpha-KBr', len(KBr_list))
print('samples tested with alpha-ZnSe', len(ZnSe_list))
print('samples tested with Tensor27', len(HTSXT_list))

print ("difference samples alpha spectrometers:",len(KBr_list) - len(ZnSe_list))
print ("difference samples alpha_kbr to tensor27 spectrometers:", len(KBr_list) - len(HTSX
```

```
samples tested with alpha-KBr 1888
samples tested with alpha-ZnSe 1835
samples tested with Tensor27 1839
difference samples alpha spectrometers: 53
difference samples alpha_kbr to tensor27 spectrometers: 49
```

```
diff_list1 = np.setdiff1d(KBr_list,ZnSe_list)
print("samples tested using the Alpha-KBr and not the Alpha-ZnSe spectrometer")
print(len(diff_list1))
```

```
samples tested using the Alpha-KBr and not the Alpha-ZnSe spectrometer
53
```

```
diff_list_KBr = np.setdiff1d(HTSXT_list, KBr_list)
print("samples tested using the Tensor27 and not the Alpha-KBr spectrometer")
print(len(diff_list_KBr))
```

```
samples tested using the Tensor27 and not the Alpha-KBr spectrometer
8
```

```
mask_diff_kbr = kbr_df[kbr_df.index.isin(diff_list )]
mask_diff_znse = ZnSe_df[ZnSe_df.index.isin(diff_list )]
mask_diff_htsxt = gb_htsxt[gb_htsxt.index.isin(diff_list )]
print('KBr',len(mask_diff_kbr.index) ,'ZnSe', len(mask_diff_znse.index), 'HTSXT', len(mask
```

```
KBr 1616 ZnSe 1616 HTSXT 1615
```

- Most information from Alpha spectrometers and MPA is redundant. Tensor27 NIR peaks provide the same information for both MID and Near IR range

4. Wet chemistry

```
WET_CHEM_PATH1 = 'afsis/2009-2013/Wet_Chemistry/CROPNUTS/Wet_Chemistry_CROPNUTS.csv'

wet_chem_df = pd.read_csv(WET_CHEM_PATH1)#, usecols=columns_to_load)
elements = ['SSN','M3 Ca', 'M3 K', 'M3 Al', 'M3 P', 'M3 S', 'PH']
wet_chem_df = wet_chem_df[elements]

print(wet_chem_df.shape)
wet_chem_df.head()
```

```
(1907, 7)
```

	SSN	M3 Ca	M3 K	M3 Al	M3 P	M3 S	PH
0	icr006475	207.1	306.30	1095.0	4.495	18.960	4.682
1	icr006586	1665.0	1186.00	1165.0	12.510	13.600	7.062
2	icr007929	2518.0	72.57	727.6	21.090	14.810	7.114
3	icr008008	734.3	274.60	1458.0	109.200	11.400	5.650
4	icr010198	261.8	91.76	2166.0	3.958	5.281	5.501

```
WET_CHEM_PATH2 = 'afsis/2009-2013/Wet_Chemistry/RRES/Wet_Chemistry_RRES.csv'

#columns_to_load = elements + ['SSN']


wet_chem_df1 = pd.read_csv(WET_CHEM_PATH2)#, usecols=columns_to_load)
```

```
elements = ['SSN','pH', '%N', 'C % Org', 'ICP OES K mg/kg ', 'ICP OES P mg/kg ']
wet_chem_df1 = wet_chem_df1[elements]
wet_chem_df1 = wet_chem_df1.rename(columns={"%N": "Leco_N_ppm"})
wet_chem_df1['Leco_N_ppm'] = wet_chem_df1['Leco_N_ppm']*10000
print(wet_chem_df1.columns)
wet_chem_df1.head()
```

```
Index(['SSN', 'pH', 'Leco_N_ppm', 'C % Org', 'ICP OES K mg/kg ',
       'ICP OES P mg/kg '],
      dtype='object')
```

	SSN	pH	Leco_N_ppm	C % Org	ICP OES K mg/kg	ICP OES P mg/kg
0	icr006454	7.85	800.0	0.94	8517.919223	96.575131
1	icr006455	8.03	600.0	0.70	10859.303780	117.423139
2	icr006474	5.01	500.0	0.57	1343.124117	87.040073
3	icr006475	4.57	500.0	0.47	1487.768795	83.555482
4	icr006492	6.78	900.0	0.98	2999.240760	150.936463

```
WET_CHEM_PATH3 = 'afsis/2009-2013/Wet_Chemistry/ICRAF/Wet_Chemistry_ICRAF.csv'
#elements = ['M3 Ca', 'M3 K', 'M3 Al']
#columns_to_load = elements + ['SSN']


wet_chem_df2 = pd.read_csv(WET_CHEM_PATH3)#, usecols=columns_to_load)
#print(wet_chem_df2.columns)
elements = ['SSN','Psa asand', 'Psa asilt','Psa aclay', 'Volfr', 'Awc1','Lshrinkpct', 'Aci
       'Acidified carbon']
wet_chem_df2 = wet_chem_df2[elements]
wet_chem_df2['Acidified nitrogen'] = wet_chem_df2['Acidified nitrogen']*10000
wet_chem_df2 = wet_chem_df2.rename(columns={"Acidified nitrogen": "Flash2000_N_ppm"})

print(wet_chem_df2.shape)
wet_chem_df2.head()
```

```
(1907, 9)
```

	SSN	Psa asand	Psa asilt	Psa aclay	Volfr	Awc1	Lshrinkpct	Flash2000_N_ppm	A
0	icr005928	90.993000	8.111667	0.896333	1.190000	0.070768	0.000000	296.21345	0
1	icr005929	87.847000	11.416000	0.737000	1.192000	0.061710	5.000000	230.68986	0
2	icr005946	94.408333	5.335333	0.256000	1.171280	0.115414	5.714286	313.39549	0
3	icr005947	94.601333	5.239333	0.159000	1.198744	0.122856	0.000000	170.62043	0
4	icr005965	90.015333	9.195667	0.789000	1.081575	0.100874	5.000000	831.45402	0

5. Join and clean datasets

5.1 Elemental analysis

```
df_elements1 = pd.merge(left=wet_chem_df1, right=df_xrf_reduced, left_on='SSN', right_on='
print(df_elements1.shape)


df_elements2 = pd.merge(left=wet_chem_df2, right=df_elements1, left_on='SSN', right_on='SS
print(df_elements2.shape)


df_elements = pd.merge(left=wet_chem_df, right=df_elements2, left_on='SSN', right_on='SSN'
print(df_elements.shape)
print(df_elements.columns)

df_elements.head()
```

```
(467, 17)
(467, 25)
(467, 31)
Index(['SSN', 'M3 Ca', 'M3 K', 'M3 Al', 'M3 P', 'M3 S', 'PH', 'Psa asand',
       'Psa asilt', 'Psa aclay', 'Volfr', 'Awc1', 'Lshrinkpct',
       'Flash2000_N_ppm', 'Acidified carbon', 'pH', 'Leco_N_ppm', 'C % Org',
       'ICP OES K mg/kg ', 'ICP OES P mg/kg ', 'P', 'K', 'S', 'Ca', 'Mg', 'Cu',
       'Cl', 'Zn', 'Fe', 'Mn', 'Mo'],
      dtype='object')
```

	SSN	M3 Ca	M3 K	M3 Al	M3 P	M3 S	PH	Psa asand	Psa asilt	Psa aclay	...
0	icr006475	207.1	306.30	1095.000	4.495	18.960	4.682	97.848667	1.845333	0.306000	...

	SSN	M3 Ca	M3 K	M3 Al	M3 P	M3 S	PH	Psa asand	Psa asilt	Psa aclay	...
1	icr006586	1665.0	1186.00	1165.000	12.510	13.600	7.062	89.520000	9.553667	0.926333	...
2	icr021104	258.7	35.25	441.400	4.424	3.608	5.522	89.950000	5.205000	4.845000	...
3	icr033622	11858.3	1156.00	108.286	31.233	25.460	8.583	91.445000	6.310000	2.245000	...
4	icr006570	896.2	607.30	1151.000	5.986	20.080	6.661	97.789667	1.885000	0.325667	...

```
#check for possible negative values
for col in df_elements.columns.tolist()[1:]:
    if df_elements[col].dtype == np.float64:
         df_elements[col][df_elements[col] < 0] =np.nan

print(df_elements.isna().sum().sum())
```

```
54
```

```
SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide
  df_elements[col][df_elements[col] < 0] =np.nan
```

merge geographical and chemical data

```
df_geoelements = pd.merge(left=df_elements, right=df_geo, left_on='SSN', right_on='SSN')

print(df_geoelements.shape)
print(df_geoelements.columns)
df_geoelements.head()
```

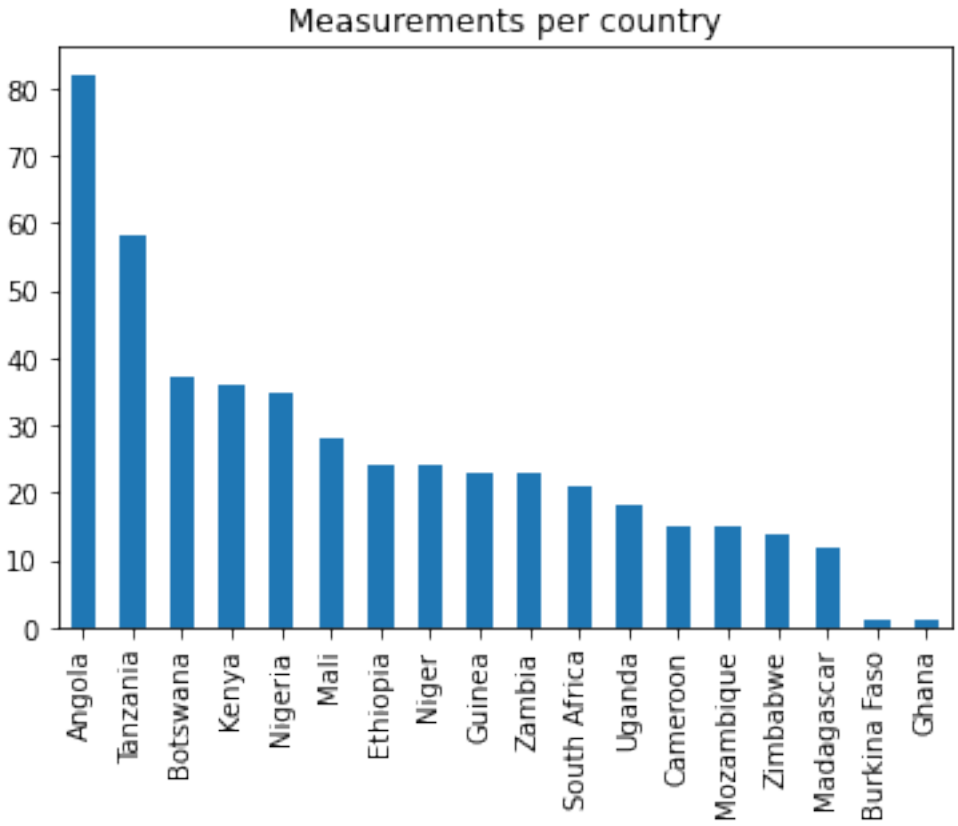
```
(467, 37)
Index(['SSN', 'M3 Ca', 'M3 K', 'M3 Al', 'M3 P', 'M3 S', 'PH', 'Psa asand',
       'Psa asilt', 'Psa aclay', 'Volfr', 'Awc1', 'Lshrinkpct',
       'Flash2000_N_ppm', 'Acidified carbon', 'pH', 'Leco_N_ppm', 'C % Org',
       'ICP OES K mg/kg ', 'ICP OES P mg/kg ', 'P', 'K', 'S', 'Ca', 'Mg', 'Cu',
       'Cl', 'Zn', 'Fe', 'Mn', 'Mo', 'Latitude', 'Longitude', 'Cluster',
       'Depth', 'Country', 'Cultivated'],
      dtype='object')
```

	SSN	M3 Ca	M3 K	M3 Al	M3 P	M3 S	PH	Psa asand	Psa asilt	Psa aclay	...
0	icr006475	207.1	306.30	1095.000	4.495	18.960	4.682	97.848667	1.845333	0.306000	...
1	icr006586	1665.0	1186.00	1165.000	12.510	13.600	7.062	89.520000	9.553667	0.926333	...
2	icr021104	258.7	35.25	441.400	4.424	3.608	5.522	89.950000	5.205000	4.845000	...
3	icr033622	11858.3	1156.00	108.286	31.233	25.460	8.583	91.445000	6.310000	2.245000	...
4	icr006570	896.2	607.30	1151.000	5.986	20.080	6.661	97.789667	1.885000	0.325667	...

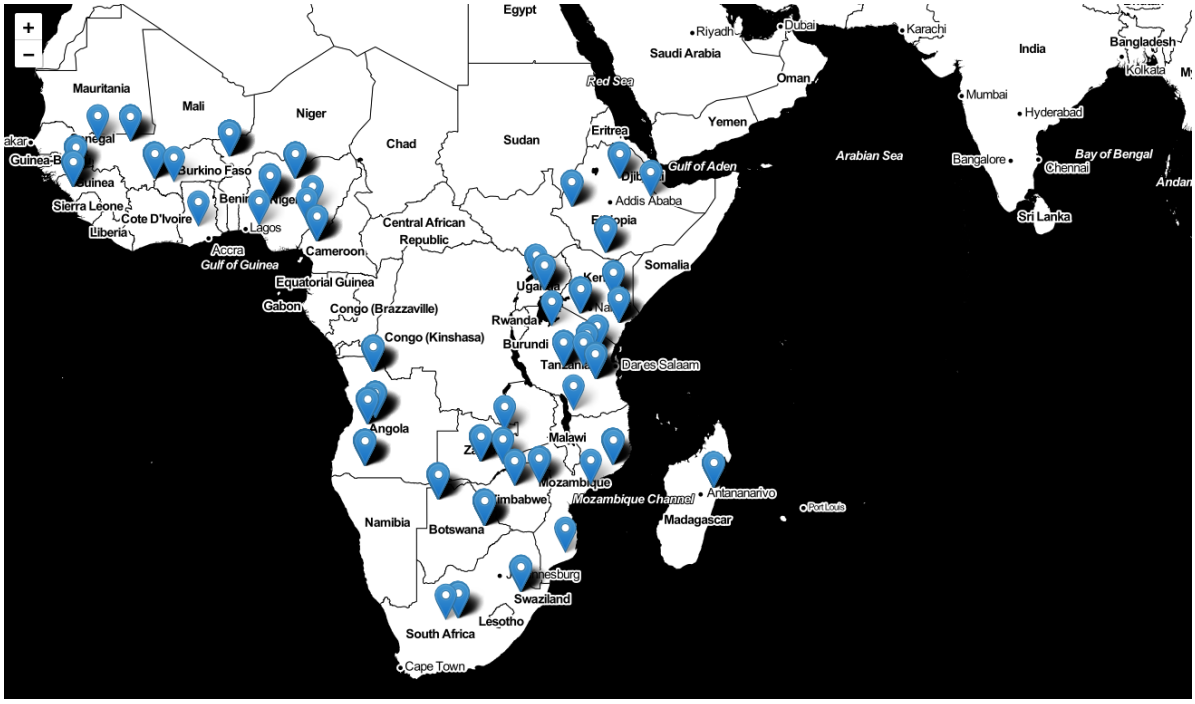
geographical distribution of the selected samples

```
pd.value_counts(df_geoelements['Country']).plot.bar(title='Measurements per country')
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7fd0c8193b20>
```



```
 #Draw map


m = folium.Map(location=[-3.5, 35.6], tiles="stamentoner", zoom_start=5)

for _, row in df_geoelements.iterrows():
    if row[['Latitude', 'Longitude']].notnull().all():
        folium.Marker([row['Latitude'],
                       row['Longitude']],
                      popup=row['SSN']
                     ).add_to(m)

#m

Image(filename='img/folium.png')
```



imputation of missing values

```
def replace_missings(data):
    # this replaces missings with medians
    # NOTE: mixed string num columns it does not do anything with
    for cols in data._get_numeric_data().columns:
        data[cols].fillna(value=data[cols].median(), inplace=True)


replace_missings(df_geoelements)

print(df_geoelements['Cultivated'].unique())
df_geoelements['Cultivated'] = df_geoelements['Cultivated'].fillna('unknown')
print(df_geoelements['Cultivated'].unique())
print(df_geoelements.isna().sum().sum())
```

```
[False 'unknown' True]
[False 'unknown' True]
0
```

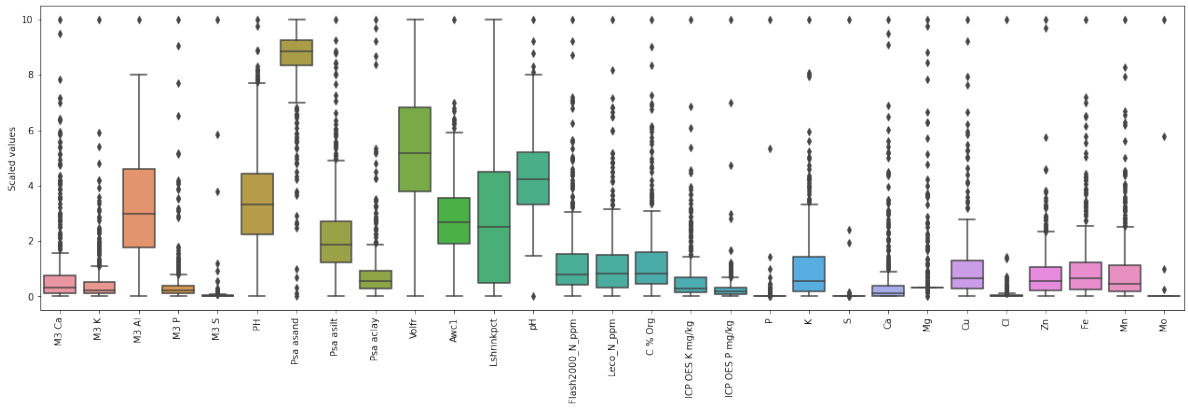
outliers

```
def detect_outliers(df, n, features):
    """
    Takes a dataframe df of features and returns a list of the indices
    corresponding to the observations containing more than n outliers according
    to the Tukey method.
    """
    outlier_indices = []

    # iterate over features(columns)
    for col in features:
        # 1st quartile (25%)
        Q1 = np.percentile(df[col], 25)
        # 3rd quartile (75%)
        Q3 = np.percentile(df[col], 75)
        # Interquartile range (IQR)
        IQR = Q3 - Q1

        # outlier step
```

```
        outlier_step = 3 * IQR

        # Determine a list of indices of outliers for feature col
        outlier_list_col = df[(df[col] < Q1 - outlier_step) | (df[col] > Q3 + outlier_step
        # append the found outlier indices for col to the list of outlier indices
        outlier_indices.extend(outlier_list_col)

    # select observations containing more than 1 outlier
    outlier_indices = Counter(outlier_indices)


    return outlier_indices

# detect outliers from list of features
lof = ['M3 Ca', 'M3 K', 'M3 Al', 'M3 P', 'M3 S', 'PH', 'Psa asand',
       'Psa asilt', 'Psa aclay', 'Volfr', 'Awc1', 'Lshrinkpct', 'pH', 'Flash2000_N_ppm','L
       'C % Org', 'ICP OES K mg/kg ', 'ICP OES P mg/kg ', 'P', 'K', 'S', 'Ca',
       'Mg', 'Cu', 'Cl', 'Zn', 'Fe', 'Mn', 'Mo']#,
Outliers_to_drop = detect_outliers(df_geoelements, 1, lof)

print(len(Outliers_to_drop), 'outliers according to Tukey method')
if len(Outliers_to_drop)>50:
    print('loss of information would be too high if Tukey method would be applied')
```

```
209 outliers according to Tukey method
loss of information would be too high if Tukey method would be applied
```

```
df_chem = df_geoelements[lof]
df_chem_scaled =((df_chem -df_chem.min())/(df_chem.max()-df_chem.min()))*10

%matplotlib inline
plt.figure(figsize= (22,6))
box_plot_scaled = sns.boxplot( data= df_chem_scaled)
fig = box_plot_scaled.get_figure()
plt.xticks(rotation=90)
plt.ylabel("Scaled values")
fig.savefig("box.png", dpi= 100)
```




```
df_chem.describe()
```

	M3 Ca	M3 K	M3 Al	M3 P	M3 S	PH	Psa asand	Psa
count	467.000000	467.000000	467.000000	467.000000	467.000000	467.000000	467.000000	467
mean	1605.142957	186.569448	802.767263	10.296321	23.906516	6.133593	84.902406	8.0
std	2780.256854	303.097846	423.564349	22.179751	154.640351	1.151291	14.436237	5.7
min	0.001000	5.110000	14.300000	0.001000	1.490000	4.000000	0.440000	0.0
25%	236.800000	47.200000	446.543000	2.495000	4.732000	5.315000	83.500000	4.3
50%	560.700000	82.200000	735.486000	4.495000	7.530000	5.950000	88.525000	6.7
75%	1375.400000	181.900000	1130.000000	8.590500	12.300000	6.603000	92.545000	9.6
max	18510.000000	3432.000000	2444.000000	221.800000	2728.860000	9.860000	100.005000	35.

```
# export to csv
df_geoelements.to_csv( 'elemental_analysis_dataset.csv',index=False)
```

5.2 FTIR

```
df_FTIR_reindexed = df_KBR_FTIRspectra.set_index('labda')
mid_infrared_df = df_FTIR_reindexed.T.reset_index()
mid_infrared_df = mid_infrared_df.rename(columns={'index': 'SSN'})
```

I select only the sample that are in the compositional dataframe "geoelements"

The composition and FTIR dataframes have same sample numbers (SSN) column

Each infrared spectrum corresponds to an elemental analysis

```
complete_measurements_list = df_geoelements_reduced.SSN.tolist()
```

- mid infrared

```
df_FTIRdata = mid_infrared_df[mid_infrared_df.SSN.isin(complete_measurements_list)]
print(df_FTIRdata.shape)
#print(df_FTIRdata.isna().sum())
```

```
(467, 2543)
```

```
df_FTIRdata.to_csv( 'middle_infrared_spectra_dataset.csv',index=False)
```

- near infrared

```
df_FTIR_reindexed1 = df_NIR_FTIRspectra.set_index('labda')
near_infrared_df = df_FTIR_reindexed1.T.reset_index()
near_infrared_df = near_infrared_df.rename(columns={'index': 'SSN'})
# I select only the sample that are in the compositional dataframe "geoelements"

complete_measurements_list = df_geoelements_reduced.SSN.tolist()

df_FTIRdataM = near_infrared_df[near_infrared_df.SSN.isin(complete_measurements_list)]
print(df_FTIRdata.shape)
#print(df_FTIRdata.isna().sum())
df_FTIRdataM.to_csv( 'near_infrared_spectra_dataset.csv',index=False)
```

```
(467, 2543)
```