SpMap: Hyperspectral library for spectroscopists in Python

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A. Introduction to *SpectraMap (SpMap)*

Hyperspectral imaging presents important applications in medicine, agriculture, pharmaceutical, space, food, and many upcoming applications. The analysis of hyperspectral images requires advanced software. The forthcoming developments related to fast hyperspectral imaging, automation and deep learning applications demand innovative software developments for analyzing hyperspectral data. Along this chapter a new software is development based on Python 3. The library is defined as hyperspectral imaging *SpectraMap(SpMap).*

SpMap is a python package for high level hyperspectral data processing scripting. The type of datasets can be any optical spectroscopic data with intensity and wavenumber axes. The coming content shows how to handle the data from an imaging spectroscopic point of view rather pure programming and developing approach. A high-level programming holds a short scripting structure for fast and efficient hyperspectral data analysis. *SpMap* comes with 6 dataset-examples for understanding and practicing the tools implemented in *SpMap*.

Table A.1 datasets and examples in *SpMap*

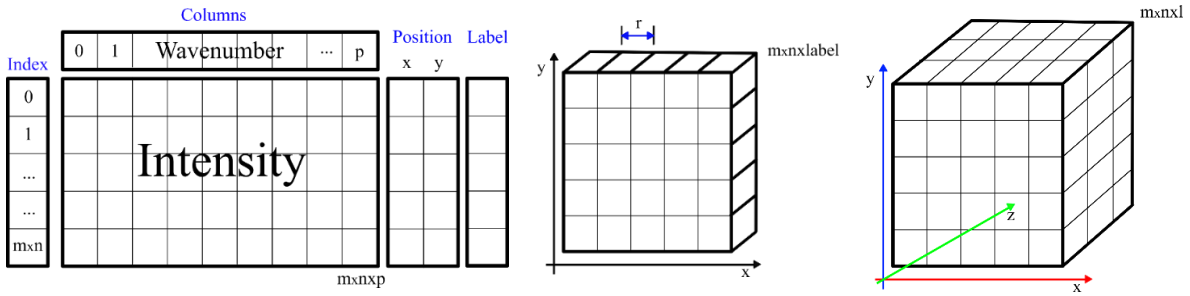
Plastics	Datasets of different plastics
Microplastics on tissue	Raman Map of tissue model and microplastics
Multi-layer of plastics	Z scanning of transparent plastic layers
Bladder	Cancer and noncancer tissue models
3D imaging	3D Raman Imaging of translucent tissue and plastics
Paracetamol	Wavenumber calibration

The previous datasets will illustrate and help how to process raw datasets and obtain a processed result by several *SpMap* tools. A complete information regarding *SpMap* functions is shown in the open-source *SpMap* code.

A.1. Hyperspectral object structure

Fig. A.1 shows the hyperspectral data object that is established in the *spmap.py* package. The object holds an index and columns along x axis or wavenumber. The rows contain the Raman intensity (Fig. A.2(a)). Datasets from 2D imaging provide spatial information that are represented as *x* and *y* in a position table. The *label* is associated to the naming and meaning of the pixel.

Hyperspectral imaging is represented by a 2D matrix considering *x* and *y* coordinates and the information of label table. Confocal Raman microscopy supplies *z* or depth information and thereby is possible to plot 3D images through voxels Fig. A.2 (c) (also included in the library).



(a) (b) (c)

Figure A.1. Hyperspectral object. (a) representation of hyperspectral object, (b) 2D plotting of hyperspectral data and (c) voxel illustration for 3D imaging.

A.2. Python, Anaconda and Spyder interface

The predetermined work interface is Spyder. For further information concerning how to install the required requirements, check the link: https://www.anaconda.com/. The required external libraries are: scikit-learn [1], standard libraries: matplotlib, NumPy and pandas, besides complex algorithms: vertex component analysis [2], alternative iterative reweighted penalized least squares [3] and hierarchical density based clustering with applications with noise HDBSCAN [4].

A.3. SpMap objects, functions, and assignment

SpMap is based on dataframe structure (Fig. A.2) that contains properties (attributes) and methods for reading, manipulation, preprocessing, processing, and visualization of hyperspectral data.

1. Download the files that are in the link: https://github.com/spectramap/spectramap
2. Set the files with examples in a working path
3. Follow the instruction of the link for the installation
4. Read *SpMap* library by: `from spectramap import spmap as sp`

A.3.1. Creating/Deleting an *SpMap* object

Creating a hyperspectral instance/object. The hyper object can contain any kind of data, spc, csv, txt or custom if it keeps the standard dataframe shape (Fig. A.2). Creating and deleting objects:

Creating
```
mapa = sp.hyper_object('name') ## creating mapa object
```
Deleting
```
del mapa ## deleting mapa object
```

A.3.2. Reading/saving csv, spc, mat and any common file

Some standard data files are spc, csv and txt, the next lines show some reading methods. The variable path may be the directory path and name for single readings and for multi readings path is the directory file of the datasets.

Reading single spc	`mapa.read_single_spc(path)`
Reading several spc	`mapa.read_multi_spc(path)`
Reading a hologram map	`mapa.read_spc_holomap(path)`
Csv (standard file in SpMap)	`mapa.read_csv(path)`
Any file (custom reading)	`pandas.read_table(parameters) # (see coming example)`
Mat (read a raw Mat)	`mat = read_mat(path) # (require custom reading)`
Show spectral data	`mapa.show(True), mapa.show(False)`
Save spectral data	`mapa.save_data(path, 'name')`

A.3.3. Basic Data Handling methods

This section provides methods for data manipulation such as getting intensity or position data. For example, the user can build the hyperobject using manually methods such as set_data(data) and set_position(position) and set_label(label). The upcoming examples will explain how to use most of the following methods:

`data = mapa.get_data()`	`mapa.set_data(data)`
`position = mapa.get_position()`	`mapa.set_position(position)`
`wavenumber = mapa.get_wavenumber()`	`mapa.set_wavenumber(calibration)`
`copied = mapa.copy()`	`mapa.set_resolution(res)`
`label = mapa.get_label()`	`mapa.set_label(label)`
`name = mapa.get_name()`	`mapa.set_name(name)`
`number = mapa.get_number_spectra()`	`mapa.append(hyperobject)`
`spectrum = mapa.get_pixel(x, y)`	`mapa.reset_index()`
`label = mapa.select_label(list)`	`mapa.concat([hyperobject1, ...])`
`wavenumber = mapa.get_wavenumber()`	`mapa.remove_spectrum([index])`
	`mapa.clean_data()`
	`mapa.rename_label([before], [after])`
	`mapa.remove_label([list])`
	`mapa.add_peaks(0.5, 'red')`

A.4. Pre-Processing

A.4.1. Selecting wavelength ranges

The selection of work range defines the spectral region of interest. Fig. A.3 shows the full spectral range and examples of range selections.

Fingerprint region (Fig. A.3(b))	`mapa.keep(lower = 400, upper = 1800)`
High wavenumber region (Fig. A.3(c))	`mapa.keep(lower = 2800, upper = 3200)`
Without silent region (Fig. A.3(d))	`mapa.keep(lower = 400, upper = 3200)` `mapa.remove(lower = 1800, upper = 2700)`

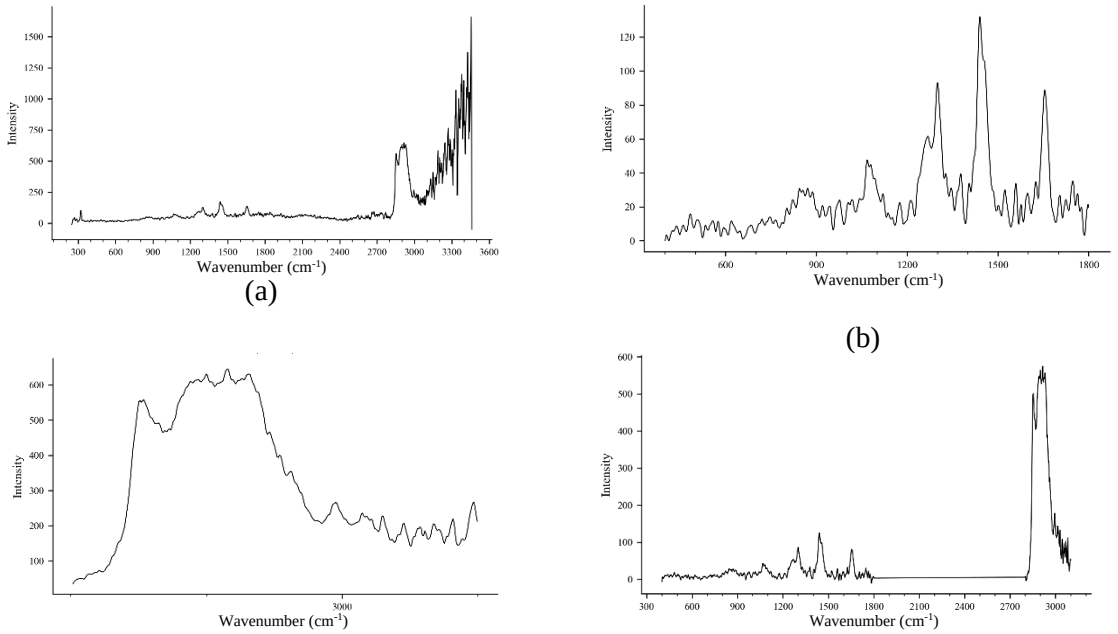


Figure A.2. Selection of work range. (a) full range, (b) low wavenumber (fingerprint region), (c) high wavenumber and (d) selection of low and high wavenumber regions without the silent region.

A.4.2. Pre-processing

Methods for removing noise, outliers, baseline correction, normalization are presented in the next lines.

Removing Outliers

Intensity threshold	`mapa.threshold(peak, lower = 50, upper = 500)`
Cosmic Ray removal tool	`mapa.spikes(threshold = 7, window = 3)`

Smoothing

Savitzky golay filter	`mapa.gol(window = 7, interpolation = 3, order = 0)`
Gaussian filter	`mapa.gaussian(variance = 2)`

Baseline correction

Rubber Band correction	`mapa.rubber()`
Snip baseline	`mapa.snip(iterations = 100)`
Alternative iterative reweighted partial least squares	`mapa.airpls(landa = 100)`

Normalization

Value / (Max - Min)	`mapa.norm()`
Considering a peak as reference	`mapa.norm_at_peak(peak = 1001)`
Vector normalization	`mapa.vector()`

A.5. Processing

The next lines provide an overview of the functions in SpMap as processing tools.

Principal component analysis	`components, loadings = mapa.pca(num_components = 3 ,norm = 'False' )`

Partial least square and linear discriminant analysis	`components, loadings = mapa.pls_lda(num_components = 3 ,norm = 'False', 1)`
Vertex component analysis	`endmembers = mapa.vca(num_components = 3)`
*Multi curve resolution	`components = mapa.mcr_als(spectra, constrain = 'NNLS', num_iterations = 100)`
Kmeans	`mapa.kmeans(3); mapa.kmeans('auto')`
Hierchical clustering	`mapa.hca('euclidean', 'ward', 2, 3)`
Abundance	`concentrations = mapa.abundance(endmembers, constrain = 'NNLS')`
dbscan	`mapa.dbscan(min_samples, eps)`
*hdbscan	`mapa.hdbscan(min_samples, min_cluster)`

*Not available (still developing and debugging)

A.6. Visualization

The final product of processing is the correct visualization of the data by different methods such as plotting spectra, maps, or scatter plots.

Overlapped plot of spectra	`mapa.show_spectra(0,0,'auto')`
Stack of spectra	`mapa.show_stack(0,0,'auto')`
Profile	`mapa.profile('auto')`
Map	`mapa.show_map('auto', None, 1)`
Show scatter points	`scores.show_scatter('auto', label, size)`
Show scatter points 3d	`scores.show_scatter_3d('auto', label, size)`
*Show 3d map	`mapa.scatter3D()`
Show intensity map	`intensity.show_intensity()`

*Not available (developing and debugging)

A.7. Hyperspectral imaging examples

Set the work file path to the file of examples path is located.

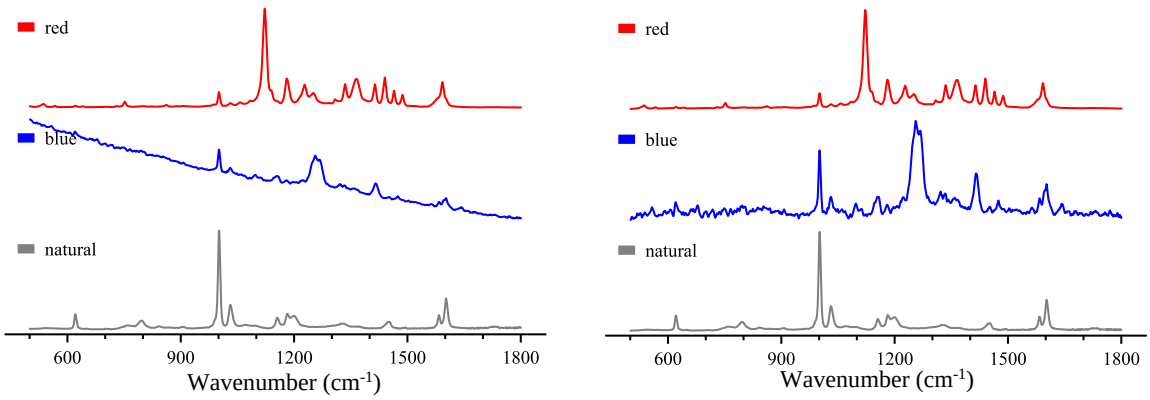
A.7.1 Plastics

The following script shows how to use *SpMap* library for reading some spectra data and apply baseline correction. Fig. A.4 illustrates the results after the script.

```
from spectramap import spmap as sp
### Defining paths ###
blue_path = 'examples/plastics/blue'
red_path = 'examples/plastics/red'
natural_path = 'examples/plastics/natural'
### Creating and reading the files ###
red = sp.hyper_object('red') ## Declaring the first hyper object for red sample
red.read_csv(red_path) ## Reading the comma separated vector file
red.set_label('red') ## Setting red name to the whole data set spectra
red.keep(500, 1800) ## Keep finger region
meanred = red.mean() ## Compute mean of all red spectra
```

```
blue = sp.hyper_object('blue') ## Same procedure for the blue sample
blue.read_csv(blue_path)
blue.set_label('blue')
blue.keep(500, 1800)
blue.rubber() ## Baseline correction rubber band
meanblue = blue.mean()

natural = sp.hyper_object('natural') ## Same procedure for the natural sample
natural.read_csv(natural_path)
red.set_label('natural')
natural.keep(500, 1800)
meannatural = natural.mean()
### Concataneting the three hyperspectral objects
concat = hyper_object('concat') ## create a new empty object
concat.concat([meanred, meanblue, meannatural])
concat.show_stack(0,0,['red', 'blue', 'gray']) ## show the spectra (see Fig. 5.4)
```



(a) (b)

Figure A.3. Modified plastics: (a) raw data and (b) result

A.7.2. Bladder

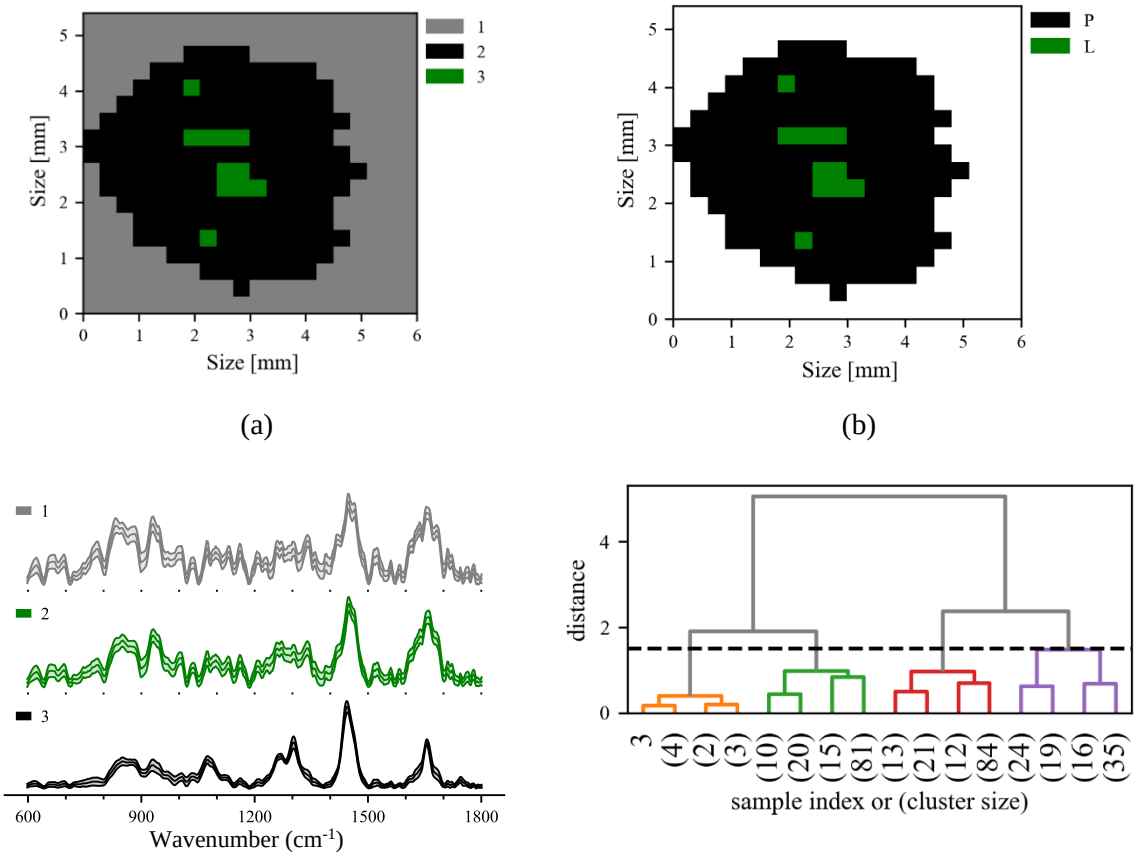
The next example displays how to process a hyperspectral image by clustering for obtaining the classification of different tissue signatures. Fig. A.5 illustrates the results after the script.

```
from spectramap import spmap as sp
### reading ###
path = 'H:/Thesis IPHT/Python/examples/bladder/data'
mapa = sp.hyper_object('Patient')
mapa.read_csv(path)
mapa.set_resolution(0.3) ## 300 µm step size resolution
mapa.vector() # vector normalization
original = mapa.get_data() ## get data
### K-means clustering
mapa.kmeans(3) #K-means clustering: 3 components
colors = mapa.show_map(['gray', 'black', 'green'], None, 1) # show 2D map (Fig.
5.5(a))
mapa.show_stack(0, 0, colors) #show stack of the clusters (Fig. 5.5(c))
```

```
mapa.remove_label([1]) # remove the noisy cluster
mapa.rename_label([2, 3], ['P', 'L']) # rename the remaining clusters

colors = mapa.show_map(['black', 'green'], None, 1) # show 2D map (Fig. 5.5 (b))
mapa.show_stack(0, 0, colors) #show stack of the clusters

### Hierarchical clustering
mapa.set_data(original)
mapa.hca('euclidean', 'ward', 1.5, 3) # hca clustering with 1.5 distance  (Fig.
5.5(d))
colors = mapa.show_map(['gray', 'black', 'lightgray', 'green'], None, 1)
### Saving data
mapa.save_data(path, 'clustering') # saving data
```



(a) (b)

(c) (d)

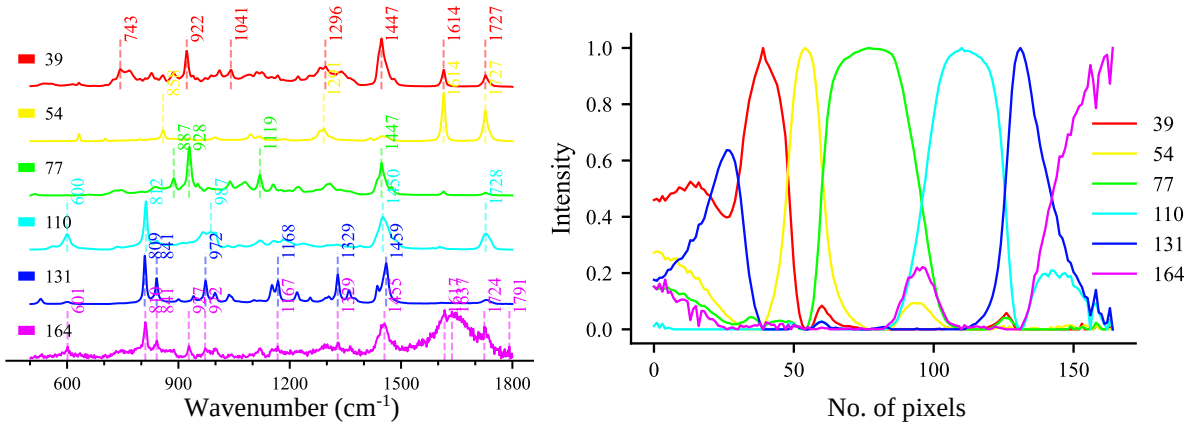
Figure A.4. Clustering results: (a) K-means clustering map, (b) Clean clustering map (without background), (c) cluster means and (d) dendrogram of hierarchical clustering

A.7.3. Multilayer of plastics

The following example: multi-layer of plastics illustrates how to analyze the data of a hyperspectral profile. Fig. A.6 illustrates the results after the script.

```
from spectramap import spmap as sp
### reading ###
path = 'examples/layers/data'
stack = sp.hyper_object('layers') #creating the hyper object
stack.read_csv(path) #reading the csv file
```

```
### preprocessing ###
stack.keep(500, 1800) #finger print selection
stack.rubber() #baseline correction
stack.vector() #vector normalization
### processing ###
endmember = stack.vca(6) # vertex component analysis
endmember.show_stack(1, 0, 'auto') # visualization of spectra and strong
peaks(Fig.5.6(a))
abundance = stack.abundance(endmember, 'NNLS') # concentration estimation by NNLS
abundance.set_resolution(0.02) # set resolution of 20 µm for the profile
abundance.profile('auto') # plot profile (Fig.5.6(b))
```

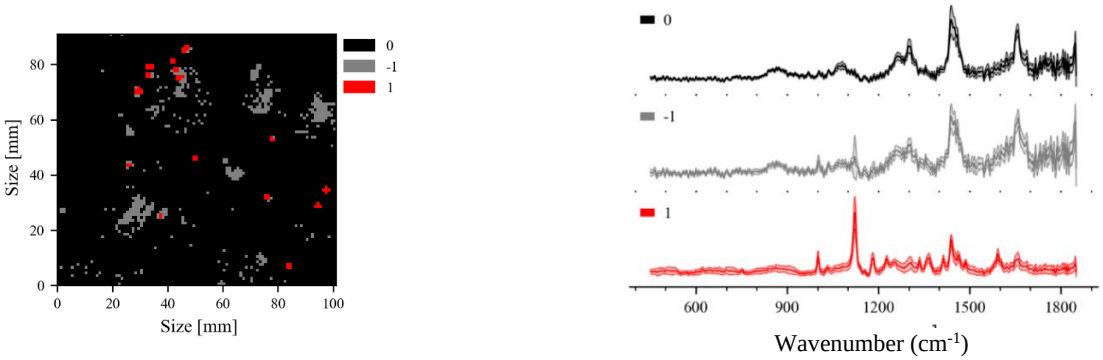


(a) (b)

Figure A.5. Hyperspectral profile analysis: (a) stack of plastics components found by VCA and (b) concentration profile.

A.7.4. Microplastic in tissue

The next examples illustrate the detection of pixel-sized microplastics on a tissue matrix using advanced clustering tools. Fig. A.7 illustrates the results after the script.



(a) (b)

Figure A.6. Density based clustering or detection of small pixels details: (a) hyperspectral image and (b) spectral cluster means.

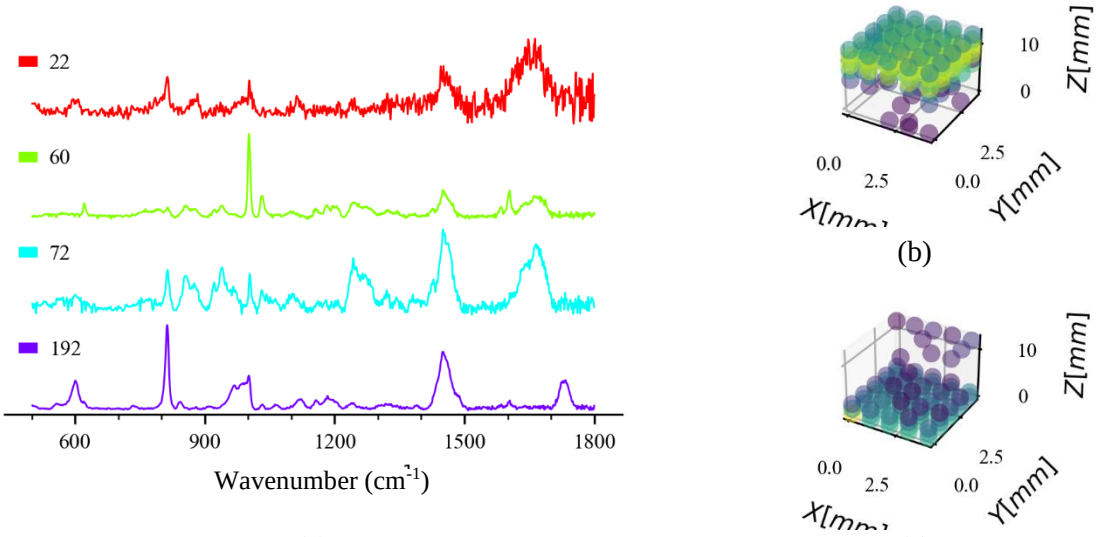
```
from spectramap import spmap as sp
### reading ###
path = 'examples/microplastic+tissue/data'
micro = sp.hyper_object('MP') #creating the hyper object
```

```
micro.read_csv(path) #reading the csv file
### processing ###
micro.hdbscan(2, 15) # hierarchical density-based clustering
colors = micro.show_map(['gray', 'k', 'r'], None, 1) # 2D map of the clusters
(Fig.5.6(a))
micro.show_stack(0,0, colors) # stack of the spectral clusters (Fig. 5.6(b))
```

A.7.5. 3D hyperspectral imaging

The final example shows how to handle basically 3D hyperspectral data and scatter 3D visualization as voxel. Fig. A.8 illustrates the results after the script.

```
from spectramap import spmap
### reading ###
path = 'examples/3D/data'
cube = spmap.hyper_object('cube') #creating the hyper object
cube.read_csv_3D(path, 0.06, 0.07) #reading the 3d csv file and placing the
resolutions xy = 60 µm and z = 70 µm
### preprocessing ###
cube.keep(500, 1800) #finger print selection
cube.airpls(100) #advanced baseline correction
cube.vector() #vector normalization
### processing ###
vca = cube.vca(4) # number of expected components
vca.show_stack(0, 0, 'auto')
abundance = cube.abundance(vca, 'NNLS') # concentration estimation by NNLS
aux = abundance.show_intensity_3d(0.3) # 3d plot of all clusters (Fig. 5.8(b-c))
```



(a) (b) (c)

Figure A.7 3D imaging: (a) stack of the endmembers, (b) 3D concentration map of first layer 72 label and (c) 3D concentration map of

A.7.6. Further information

Further information and examples are found on https://pypi.org/project/spectramap/ and advances in imaging on https://advancesimaging.blogspot.com/ .

References

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