data_lib

October 13, 2023

[ ]:
```
import numpy as np
import pandas as pd
import sklearn.cluster as cl
import matplotlib.pyplot as plt
import itertools
from typing import Dict
import data_lib
```

1 Data Lib examples

1.0.1 data_lib.explore_datasets(datafolder : str = "../Data", verbose=False) -> Dict[str, List[str]]:

This method is to gather all the datasets in the Data folder and ouput them as a list. The output of the function is not very intersting to the user, it is mostly used internaly with function calls like `data_lib.load_dataset`.

The only intersting feature, is that with the option `verbose = True` it lists all available datasets orderd by their folder.

[ ]:
```
# print available data summary
_ = data_lib.explore_datasets(datafolder="../Data",verbose=True)
print(data_lib.LABELS_LIST)
```

```
--------------------------------------------------------------------------------
--------------
-- The following 4 groups were found
-- They contain 40 datasets
-- The first printed entity is the key to the returned dictionary
-----------------------------------
Group: ../Data/6P-positive-dilution-series-2-labelled/droplet-level-data/RawData
po-di-se-2-A4, files: 13                po-di-se-2-C4, files: 13
po-di-se-2-A1, files: 13
po-di-se-2-B1, files: 13                po-di-se-2-D1, files: 13
po-di-se-2-B4, files: 13
-----------------------------------
Group: ../Data/6P-positive-dilution-series-1-labelled/droplet-level-data/RawData
po-di-se-1-D4, files: 13                po-di-se-1-A4, files: 13
po-di-se-1-A1, files: 13
```

```
po-di-se-1-D1, files: 13                po-di-se-1-B1, files: 13
po-di-se-1-C1, files: 13
-----------------------------------
Group: ../Data/6P-positive-dilution-series-labelled/droplet-level-data/RawData
po-di-se-B8, files: 13                  po-di-se-A8, files: 13
po-di-se-C8, files: 13
-----------------------------------
Group: ../Data/6P-wastewater-samples-labelled/droplet-level-data/RawData
wa-sa-A2, files: 13                     wa-sa-B4, files: 13
wa-sa-C5, files: 13
wa-sa-C4, files: 13                     wa-sa-B3, files: 13
wa-sa-B2, files: 13
wa-sa-A5, files: 13                     wa-sa-A3, files: 13
wa-sa-C2, files: 13
wa-sa-C3, files: 13                     wa-sa-D3, files: 13
wa-sa-D4, files: 13
wa-sa-B1, files: 13                     wa-sa-A4, files: 13
wa-sa-A1, files: 13
wa-sa-D2, files: 13                     wa-sa-D5, files: 13
wa-sa-C1, files: 13
-----------------------------------
['IAV-M_POS', 'IAV-M_NEG', 'IBV-M_POS', 'IBV-M_NEG', 'MHV_POS', 'MHV_NEG', 'RSV-
N_POS', 'RSV-N_NEG', 'SARS-N1_POS', 'SARS-N1_NEG', 'SARS-N2_POS', 'SARS-N2_NEG']
```

1.0.2 data_lib.load_dataset(labels : List[str] = None, datasets : List[str] = None, datafolder : str = "../Data") -> pd.DataFrame:

This function probably the most usefull, as it allows to create custom combinations of datasets and labels in ONE dataframe.

The first parameter takes a list of desired labels to be collected. For each of the indicated labels, one columns with the one-hot-encodings will be added.

The next parameter is a list of datasets to be merged into one single dataset. The entries of the indicated sets are combined in the order given along the rows, i.e. there will be much more rows in the output dataset than in the individual datasets.

[ ]:
```
# load a single dataset without labels
df = data_lib.load_dataset([], ["po-di-se-2-A4"], "../Data")
print(f"shape: {df.shape}")
print(f"head {df.head()}")
```

```
shape: (24044, 6)
head    Chan1_FluoValue  Chan2_FluoValue  Chan3_FluoValue  Chan4_FluoValue  \
0              5012             7032             5329             4326
1              5091            10959            15297            13063
2              5056             6453             5914            11799
3             12156            13688             5830            10977
4              4774             6879             5458             4487
```

```
   Chan5_FluoValue  Chan6_FluoValue
0             2774             9374
1            17206            19029
2             2319             8796
3             2754             9151
4             2756             8994
```

[ ]:
```
# load three datasets with two labels
df = data_lib.load_dataset(["IAV-M_POS", "SARS-N1_POS"], ["po-di-se-2-A4",␣
 ↪"po-di-se-2-A1"], "../Data")
print(f"shape: {df.shape}")
print(f"head {df.head()}")
```

```
shape: (50755, 8)
head    Chan1_FluoValue  Chan2_FluoValue  Chan3_FluoValue  Chan4_FluoValue  \
0              5012             7032             5329             4326
1              5091            10959            15297            13063
2              5056             6453             5914            11799
3             12156            13688             5830            10977
4              4774             6879             5458             4487

   Chan5_FluoValue  Chan6_FluoValue  IAV-M_POS  SARS-N1_POS
0             2774             9374          0            0
1            17206            19029          1            0
2             2319             8796          0            0
3             2754             9151          0            0
4             2756             8994          0            0
```

[ ]:
```
# load three datasets with all POSITIVE labels
df = data_lib.load_dataset(None, ["po-di-se-2-A4", "po-di-se-2-A1"], "../Data")
print(f"shape: {df.shape}")
print(f"head {df.head()}")
```

```
shape: (50755, 12)
head    Chan1_FluoValue  Chan2_FluoValue  Chan3_FluoValue  Chan4_FluoValue  \
0              5012             7032             5329             4326
1              5091            10959            15297            13063
2              5056             6453             5914            11799
3             12156            13688             5830            10977
4              4774             6879             5458             4487

   Chan5_FluoValue  Chan6_FluoValue  IAV-M_POS  IBV-M_POS  MHV_POS  RSV-N_POS  \
0             2774             9374          0          0        0          0
1            17206            19029          1          1        0          1
2             2319             8796          0          0        0          1
3             2754             9151          0          0        0          1
4             2756             8994          0          0        0          0
```

```
   SARS-N1_POS  SARS-N2_POS
0            0            0
1            0            0
2            0            0
3            0            1
4            0            0
```

[ ]:
```
# load all available data
df = data_lib.load_dataset(datafolder="../Data")
print(f"shape: {df.shape}")
print(f"head {df.head()}")
```

```
shape: (916501, 12)
head    Chan1_FluoValue  Chan2_FluoValue  Chan3_FluoValue  Chan4_FluoValue  \
0             5012             7032             5329             4326
1             5091            10959            15297            13063
2             5056             6453             5914            11799
3            12156            13688             5830            10977
4             4774             6879             5458             4487

   Chan5_FluoValue  Chan6_FluoValue  IAV-M_POS  IBV-M_POS  MHV_POS  RSV-N_POS  \
0             2774             9374          0          0        0          0
1            17206            19029          1          1        0          1
2             2319             8796          0          0        0          1
3             2754             9151          0          0        0          1
4             2756             8994          0          0        0          0

   SARS-N1_POS  SARS-N2_POS
0            0            0
1            0            0
2            0            0
3            0            1
4            0            0
```

1.0.3 data_lib.pairwise_plots(label : str, data_sets : List[str], classifier : skl.base.ClusterMixin, data_folder : str = "../Data", verbose : bool = False):

This function generates clusters and compares them with the labels.

The function takes the desired label to be compared as a first input

Then a list of datasets to generate the datasets on which to do the classification.

Next it needs a classifier, which is just an object instance of a class with the `fit_predict` function.

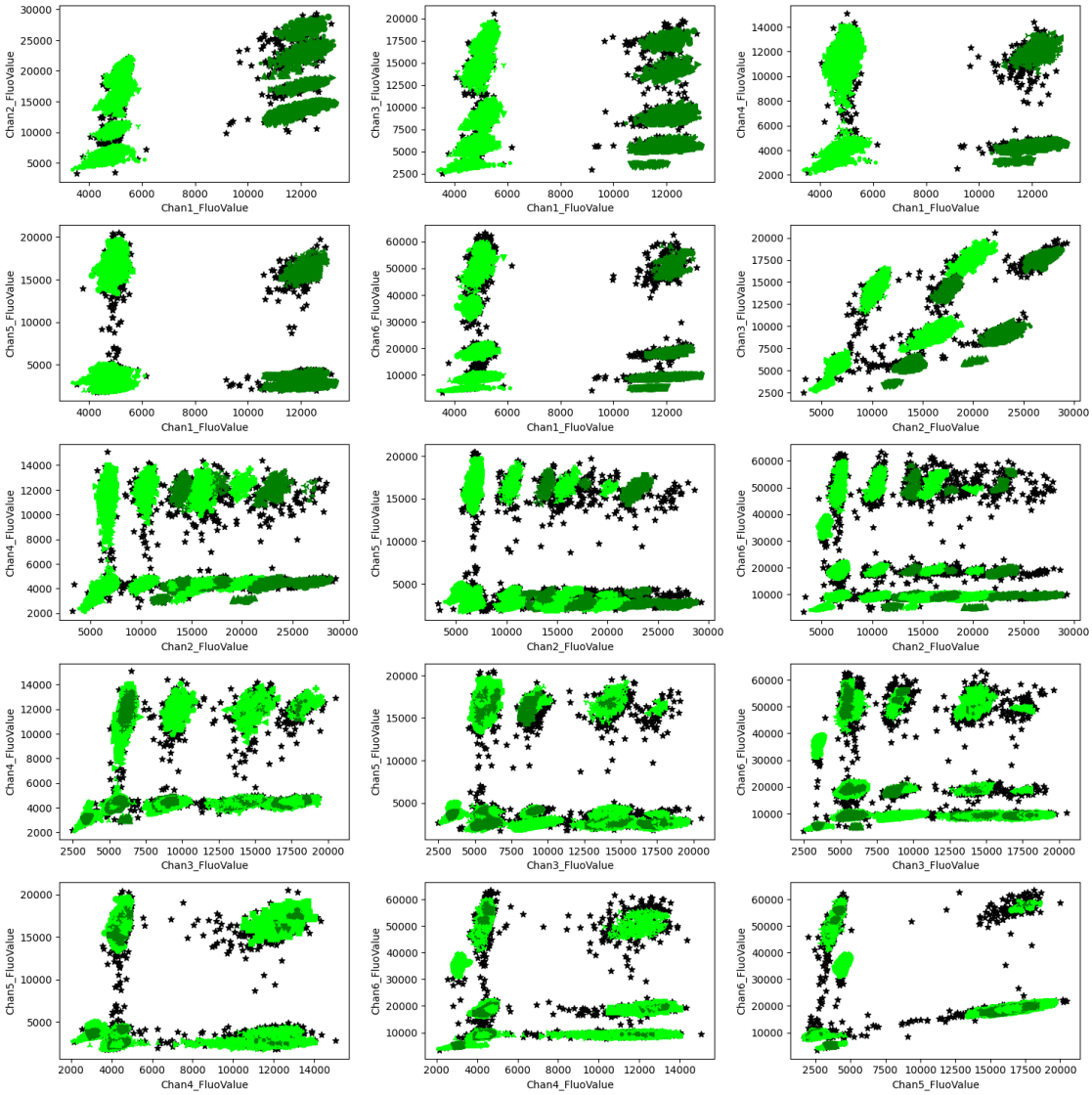
If `verbose = True`, the output will then be a list of clusters generated, and the association with the "best" label and their accuracies. The plot will in any case contain all datapoints, with a different **Marker** per **Cluster** and **Color** for **Labels** whereas red labels are falsely classified point (indicating too little clusters).

[ ]:
```
# DBSCAN on two combined datasets
classifier = cl.DBSCAN(eps = 700, min_samples = 5)
df = data_lib.pairwise_plots("SARS-N2_POS", ["wa-sa-A3", "po-di-se-2-A1"],␣
 ↪classifier, "../Data", verbose=True)
```

```
Cluster  0, num points    18537, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster  1, num points      293, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster  2, num points       21, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster  3, num points       54, POS labelled     54,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster  4, num points       22, POS labelled     22,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster  5, num points     2388, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster  6, num points      130, POS labelled    130,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster  7, num points     2507, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster  8, num points    10680, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster  9, num points     1244, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 10, num points      270, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 11, num points     1510, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 12, num points      328, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 13, num points     1131, POS labelled   1131,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 14, num points      295, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 15, num points       24, POS labelled     24,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 16, num points      682, POS labelled    682,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 17, num points      297, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 18, num points      261, POS labelled    261,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 19, num points      241, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 20, num points     1317, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 21, num points      259, POS labelled    259,   100.0%, for SARS-N2_POS,
```

```
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 22, num points      574, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 23, num points      323, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 24, num points      164, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 25, num points      137, POS labelled    137,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 26, num points       42, POS labelled     42,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 27, num points      145, POS labelled    145,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 28, num points       65, POS labelled     65,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 29, num points       11, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 30, num points       60, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 31, num points       59, POS labelled     59,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 32, num points       42, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 33, num points       23, POS labelled     23,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 34, num points       73, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 35, num points       35, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 36, num points       12, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 37, num points       14, POS labelled     14,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 38, num points       15, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 39, num points       11, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 40, num points       10, POS labelled     10,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 41, num points        5, POS labelled      5,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 42, num points        5, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 43, num points        6, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 44, num points        9, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 45, num points        7, POS labelled      7,   100.0%, for SARS-N2_POS,
```

```
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 46, num points        5, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 47, num points       15, POS labelled     15,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 48, num points        8, POS labelled      8,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 49, num points        6, POS labelled      6,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 50, num points        5, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 51, num points        5, POS labelled      5,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 52, num points        6, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 53, num points        9, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 54, num points       14, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 55, num points        5, POS labelled      5,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 56, num points        5, POS labelled      5,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 57, num points        9, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 58, num points        5, POS labelled      0,     0.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 59, num points        4, POS labelled      4,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
Cluster 60, num points        5, POS labelled      5,   100.0%, for SARS-N2_POS,
on ['wa-sa-A3', 'po-di-se-2-A1'].
```


Chan2_FluoValue
Chan1_FluoValue
Chan3_FluoValue
Chan1_FluoValue
Chan4_FluoValue
Chan1_FluoValue
Chan5_FluoValue
Chan1_FluoValue
Chan6_FluoValue
Chan1_FluoValue
Chan3_FluoValue
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