APSC-5984 Lab 5: Dataframe manipulation

Due: 2023-02-20 (Monday) 23:59:59

0. Overview

We will introduce the concept of `DataFrame` in this lab. You will be intstructed to use the Python library `pandas` to manipulate dataframes. First, let's import the library. Conventionally, we import it as `pd`.

```
import pandas as pd
import os
os.chdir("data")
pd.set_option("display.notebook_repr_html", False)
```

1. Data Loading and Saving

We will work on the several files in the `lab_05` folder to practice how to load and save files

1.1 CSV and tab-delimited files

1.1.1 Separators

The basic function to load data in `pandas` is `pd.read_csv()`. It can read data from a CSV file or a tab-delimited file. The default delimiter is comma "`,`", but it also allows you to specify other delimiters, such as tab "`\t`".

The file `file_A.csv` is a CSV file with comma as the delimiter:

```
!cat file_A.csv
```

```
id,A,B,C
a1,1,1,1
a2,0,1,0
a3,1,0,1
```

```
pd.read_csv('file_A.csv')
```

```
   id  A  B  C
0  a1  1  1  1
```

```
1  a2  0  1  0
2  a3  1  0  1
```

The file `file_A.csv` was correctly loaded into Python. The dataframe has 3 rows and 4 columns. What if we use the same way to load the file `file_B.txt` that is tab-delimited?

```
!cat file_B.txt
```

```
id  A   B   C
a1  1   1   1
a2  0   1   0
a3  1   0   1
```

```
pd.read_csv('file_B.txt')
```

```
   id\tA\tB\tC
0  a1\t1\t1\t1
1  a2\t0\t1\t0
2  a3\t1\t0\t1
```

The result was not what we expected. The reason is that the default delimiter is comma, but the file is tab-delimited. We can specify the delimiter as tab "`\t`" to fix the problem.

```
pd.read_csv('file_B.txt', sep='\t')
```

```
   id  A  B  C
0  a1  1  1  1
1  a2  0  1  0
2  a3  1  0  1
```

Great! Noted that `sep` can be any character, such as "`|`", "`;`", "`:`", etc. So, always check the delimiter before loading the file.

1.1.2 Header

In some cases, the first row of the file is not the header. We can use the argument `header` to specify the row number of the header.

This example shows what would happen if we do not specify the header wiht a non-header file `file_A_nh.csv`.

```
!cat file_A_nh.csv
```

```
a1,1,1,1
a2,0,1,0
a3,1,0,1
```

```
pd.read_csv('file_A_nh.csv')
```

```
   a1  1  1.1  1.2
0  a2  0    1    0
1  a3  1    0    1
```

The first row was loaded as the header. Here is the fix.

```
pd.read_csv('file_A_nh.csv', header=None)
```

```
    0  1  2  3
0  a1  1  1  1
1  a2  0  1  0
2  a3  1  0  1
```

Some files may be coded with two headers:

```
!cat file_A_2h.csv
```

```
id,A,B,C
a1,1,1,1
a2,0,1,0
a3,1,0,1
id,D,E,F
a4,1,1,1
a5,0,1,0
a6,1,0,1
```

If we want the 5th row to be the header, we can use `header=4` (again, it is 0-based).

```
pd.read_csv('file_A_2h.csv', header=4)
```

```
   id  D  E  F
0  a4  1  1  1
1  a5  0  1  0
2  a6  1  0  1
```

1.2 Excel spreadsheet (.xlsx)

Excel spreadsheet is a common format for data storage. However, given it is a format that contains multiple sheets, it is not straightforward to load it into a tabular format.

1.2.1 Load a single sheet

Here is an example of using `pd.read_excel()` to load the spreadsheet `file_C.xlsx`:

```
pd.read_excel('file_C.xlsx')
```

```
   id  A  B  C
0  a1  1  1  1
1  a2  0  1  0
2  a3  1  0  1
```

By default, it only loads the first sheet. We can specify the sheet name or the sheet number to load other sheets.

```
pd.read_excel('file_C.xlsx', sheet_name='Sheet2')
```

```
   id  D  E  F
0  a4  0  1  0
1  a5  0  0  0
2  a6  1  1  0
3  a7  2  2  0
4  a8  3  3  0
5  a9  4  4  0
```

```
pd.read_excel('file_C.xlsx', sheet_name='Sheet3')
```

```
          A         B
0  0.631007  0.034287
1  0.114071  0.370723
2  0.156949  0.851093
3  0.051913  0.089328
4  0.089216  0.861941
5  0.572473  0.364972
6  0.452546  0.152391
7  0.052752  0.024641
```

1.2.2 Dictionary of dataframes

In `pandas`, Excel spreadsheet is loaded as a dictionary of dataframes. The keys are the sheet names, and the values are the dataframes.

To load the entire spreadsheet taht contains all sheets, we can use `pd.read_excel()` with `sheet_name=None`:

```
data = pd.read_excel('file_C.xlsx', sheet_name=None)
print(data)
```

```
{'Sheet1':    id  A  B  C
0  a1  1  1  1
1  a2  0  1  0
2  a3  1  0  1, 'Sheet2':    id  D  E  F
0  a4  0  1  0
1  a5  0  0  0
2  a6  1  1  0
3  a7  2  2  0
4  a8  3  3  0
5  a9  4  4  0, 'Sheet3':           A         B
0  0.631007  0.034287
1  0.114071  0.370723
2  0.156949  0.851093
3  0.051913  0.089328
4  0.089216  0.861941
5  0.572473  0.364972
6  0.452546  0.152391
7  0.052752  0.024641}
```

The sheets might not be displayed well aligned, but you can still see the keys as each sheet name and its corresponding dataframe. You can use the 'lookup' function we learned in the previous lecture to find the dataframe of a specific sheet:

```
data["Sheet3"]
```

```
          A         B
0  0.631007  0.034287
1  0.114071  0.370723
2  0.156949  0.851093
3  0.051913  0.089328
4  0.089216  0.861941
5  0.572473  0.364972
6  0.452546  0.152391
7  0.052752  0.024641
```

1.3 Save data

1.3.1 Save as CSV

We can use `df.to_csv()` to save a dataframe as a CSV file. Here are parameters that we can use:

- `sep`: the delimiter. Default is comma ",".
- `index`: whether to save the index column. Default is `True`.
- `header`: whether to save the header. Default is `True`.
- `columns`: the columns to save. Default is `None` (all columns).
- `mode`: the mode to open the file. Default is `"w"` (write). Other options are `"a"` (append) and `"r"` (read).

```
data["Sheet1"].to_csv('out_A.csv')
!cat out_A.csv
```

```
,id,A,B,C
0,a1,1,1,1
1,a2,0,1,0
2,a3,1,0,1
```

```
data["Sheet1"].to_csv('out_A.csv', index=False)
!cat out_A.csv
```

```
id,A,B,C
a1,1,1,1
a2,0,1,0
a3,1,0,1
```

```
data["Sheet1"].to_csv('out_A.csv', index=False, header=None)
!cat out_A.csv
```

```
a1,1,1,1
a2,0,1,0
a3,1,0,1
```

```
data["Sheet1"].to_csv('out_A.csv', index=False, header=None, sep='\t')
!cat out_A.csv
```

```
a1  1   1   1
a2  0   1   0
a3  1   0   1
```

```
data["Sheet1"].to_csv('out_A.csv', index=False, columns=['A', 'B'])
!cat out_A.csv
```

```
A,B
1,1
0,1
1,0
```

1.3.2 Save as Excel spreadsheet

Pandas also allows us to save a dataframe as an Excel spreadsheet. It is highly recommended to interact with Excel spreadsheet using `with` statement when you want to work with multiple sheets. Here is an example:

```
with pd.ExcelWriter('out_C2.xlsx') as writer:
    data["Sheet1"].to_excel(writer, sheet_name='Sheet1')
```

```
    data["Sheet2"].to_excel(writer, sheet_name='Sheet2')
    data["Sheet3"].to_excel(writer, sheet_name='Sheet3')
```

An example to append a new sheet to an existing spreadsheet:

```
with pd.ExcelWriter('out_C2.xlsx', mode="a") as writer:
    data["Sheet1"].to_excel(writer, sheet_name='Sheet4', index=False)
    data["Sheet2"].to_excel(writer, sheet_name='Sheet5', index=False)
    data["Sheet3"].to_excel(writer, sheet_name='Sheet6', index=False)
```

2. Construct a dataframe

We can also construct a dataframe from scratch. We can start with a dictionary of lists to define our dataframe:

```
data = dict()
data["id"] = ["id1", "id2", "id3", "id4"]
data["factor"] = ["A", "B", "A", "B"]
data["value"] = [1, 2, 3, 4]
print(data)
```

```
{'id': ['id1', 'id2', 'id3', 'id4'], 'factor': ['A', 'B', 'A', 'B'],
'value': [1, 2, 3, 4]}
```

And we can put the dictionary into a dataframe using `pd.DataFrame()`:

```
df = pd.DataFrame(data)
df
```

```
    id factor  value
0  id1      A      1
1  id2      B      2
2  id3      A      3
3  id4      B      4
```

3. Dataframe manipulation

3.1 Index location (.iloc)

We can use `.iloc()` method to access the data by numeric index location. The indexing rule is the same as what we have learned in the sections of `list` and `numpy`. In `.iloc()`, the first argument is the row index, and the second argument is the column index.

Here is an example dataframe:

```
data = pd.read_excel('file_C.xlsx', sheet_name="Sheet1")
data
```

```
   id  A  B  C
0  a1  1  1  1
1  a2  0  1  0
2  a3  1  0  1
```

Get the second and third row:

```
data.iloc[[1, 2], :]
```

```
   id  A  B  C
1  a2  0  1  0
2  a3  1  0  1
```

Get multiple (first and second) columns. (Note we use `:` to specify all rows.)

```
data.iloc[:, [0, 1]]
```

```
   id  A
0  a1  1
1  a2  0
2  a3  1
```

It is equivalent to using slicing:

```
data.iloc[:, :2]
```

```
   id  A
0  a1  1
1  a2  0
2  a3  1
```

3.2 Label-based indexing (.loc)

The `.loc()` method is another way to access the data. It works with either column/index names or boolean arrays.

```
data.loc[[0, 1], :]
```

```
   id  A  B  C
0  a1  1  1  1
1  a2  0  1  0
```

```
data.loc[:, ['id', 'B']]
```

```
   id  B
0  a1  1
1  a2  1
2  a3  0
```

Use boolean to select column containing a letter "B". (We can use `df.columns` to list all column names)

```
colnames = data.columns
bol_B = ["B" in col for col in colnames]
print(bol_B)
```

```
[False, False, True, False]
```

```
data.loc[:, bol_B]
```

```
   B
0  1
1  1
2  0
```

```
data
```

```
   id  A  B  C
0  a1  1  1  1
1  a2  0  1  0
2  a3  1  0  1
```

3.3 Create a new column

The `.loc()` method is also a recommended way (compared to `df["new_column"]`) to create a new column. Simply put a desired column name in the second argument, and assign a value to it.

```
data.loc[:, "new_col"] = ["new"] * 3
# or
data.loc[:, "new_col"] = "new"
data
```

```
   id  A  B  C new_col
0  a1  1  1  1     new
1  a2  0  1  0     new
2  a3  1  0  1     new
```

3.4 Miscellaneous

3.4.1 Drop a column

```
data.drop(columns=["B"])
```

```
   id  A  C new_col
0  a1  1  1     new
1  a2  0  0     new
2  a3  1  1     new
```

3.4.2 Drop a row

```
data.drop(index=[0, 1])
```

```
   id  A  B  C new_col
2  a3  1  0  1     new
```

3.4.3 inspect the dimension and summary

`df.shape` returns the dimension of the dataframe. This tells us that the dataframe has 3 rows and 5 columns.

```
data.shape
```

```
(3, 5)
```

df.info() is another way to inspect the dataframe of its dimension and data types of each column.

```
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 3 entries, 0 to 2
Data columns (total 5 columns):
 #   Column   Non-Null Count  Dtype 
---  ------   --------------  ----- 
 0   id       3 non-null      object
 1   A        3 non-null      int64 
 2   B        3 non-null      int64 
 3   C        3 non-null      int64 
 4   new_col  3 non-null      object
dtypes: int64(3), object(2)
memory usage: 248.0+ bytes
```

`df.describe()` returns the summary statistics of the dataframe. Only numeric columns are included in the summary statistics.

```
data.describe()
```

```
              A         B         C
count  3.000000  3.000000  3.000000
mean   0.666667  0.666667  0.666667
std    0.577350  0.577350  0.577350
min    0.000000  0.000000  0.000000
25%    0.500000  0.500000  0.500000
50%    1.000000  1.000000  1.000000
75%    1.000000  1.000000  1.000000
max    1.000000  1.000000  1.000000
```

`df["column"].value_counts()` returns the counts of unique values in that specified column. Below the example tells us that there are two rows with value 1 and one row with value 0.

```
data["B"].value_counts()
```

```
1    2
0    1
Name: B, dtype: int64
```

4.Querying with an example dataframe

Let's create a mock dataframe for this section:

```
import numpy as np
import pandas as pd

factors = [i for _ in range(30) for i in ["A", "B", "C", "D"]]
# random sample from id {1, 2, 3, 4, 5, 6}
ids = np.random.choice(["id_%d" % (i + 1) for i in range(6)], 120)
envs = [i for _ in range(60) for i in ["env_1", "env_2"]]
obs = np.random.normal(0, 1, 120)
data = pd.DataFrame({"factor": factors, "id": ids, "env": envs, "obs":
obs})
data.to_csv("file_D.csv", index=False)
```

```
data = pd.read_csv("file_D.csv")
data.info()
data
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 120 entries, 0 to 119
Data columns (total 4 columns):
 #   Column  Non-Null Count  Dtype
---  ------  --------------  -----
 0   factor  120 non-null    object
 1   id      120 non-null    object
 2   env     120 non-null    object
 3   obs     120 non-null    float64
dtypes: float64(1), object(3)
memory usage: 3.9+ KB
```

```
    factor    id    env       obs
0        A  id_4  env_1 -0.103541
1        B  id_5  env_2 -0.743779
2        C  id_3  env_1  1.367427
3        D  id_1  env_2  1.277709
4        A  id_5  env_1 -0.036865
..     ...   ...    ...       ...
115      D  id_2  env_2  1.090125
116      A  id_3  env_1  1.992980
117      B  id_2  env_2 -1.098938
118      C  id_5  env_1  0.973049
119      D  id_3  env_2 -0.049207

[120 rows x 4 columns]
```

4.1 Check the distribution of each column

```
data["factor"].value_counts()
```

```
A    30
B    30
C    30
D    30
Name: factor, dtype: int64
```

```
data["id"].value_counts()
```

```
id_3    26
id_5    21
id_2    20
id_6    20
id_4    17
id_1    16
Name: id, dtype: int64
```

```
data["env"].value_counts()
```

```
env_1    60
env_2    60
Name: env, dtype: int64
```

```
data["obs"].value_counts()
```

```
-0.103541    1
-0.743779    1
-0.420372    1
-0.974859    1
 0.847130    1
            ..
-0.801611    1
 0.609561    1
-0.305139    1
 0.960369    1
-0.049207    1
Name: obs, Length: 120, dtype: int64
```

```
data["obs"].describe()
```

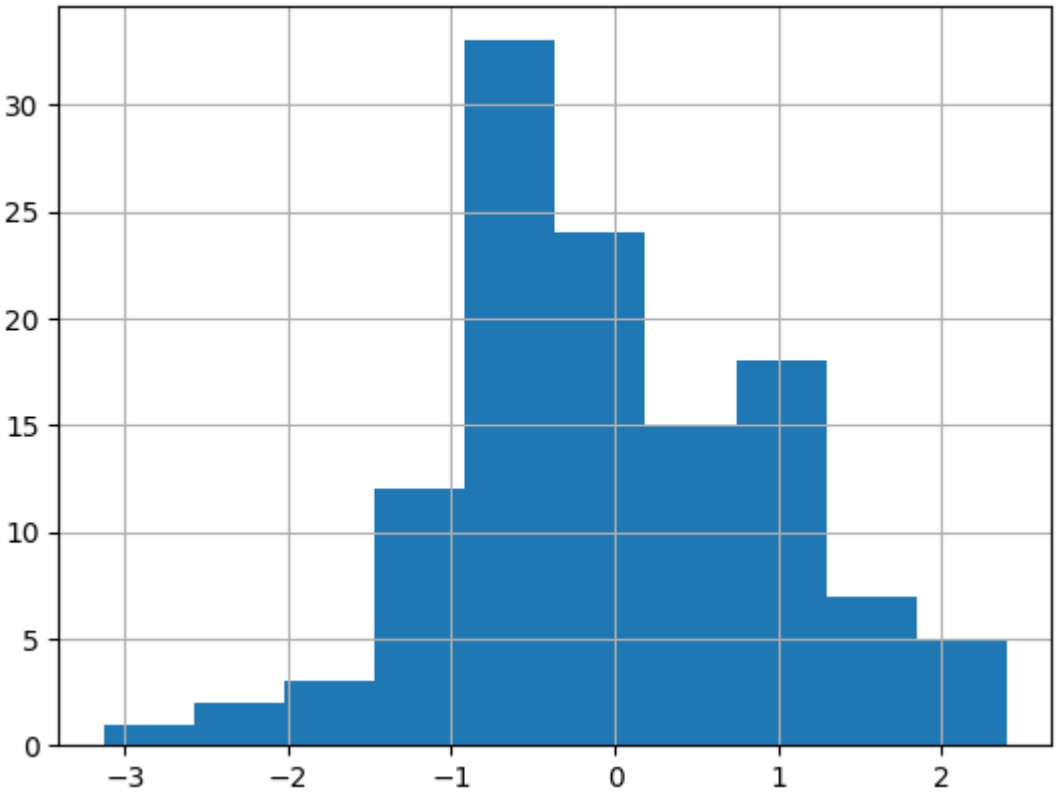
```
count    120.000000
mean      -0.007360
std        0.996616
min       -3.128698
25%       -0.673746
50%       -0.078736
```

```
75%         0.718717
max         2.401238
Name: obs, dtype: float64
```

For better visualization, we can use `df.hist()` to plot the histogram of each column.

```
data["obs"].hist()
```

```
<AxesSubplot: >
```



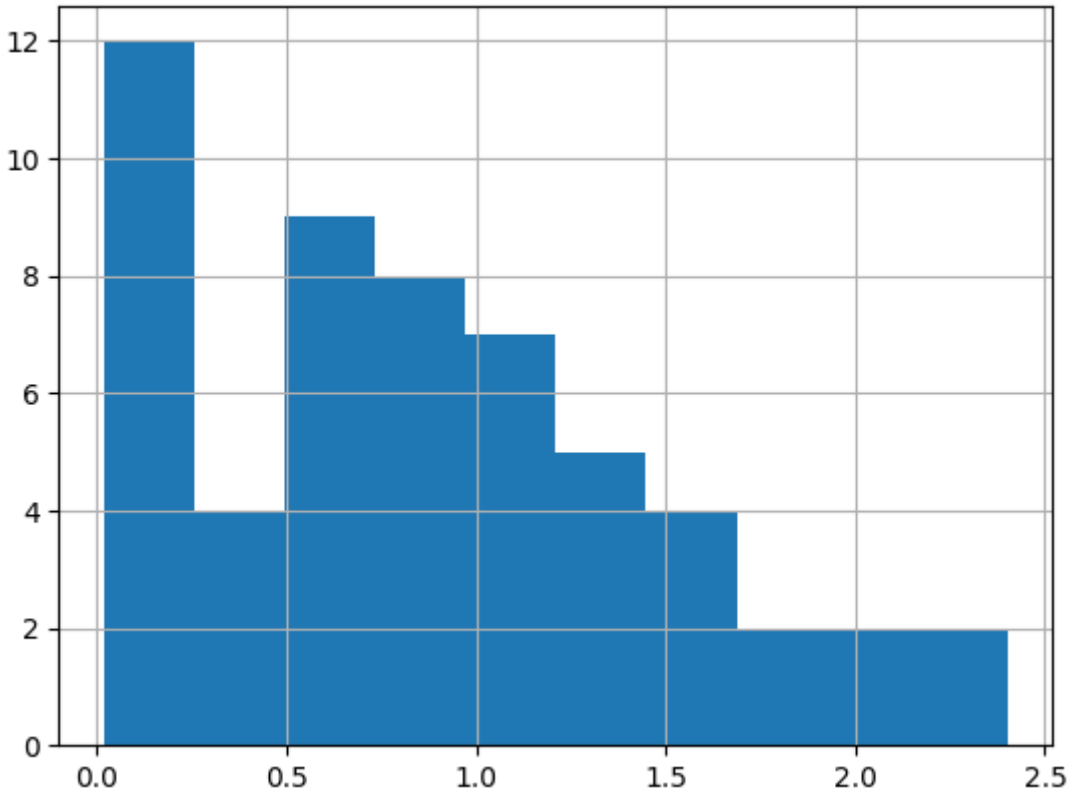
4.2 Subset the dataframe (query)

```
data_sub = data.query("obs > 0")
data_sub[:5]
```

	factor	id	env	obs
2	C	id_3	env_1	1.367427
3	D	id_1	env_2	1.277709
5	B	id_4	env_2	0.018896
6	C	id_3	env_1	0.697119
10	C	id_2	env_1	0.129155

```
data_sub["obs"].hist()
```

```
<AxesSubplot: >
```

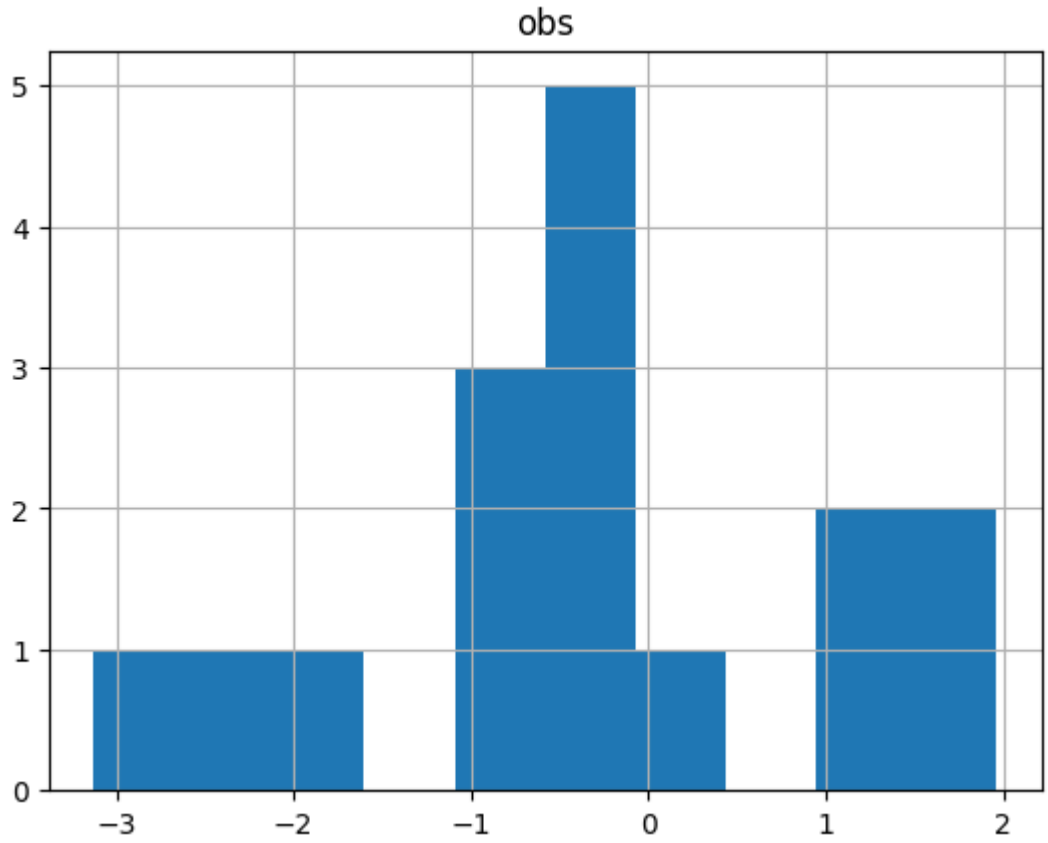



```
data_id1 = data.query("id == 'id_1'")
data_id1[:5]
```

```
   factor    id    env       obs
3       D  id_1  env_2  1.277709
12      A  id_1  env_1 -0.514876
15      D  id_1  env_2 -0.910731
18      C  id_1  env_1  0.324932
23      D  id_1  env_2 -0.915508
```

```
data_id1.hist()
```

```
array([[<AxesSubplot: title={'center': 'obs'}>]], dtype=object)
```



Multiple conditions can be combined using & (and) and | (or).

```
data.query("id == 'id_1' and (obs > 1 or obs < -1)")
```

```
    factor    id    env       obs
3        D  id_1  env_2  1.277709
30       C  id_1  env_1  1.959333
50       C  id_1  env_1 -1.807202
53       B  id_1  env_2  1.226145
95       D  id_1  env_2 -2.187798
102      C  id_1  env_1 -3.128698
113      B  id_1  env_2  1.556891
```

4.3 Grouping

```
data.groupby("id")["obs"].mean()
```

```
id
id_1   -0.353290
```

```
id_2    0.010237
id_3    0.338903
id_4    0.089247
id_5   -0.069404
id_6   -0.215322
Name: obs, dtype: float64
```

```
data.groupby(["id", "factor"])["obs"].mean()
```

```
id    factor
id_1  A        -0.572145
      B         0.800764
      C        -0.662909
      D        -0.622944
id_2  A        -0.035847
      B        -0.379162
      C        -0.028974
      D         0.710803
id_3  A         0.537934
      B         0.016166
      C         0.474403
      D         0.337999
id_4  A         0.344797
      B        -0.510488
      D         0.190927
id_5  A        -0.078994
      B        -0.326861
      C         0.162713
      D         0.018248
id_6  A        -0.401546
      B         0.269396
      C        -0.271808
      D        -0.718168
Name: obs, dtype: float64
```

```
# multiple calculation
cus_fun = lambda x: x.max() - x.min()
pivot = data.groupby(["id", "factor"])["obs"].agg(["mean", "std", "count",
cus_fun])
pivot
```

```
                mean       std  count  <lambda_0>
id   factor
```

```
id_1 A      -0.572145  0.275969      4    0.600521
     B       0.800764  1.036493      3    1.937635
     C      -0.662909  2.253997      4    5.088031
     D      -0.622944  1.253941      5    3.465507
id_2 A      -0.035847  0.835036      5    2.113688
     B      -0.379162  0.991673      4    2.105734
     C      -0.028974  1.273576      8    3.951148
     D       0.710803  0.338261      3    0.649650
id_3 A       0.537934  1.056636      5    2.838498
     B       0.016166  1.082023      6    2.891030
     C       0.474403  0.646405      7    1.984283
     D       0.337999  1.121005      8    3.527217
id_4 A       0.344797  0.761420      7    2.389062
     B      -0.510488  0.353390      4    0.731529
     D       0.190927  1.028478      6    2.801286
id_5 A      -0.078994  0.091463      3    0.167741
     B      -0.326861  0.728683      7    2.330027
     C       0.162713  0.888686      6    2.129052
     D       0.018248  0.861026      5    2.056391
id_6 A      -0.401546  1.009011      6    2.810509
     B       0.269396  0.824500      6    2.113502
     C      -0.271808  1.400287      5    3.316543
     D      -0.718168  0.471266      3    0.931386
```

```
pivot.loc["id_5"]
```

```
            mean       std  count  <lambda_0>
factor
A      -0.078994  0.091463      3    0.167741
B      -0.326861  0.728683      7    2.330027
C       0.162713  0.888686      6    2.129052
D       0.018248  0.861026      5    2.056391
```

```
pivot.loc["id_3"].loc["A"]
```

```
mean          0.537934
std           1.056636
count         5.000000
<lambda_0>    2.838498
Name: A, dtype: float64
```

```
data_pivot = pivot.reset_index()
data_pivot
```

	id	factor	mean	std	count	<lambda_0>
0	id_1	A	-0.572145	0.275969	4	0.600521
1	id_1	B	0.800764	1.036493	3	1.937635
2	id_1	C	-0.662909	2.253997	4	5.088031
3	id_1	D	-0.622944	1.253941	5	3.465507
4	id_2	A	-0.035847	0.835036	5	2.113688
5	id_2	B	-0.379162	0.991673	4	2.105734
6	id_2	C	-0.028974	1.273576	8	3.951148
7	id_2	D	0.710803	0.338261	3	0.649650
8	id_3	A	0.537934	1.056636	5	2.838498
9	id_3	B	0.016166	1.082023	6	2.891030
10	id_3	C	0.474403	0.646405	7	1.984283
11	id_3	D	0.337999	1.121005	8	3.527217
12	id_4	A	0.344797	0.761420	7	2.389062
13	id_4	B	-0.510488	0.353390	4	0.731529
14	id_4	D	0.190927	1.028478	6	2.801286
15	id_5	A	-0.078994	0.091463	3	0.167741
16	id_5	B	-0.326861	0.728683	7	2.330027
17	id_5	C	0.162713	0.888686	6	2.129052
18	id_5	D	0.018248	0.861026	5	2.056391
19	id_6	A	-0.401546	1.009011	6	2.810509
20	id_6	B	0.269396	0.824500	6	2.113502
21	id_6	C	-0.271808	1.400287	5	3.316543
22	id_6	D	-0.718168	0.471266	3	0.931386

```
data_pivot.to_csv("out_pivot.csv", index=False)
```

```
!cat out_pivot.csv
```

```
id,factor,mean,std,count,<lambda_0>
id_1,A,-0.5721451319957364,0.2759691621869315,4,0.6005207714131151
id_1,B,0.8007641707797974,1.0364934807700155,3,1.9376345238846369
id_1,C,-0.6629089104632997,2.253996983629481,4,5.088031295812392
id_1,D,-0.6229444416720034,1.2539408642924903,5,3.465507221194403
id_2,A,-0.035846506594991834,0.8350360108995132,5,2.113687559524173
id_2,B,-0.379161981588368,0.9916730486129572,4,2.105734163902122
id_2,C,-0.028973912570866345,1.2735759529812984,8,3.9511482250204737
id_2,D,0.7108034172724883,0.33826146647224276,3,0.6496501604168332
id_3,A,0.5379337768185726,1.0566362183461382,5,2.838498093174227
```

```
id_3,B,0.016166265985501038,1.0820228345659655,6,2.8910301815434467
id_3,C,0.474403439830994,0.646404644751632,7,1.9842826893508816
id_3,D,0.3379989349365774,1.1210052264622168,8,3.5272166799089844
id_4,A,0.3447970839358367,0.7614202452739026,7,2.389062256967856
id_4,B,-0.5104878699033722,0.35339019404120087,4,0.7315285533460211
id_4,D,0.19092723591472208,1.0284776900867785,6,2.8012856309176444
id_5,A,-0.07899438127161257,0.09146273308524398,3,0.167740923053321
id_5,B,-0.32686142994641176,0.728683117065449,7,2.3300269181696964
id_5,C,0.16271334666682133,0.8886856920836689,6,2.1290522592475236
id_5,D,0.018248250423816382,0.8610262343729462,5,2.056390978154677
id_6,A,-0.40154626931806864,1.00901117222255,6,2.810509048350021
id_6,B,0.2693955898375124,0.8244996811829504,6,2.113501718226548
id_6,C,-0.27180772132303965,1.4002872099962633,5,3.3165427766752997
id_6,D,-0.7181675436798494,0.4712663301452729,3,0.9313858318138433
```