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1 ICW1

package will use

```
[]: #import and load the package
     import pandas as pd
     import numpy as np
     import matplotlib.pyplot as plt
     from sklearn.ensemble import IsolationForest
     import statsmodels.api as sm
     import seaborn as sns
     from sklearn.experimental import enable_iterative_imputer
     from sklearn.impute import IterativeImputer
     from scipy import stats
     from scipy import stats
     from sklearn.preprocessing import MinMaxScaler
     from sklearn.decomposition import PCA
     from sklearn.decomposition import NMF
     from scipy.cluster.hierarchy import linkage, cophenet
     from scipy.spatial.distance import pdist
     from sklearn.model_selection import train_test_split
     import matplotlib.patches as mpatches
     from sklearn.manifold import TSNE
     from mpl_toolkits.mplot3d import Axes3D
     from sklearn.datasets import make_blobs
     from sklearn.cluster import KMeans
     from itertools import cycle
```

1.1 The Project Questions

input data from csv file:

```
[]:
                                ACTL6A_S5
                                              ADAM9_S2
                                                         ADAMTS1_S5
                                                                        ADCY7_S3
     TCGA.HF.7136.STAD.C1_
                              0.592349159
                                           0.628634428
                                                        0.570785319
                                                                     0.536637178
     TCGA.EW.A10Z.BRCA.C1
                              0.616707551
                                           0.589805879
                                                        0.546914715
                                                                      0.522103124
     TCGA.EY.A1GL.UCEC.C1_
                              0.591583228
                                            0.60137506
                                                        0.530573235
                                                                      0.470163893
     TCGA.EB.A5FP.SKCM.C1
                               0.60418886
                                           0.586197969
                                                        0.566643527
                                                                      0.523075884
     TCGA.D1.A16D.UCEC.C1_
                              0.545902837
                                           0.632497249
                                                         0.58791722
                                                                      0.533485849
     TCGA.FB.AAQ1.PAAD.C6_.2
                              0.547088474
                                           0.669353783
                                                        0.556373656
                                                                     0.575362692
     TCGA.DX.A1KU.SARC.C6_.1
                                                                     0.521712202
                               0.54993579
                                           0.652694922
                                                        0.674654449
     TCGA.A2.A4S1.BRCA.C6_
                              0.513619217
                                           0.599381792
                                                        0.589908476
                                                                      0.543181612
     TCGA.3U.A98I.MESO.C6_.1
                              0.504295371
                                           0.620086907
                                                        0.602403486
                                                                      0.542429285
     TCGA.AR.A2LJ.BRCA.C6_
                              0.540357583
                                            0.55191784
                                                        0.526152563
                                                                      0.489544812
                                 AIMP2_S5
                                             ALKBH7_S5
                                                         ALOX5AP_S3
                                                                        AMPD3_S3
     TCGA.HF.7136.STAD.C1_
                              0.509823444
                                           0.462217686
                                                        0.443087096
                                                                      0.482923423
     TCGA.EW.A10Z.BRCA.C1_
                              0.523892866
                                           0.545415692
                                                        0.518862114
                                                                      0.428246143
     TCGA.EY.A1GL.UCEC.C1_
                                                                      0.529846796
                              0.573793291
                                           0.560062178
                                                        0.408029142
     TCGA.EB.A5FP.SKCM.C1
                              0.575625221
                                           0.497917854
                                                        0.362421719
                                                                      0.428469267
     TCGA.D1.A16D.UCEC.C1_
                                                                      0.510708281
                              0.540957612
                                           0.556670227
                                                        0.518468063
     TCGA.FB.AAQ1.PAAD.C6_.2
                              0.511424709
                                           0.534338128
                                                        0.584272643
                                                                     0.474198022
     TCGA.DX.A1KU.SARC.C6_.1
                              0.510103123
                                            0.50135204
                                                        0.521481461
                                                                      0.501617299
     TCGA.A2.A4S1.BRCA.C6_
                                0.4788955
                                           0.507401046
                                                        0.570468374
                                                                      0.483157655
     TCGA.3U.A98I.MESO.C6_.1
                              0.476758106
                                           0.503558058
                                                        0.511588826
                                                                      0.457273386
     TCGA.AR.A2LJ.BRCA.C6_
                              0.518348041
                                           0.603053115
                                                        0.517177218
                                                                     0.453268531
                                APITD1_S5
                                              APOC1_S3
                                                              WIPF1_S3
     TCGA.HF.7136.STAD.C1_
                              0.418518998
                                           0.483556486
                                                           0.557670757
     TCGA.EW.A10Z.BRCA.C1_
                              0.447287266
                                           0.588167354
                                                           0.543130808
     TCGA.EY.A1GL.UCEC.C1_
                              0.516928306
                                           0.500290877
                                                           0.537821188
     TCGA.EB.A5FP.SKCM.C1_
                              0.544391175
                                           0.580779692
                                                           0.635673186
     TCGA.D1.A16D.UCEC.C1_
                              0.488153784
                                           0.585869525 ...
                                                           0.533509926
     TCGA.FB.AAQ1.PAAD.C6_.2
                              0.450351433
                                           0.575779881
                                                           0.548371597
     TCGA.DX.A1KU.SARC.C6 .1
                              0.430389962
                                           0.517204617
                                                            0.63649641
     TCGA.A2.A4S1.BRCA.C6_
                              0.441636966
                                            0.46383583 ... 0.601900974
     TCGA.3U.A98I.MESO.C6_.1
                              0.436591435
                                           0.539356545
                                                           0.585780294
     TCGA.AR.A2LJ.BRCA.C6_
                              0.484431339
                                           0.650399976
                                                           0.563844585
                                 WNT2B_S2
                                              WNT8B_S2
                                                            WSB2_S5
                                                                        ZWILCH_S5
     TCGA.HF.7136.STAD.C1_
                              0.348505759
                                            0.21001634
                                                        0.629422932
                                                                      0.515652808
     TCGA.EW.A10Z.BRCA.C1_
                              0.271636495
                                           0.215561609
                                                        0.588503202
                                                                      0.520021651
     TCGA.EY.A1GL.UCEC.C1_
                              0.370267472
                                           0.256228773
                                                        0.626341995
                                                                      0.500481153
     TCGA.EB.A5FP.SKCM.C1_
                              0.360680436
                                           0.261152768
                                                        0.612561409
                                                                      0.564330771
     TCGA.D1.A16D.UCEC.C1_
                              0.332905555
                                           0.129105571
                                                         0.60903958
                                                                     0.482094262
     TCGA.FB.AAQ1.PAAD.C6_.2 0.301071951
                                           0.202440846
                                                        0.554636793
                                                                      0.47268884
```

```
TCGA.DX.A1KU.SARC.C6_.1
                                       0.18709252 0.586367439
                         0.431338453
                                                                 0.486879106
TCGA.A2.A4S1.BRCA.C6_
                         0.340523965
                                      0.171784796
                                                   0.541963837
                                                                 0.450655279
TCGA.3U.A98I.MESO.C6_.1
                         0.476789408
                                      0.182592379
                                                   0.563271127
                                                                 0.493495531
TCGA.AR.A2LJ.BRCA.C6_
                         0.215692689
                                      0.201434471
                                                   0.558990676
                                                                 0.462621113
                              ZYX_S2
                                          MMP3_S2
                                                         PLG_S5
                                                                     RGS8_S5
TCGA.HF.7136.STAD.C1_
                         0.664830576
                                      0.548405265
                                                   0.144131649
                                                                 0.156692658
TCGA.EW.A10Z.BRCA.C1_
                         0.661330832
                                       0.48897231
                                                   0.129630028
                                                                 0.147664886
TCGA.EY.A1GL.UCEC.C1
                                      0.602703844
                                                   0.236607056
                                                                 0.236607056
                         0.650542802
TCGA.EB.A5FP.SKCM.C1_
                         0.620690208
                                      0.457935414 0.261152768
                                                                 0.261152768
TCGA.D1.A16D.UCEC.C1
                         0.670960037
                                       0.38913796
                                                   0.282478711
                                                                 0.151171985
TCGA.FB.AAQ1.PAAD.C6 .2 0.653400943
                                      0.307704021
                                                   0.332027894
                                                                 0.125693204
TCGA.DX.A1KU.SARC.C6_.1
                         0.666805202
                                      0.485531743
                                                   0.163455699
                                                                 0.216324944
TCGA.A2.A4S1.BRCA.C6_
                         0.643585011
                                       0.25990241
                                                   0.171784796
                                                                 0.171784796
TCGA.3U.A98I.MESO.C6_.1
                         0.659346701
                                      0.204456653
                                                   0.146536279
                                                                 0.182592379
TCGA.AR.A2LJ.BRCA.C6_
                         0.676615381
                                      0.476987934
                                                   0.133938618
                                                                 0.133938618
                        Subgroup
TCGA.HF.7136.STAD.C1_
                              C1
TCGA.EW.A10Z.BRCA.C1_
                              C1
TCGA.EY.A1GL.UCEC.C1
                              C1
TCGA.EB.A5FP.SKCM.C1_
                              C1
TCGA.D1.A16D.UCEC.C1
                              C1
TCGA.FB.AAQ1.PAAD.C6 .2
                              C6
TCGA.DX.A1KU.SARC.C6 .1
                              C6
TCGA.A2.A4S1.BRCA.C6
                              C6
TCGA.3U.A98I.MESO.C6_.1
                              C6
TCGA.AR.A2LJ.BRCA.C6_
                              C6
```

[588 rows x 441 columns]

```
[]: #sns.pairplot(Dataset_1)
# 440 feature not choose this to plot all feature for obsercation
```

1.1.1 Data Preparation and Addressing Missingness

a. Data Cleaning Cleaning data involves: 1. Data Separation 2. Header 3. Data Type 4. Handing Missing Data 5. Outliers 6. Duplicates 7. Scaling/Normalization 8. Data Formatting 9. Text Cleaning 10. Save Cleaned Data

Bad data in data set need to be fixxed

Bad data could be: 1. Empty cells 2. Data in wrong format 3. Wrong data 4. Duplicates

challenges: The high dimensional data not easy to find out the problem by observation and some feature have relationship between each other

check the data type Check the data type first because if the data type is wrong it will return error when we using function to operate it. And It will more effective to clean the data.

```
[]: #get the data type of the DataFrame content
Dataset_1.dtypes
```

[]: ACTL6A_S5 object ADAM9_S2 object ADAMTS1_S5 object ADCY7_S3 object AIMP2_S5 object ZYX_S2 object MMP3_S2 object PLG_S5 object RGS8_S5 object Subgroup object Length: 441, dtype: object

[]: Dataset_1.describe()

[]:		ACTL6A_S5	ADAM9_S2	ADAMTS1_S5	ADCY7_S3	AIMP2_S5		
	count	588	588	588	588	588	\	
	unique	540	540	540	540	540		
	top	0.547088474	0.669353783	0.556373656	0.575362692	0.511424709		
	freq	3	3	3	3	3		
		_	ALOX5AP_S3	_	_	_		
	count	588	588	588	588			\
	unique	540	540	540	540	540	•••	
	top	0.534338128	0.584272643	0.474198022	0.450351433	0.575779881		
	freq	3	3	3	3	3	•••	
		WTPF1 S3	WNT2B_S2	WNT8B S2	WSB2 S5	ZWILCH S5		
	count	588	588	588	588	588	\	
	unique	540	540	540	540	540	•	
	top		0.301071951					
	freq	3	3	3	3	3		
	1164	3	9	3	3	3		
		ZYX_S2	MMP3_S2	PLG_S5	RGS8_S5	Subgroup		
	count	588	588	588	588	588		
	unique	540	540	540	540	6		
	top	0.653400943	0.307704021	0.332027894	0.125693204	C1		
	freq	3	3	3	3	98		

[4 rows x 441 columns]

It shows all data are store by object(string) but if we want to do some mathmatic operation for

example, mean, max, min..... it needs to translate it to numberic

```
[]: #all data are decimal so change the object(string) to float64 -> can have 184
      ⇔digits after the decimal point
    Dataset_1[Dataset_1.columns[0:-1]] = Dataset_1[Dataset_1.columns[0:-1]].
      ⇔astype('float64')
[]: #check the data: never lost data after change data type
    Dataset 1
[]:
                             ACTL6A_S5 ADAM9_S2 ADAMTS1_S5
                                                             ADCY7_S3 AIMP2_S5
                              0.592349 0.628634
                                                   0.570785
                                                             0.536637
                                                                       0.509823
    TCGA.HF.7136.STAD.C1_
    TCGA.EW.A10Z.BRCA.C1_
                              0.616708 0.589806
                                                   0.546915
                                                             0.522103 0.523893
    TCGA.EY.A1GL.UCEC.C1
                              0.591583 0.601375
                                                   0.530573
                                                             0.470164 0.573793
    TCGA.EB.A5FP.SKCM.C1_
                              0.604189 0.586198
                                                   0.566644
                                                             0.523076 0.575625
    TCGA.D1.A16D.UCEC.C1_
                              0.545903 0.632497
                                                   0.587917
                                                             0.533486 0.540958
    TCGA.FB.AAQ1.PAAD.C6_.2
                              0.547088 0.669354
                                                   0.556374
                                                             0.575363 0.511425
    TCGA.DX.A1KU.SARC.C6_.1
                              0.549936 0.652695
                                                   0.674654
                                                             0.521712 0.510103
    TCGA.A2.A4S1.BRCA.C6_
                                                             0.543182 0.478895
                              0.513619 0.599382
                                                   0.589908
    TCGA.3U.A98I.MESO.C6_.1
                              0.504295 0.620087
                                                   0.602403
                                                             0.542429 0.476758
    TCGA.AR.A2LJ.BRCA.C6_
                              0.540358 0.551918
                                                   0.526153
                                                             0.489545 0.518348
                             ALKBH7_S5 ALOX5AP_S3
                                                   AMPD3_S3
                                                             APITD1_S5 APOC1_S3
                              0.462218
                                         0.443087
                                                   0.482923
                                                              0.418519 0.483556 \
    TCGA.HF.7136.STAD.C1_
    TCGA.EW.A10Z.BRCA.C1_
                              0.545416
                                         0.518862
                                                   0.428246
                                                              0.447287
                                                                        0.588167
    TCGA.EY.A1GL.UCEC.C1_
                              0.560062
                                         0.408029
                                                   0.529847
                                                              0.516928 0.500291
                                                              0.544391
    TCGA.EB.A5FP.SKCM.C1_
                              0.497918
                                         0.362422 0.428469
                                                                        0.580780
    TCGA.D1.A16D.UCEC.C1
                              0.556670
                                         0.518468 0.510708
                                                              0.488154 0.585870
    TCGA.FB.AAQ1.PAAD.C6_.2
                              0.534338
                                         0.584273 0.474198
                                                              0.450351 0.575780
    TCGA.DX.A1KU.SARC.C6_.1
                                                              0.430390 0.517205
                              0.501352
                                         0.521481 0.501617
    TCGA.A2.A4S1.BRCA.C6_
                              0.507401
                                         0.570468 0.483158
                                                              0.441637
                                                                        0.463836
    TCGA.3U.A98I.MESO.C6_.1
                              0.503558
                                         0.511589 0.457273
                                                              0.436591
                                                                        0.539357
    TCGA.AR.A2LJ.BRCA.C6_
                              0.603053
                                                   0.453269
                                                              0.484431 0.650400
                                         0.517177
                               WIPF1_S3
                                         WNT2B_S2
                                                   WNT8B_S2
                                                              WSB2_S5
    TCGA.HF.7136.STAD.C1_
                             ... 0.557671
                                         0.348506
                                                   0.210016
                                                             0.629423 \
    TCGA.EW.A10Z.BRCA.C1_
                             ... 0.543131
                                         0.271636 0.215562
                                                             0.588503
    TCGA.EY.A1GL.UCEC.C1_
                             ... 0.537821
                                         0.370267
                                                   0.256229
                                                             0.626342
    TCGA.EB.A5FP.SKCM.C1_
                             ... 0.635673
                                         0.360680
                                                   0.261153
                                                             0.612561
    TCGA.D1.A16D.UCEC.C1
                             ... 0.533510
                                         0.332906 0.129106
                                                             0.609040
    TCGA.FB.AAQ1.PAAD.C6 .2 ... 0.548372
                                         0.301072 0.202441
                                                             0.554637
    TCGA.DX.A1KU.SARC.C6_.1 ... 0.636496
                                         0.431338 0.187093
                                                             0.586367
    TCGA.A2.A4S1.BRCA.C6
                             ... 0.601901
                                         0.340524 0.171785
                                                             0.541964
    TCGA.3U.A98I.MESO.C6_.1 ... 0.585780 0.476789 0.182592
                                                             0.563271
```

```
0.215693 0.201434
                                                          0.558991
TCGA.AR.A2LJ.BRCA.C6_
                            0.563845
                         ZWILCH_S5
                                      ZYX_S2
                                               MMP3_S2
                                                          PLG_S5
                                                                   RGS8_S5
                          0.515653
                                    0.664831 0.548405
                                                        0.144132
                                                                  0.156693 \
TCGA.HF.7136.STAD.C1_
TCGA.EW.A10Z.BRCA.C1_
                          0.520022
                                    0.661331 0.488972
                                                        0.129630
                                                                  0.147665
TCGA.EY.A1GL.UCEC.C1_
                          0.500481
                                    0.650543 0.602704
                                                        0.236607
                                                                  0.236607
TCGA.EB.A5FP.SKCM.C1_
                          0.564331
                                    0.620690
                                              0.457935
                                                        0.261153
                                                                  0.261153
TCGA.D1.A16D.UCEC.C1_
                          0.482094
                                    0.670960 0.389138
                                                        0.282479
                                                                  0.151172
TCGA.FB.AAQ1.PAAD.C6_.2
                          0.472689
                                    0.653401 0.307704
                                                        0.332028
                                                                  0.125693
TCGA.DX.A1KU.SARC.C6_.1
                          0.486879
                                    0.666805 0.485532
                                                        0.163456 0.216325
TCGA.A2.A4S1.BRCA.C6_
                          0.450655
                                    0.643585 0.259902
                                                        0.171785 0.171785
TCGA.3U.A98I.MESO.C6_.1
                          0.493496
                                    0.659347 0.204457
                                                        0.146536 0.182592
TCGA.AR.A2LJ.BRCA.C6_
                          0.462621
                                    0.676615  0.476988  0.133939  0.133939
                         Subgroup
TCGA.HF.7136.STAD.C1_
                               C1
TCGA.EW.A10Z.BRCA.C1_
                               C1
                               C1
TCGA.EY.A1GL.UCEC.C1_
TCGA.EB.A5FP.SKCM.C1_
                               C1
TCGA.D1.A16D.UCEC.C1_
                               C1
                               C6
TCGA.FB.AAQ1.PAAD.C6_.2
TCGA.DX.A1KU.SARC.C6_.1
                               C6
TCGA.A2.A4S1.BRCA.C6_
                               C6
TCGA.3U.A98I.MESO.C6_.1
                               C6
TCGA.AR.A2LJ.BRCA.C6_
                               C6
[588 rows x 441 columns]
```

[]: Dataset_1.dtypes

[]: ACTL6A_S5 float64 ADAM9_S2 float64 ADAMTS1_S5 float64 ADCY7_S3 float64 AIMP2_S5 float64 ZYX_S2 float64 MMP3_S2 float64 PLG_S5 float64 RGS8_S5 float64 Subgroup object Length: 441, dtype: object

Now number in Dataset are store in float64 data type

Get statistic details about the dataset and data distribution

[]: #statistic details of the dataset : min max mean std....
Dataset_1.describe()

[]:		ACTL6A_S5	ADAM9_S2	ADAMTS1_S5	ADCY7_S3	AIMP2_S5	ALKBH7_S5	
	count	588.000000	588.000000	588.000000	588.000000	588.000000	588.000000	\
	mean	0.561551	0.617498	0.548594	0.530525	0.531586	0.550029	
	std	0.031263	0.045431	0.057663	0.039461	0.037694	0.045562	
	min	0.454512	0.481747	0.367899	0.420165	0.394824	0.406076	
	25%	0.540899	0.595816	0.508768	0.502042	0.504046	0.519404	
	50%	0.558783	0.617728	0.544527	0.532039	0.535152	0.551989	
	75%	0.581267	0.645072	0.586353	0.559252	0.559505	0.581758	
	max	0.710251	0.746323	0.729066	0.678374	0.636284	0.679299	
		ALOX5AP_S3	AMPD3_S3	APITD1_S5	APOC1_S3	WDR77_	S5	
	count	588.000000	588.000000	588.000000	588.000000	 588.0000	00 \	
	mean	0.483884	0.493659	0.477836	0.573563	0.5500	60	
	std	0.053663	0.044309	0.036428	0.086896	0.0310	76	
	min	0.331671	0.368469	0.322530	0.324714	0.4694	74	
	25%	0.445604	0.465907	0.452058	0.517147	0.5265	66	
	50%	0.486738	0.492044	0.477274	0.574435	0.5512	57	
	75%	0.521481	0.516225	0.502244	0.620487	 0.5718		
	max	0.616650	0.682606	0.569738	0.908518	0.648555		
		WIPF1_S3	WNT2B_S2	WNT8B_S2	WSB2_S5	ZWILCH_S5	ZYX_S2	
	count	588.000000	588.000000	588.000000	588.000000	588.000000	588.000000	\
	mean	0.568496	0.355256	0.210675	0.607736	0.494147	0.643149	
	std	0.036815	0.074243	0.063276	0.034675	0.035358	0.026195	
	min	0.445756	0.175897	0.055078	0.491753	0.393490	0.542554	
	25%	0.543102	0.303990	0.165478	0.581120	0.468319	0.626829	
	50%	0.572505	0.349658	0.208920	0.603647	0.492761	0.640914	
	75%	0.596134	0.397857	0.253542	0.634212	0.518996	0.660907	
	max	0.666154	0.611041	0.455048	0.704738	0.613592	0.745479	
		MMP3_S2	PLG_S5	RGS8_S5				
	count	588.000000	588.000000	588.000000				
	mean	0.321869	0.219206	0.192180				
	std	0.130251	0.147881	0.078831				
	min	0.056857	0.026909	0.046179				
	25%	0.220870	0.137597	0.134364				
	50%	0.287781	0.186938	0.178872				
	75%	0.420708	0.232155	0.239960				
	max	0.782070	0.833178	0.540641				

[8 rows x 440 columns]

If the data type never be Converted, it will only show the count cannot show the statistic details All data are between 0 to 1.

remove the duplicates check the duplicates, it is one of the bad data

```
[]: #check the duplicated and show how many
Dataset_1.duplicated(keep=False)
#show the location of the duplicated:
Dataset_1.loc[Dataset_1.duplicated(),:]
```

```
[]:
                              ACTL6A_S5
                                                    ADAMTS1_S5
                                          ADAM9_S2
                                                                ADCY7_S3
                                                                          AIMP2_S5
     TCGA.EB.A5FP.SKCM.C1_.1
                               0.604189
                                          0.586198
                                                      0.566644
                                                                0.523076
                                                                          0.575625
                               0.603431
                                                                0.514740
     TCGA.31.1944.0V.C1_.1
                                          0.607367
                                                      0.558262
                                                                          0.511529
     TCGA.DK.A1A7.BLCA.C1_.1
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                                                      0.588034
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     TCGA.EW.A10Z.BRCA.C1_.1
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                               0.616708
                                         0.589806
                                                      0.546915
                                                                          0.523893
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                                         0.635687
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                                                                          0.459488
     TCGA.25.2396.0V.C2_.1
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                                         0.650131
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                                                                          0.552538
     TCGA.BK.A4ZD.UCEC.C4_.1
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                                                      0.566843
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     TCGA.26.5134.GBM.C4_.1
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     TCGA.DD.AACX.LIHC.C4_.1
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     TCGA.4G.AAZO.CHOL.C4 .1
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     TCGA.E1.A7YM.LGG.C5_.1
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     TCGA.D7.A748.STAD.C6_.1
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                                    ALOX5AP S3
                                                 AMPD3 S3
                                                           APITD1 S5
                                                                      APOC1 S3
TCGA.EB.A5FP.SKCM.C1_.1
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TCGA.31.1944.0V.C1_.1
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TCGA.DK.A1A7.BLCA.C1_.1
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TCGA.FY.A3WA.THCA.C3_.1
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TCGA.BK.A4ZD.UCEC.C4 .1
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TCGA.4G.AAZO.CHOL.C4_.1
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TCGA.CZ.5454.KIRC.C4_.1
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TCGA.E1.A7YM.LGG.C5_.1
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TCGA.F6.A803.LGG.C5_.1
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TCGA.S9.A6WE.LGG.C5_.1
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TCGA.HW.7486.LGG.C5_.1
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TCGA.P5.A5EV.LGG.C5_.1
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TCGA.WY.A85D.LGG.C5_.1
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TCGA.CS.4938.LGG.C5_.1
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TCGA.HT.7483.LGG.C5_.1
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TCGA.OR.A5J8.ACC.C6_.1
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TCGA.D7.A748.STAD.C6 .1
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TCGA.DX.AB2L.SARC.C6_.1
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TCGA.BH.AOH5.BRCA.C6_.1
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TCGA.D8.A141.BRCA.C6_.1
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TCGA.A7.AODB.BRCA.C6 .1
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TCGA.FB.A4P5.PAAD.C6_.1
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TCGA.FB.AAQ1.PAAD.C6_.1
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TCGA.A8.A08Z.BRCA.C6_.1
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TCGA.AR.AOTT.BRCA.C6_.1
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TCGA.05.5715.LUAD.C6_.1
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TCGA.05.5715.LUAD.C6_.2
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TCGA.E7.A7DU.BLCA.C6_.1
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TCGA.E7.A7DU.BLCA.C6_.2
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TCGA.FB.AAQ1.PAAD.C6_.2
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                                      WNT2B_S2
                                                WNT8B_S2
                                                           WSB2_S5
TCGA.EB.A5FP.SKCM.C1_.1
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TCGA.31.1944.0V.C1_.1
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TCGA.DK.A1A7.BLCA.C1_.1 ...
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TCGA.EW.A1OZ.BRCA.C1_.1
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TCGA.25.2396.0V.C2_.1
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TCGA.FY.A3WA.THCA.C3_.1 ...
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TCGA.5L.AATO.BRCA.C3 .1
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TCGA.EM.A2CO.THCA.C3_.1 ...
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TCGA.G9.7509.PRAD.C3 .1 ...
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TCGA.BK.A4ZD.UCEC.C4_.1 ...
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TCGA.26.5134.GBM.C4_.1
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TCGA.4G.AAZO.CHOL.C4_.1 ...
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TCGA.CZ.5454.KIRC.C4_.1
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TCGA.E1.A7YM.LGG.C5_.1
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TCGA.DU.5871.LGG.C5_.1
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TCGA.F6.A803.LGG.C5_.1
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TCGA.HW.7486.LGG.C5_.1
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TCGA.P5.A5EV.LGG.C5_.1
                                                          0.659484
                         •••
TCGA.WY.A85D.LGG.C5_.1
                         ... 0.593898
                                      0.389431
                                                0.254682
                                                          0.662202
TCGA.CS.4938.LGG.C5_.1
                                      0.415060
                         ... 0.600972
                                                0.305500
                                                          0.659040
TCGA.E1.A7YU.LGG.C5_.1
                           0.590782
                                      0.410158
                                                0.280933
                                                          0.649194
TCGA.TM.A7C4.LGG.C5_.1
                            0.576507
                                      0.429955
                                                0.271722
                                                          0.669425
TCGA.HT.7483.LGG.C5_.1
                         ... 0.600827
                                      0.360948
                                                0.175140
                                                          0.655678
TCGA.OR.A5J8.ACC.C6_.1
                         ... 0.597697
                                      0.253930
                                                0.150130
                                                          0.591696
TCGA.D7.A748.STAD.C6_.1 ... 0.594324
                                      0.248820
                                                0.097389
                                                          0.573912
TCGA.DX.AB2L.SARC.C6_.1
                        ... 0.610022
                                      0.460631
                                                0.186813
                                                          0.601006
TCGA.BH.AOH5.BRCA.C6_.1 ...
                            0.632985
                                      0.191194
                                                0.154078
                                                          0.562375
TCGA.D8.A141.BRCA.C6_.1 ...
                            0.620485
                                      0.345195
                                                0.146276
                                                          0.576920
TCGA.A7.AODB.BRCA.C6_.1 ...
                            0.563253
                                      0.313447
                                                0.169471
                                                          0.591349
TCGA.FB.A4P5.PAAD.C6_.1 ...
                            0.603698
                                      0.288770
                                                0.066713
                                                          0.560555
```

```
TCGA.FB.AAQ1.PAAD.C6_.1 ...
                           0.548372
                                     0.301072
                                               0.202441
                                                         0.554637
TCGA.A8.A08Z.BRCA.C6 .1
                           0.592347
                                     0.326527
                                               0.180855
                                                         0.583227
TCGA.AR.AOTT.BRCA.C6_.1 ...
                           0.614017
                                     0.257182
                                               0.137421
                                                         0.593452
TCGA.EL.A3GP.THCA.C6_.1
                           0.593318
                                     0.306822
                                               0.130648
                                                         0.598497
TCGA.DX.AB2Z.SARC.C6_.1 ...
                                     0.303047
                           0.622022
                                               0.174420
                                                         0.565077
TCGA.05.5715.LUAD.C6_.1 ...
                           0.549089
                                     0.246295
                                               0.198633
                                                         0.598890
TCGA.XF.AAN8.BLCA.C6_.1 ...
                                     0.323108
                           0.579951
                                               0.166204
                                                         0.563020
                           0.549089
TCGA.05.5715.LUAD.C6_.2 ...
                                     0.246295
                                               0.198633
                                                         0.598890
TCGA.3U.A98H.MESO.C6_.1 ...
                           0.577190
                                     0.336248
                                               0.126303
                                                         0.551038
TCGA.E7.A7DU.BLCA.C6_.1 ...
                           0.503172
                                     0.354811
                                               0.291779
                                                         0.617974
TCGA.E7.A7DU.BLCA.C6_.2 ...
                           0.503172
                                     0.354811
                                               0.291779
                                                         0.617974
TCGA.A7.AODB.BRCA.C6_.2 ...
                           0.563253
                                     0.313447
                                               0.169471
                                                         0.591349
TCGA.FB.AAQ1.PAAD.C6_.2 ...
                           0.548372
                                     0.301072
                                               0.202441
                                                         0.554637
TCGA.DX.A1KU.SARC.C6_.1 ...
                           0.636496
                                     0.431338
                                               0.187093
                                                         0.586367
TCGA.3U.A98I.MESO.C6_.1
                           0.585780
                                     0.476789
                                               0.182592
                                                         0.563271
                                     ZYX_S2
                        ZWILCH_S5
                                                         PLG_S5
                                              MMP3_S2
                                                                  RGS8_S5
TCGA.EB.A5FP.SKCM.C1_.1
                         0.564331
                                   0.620690 0.457935
                                                       0.261153 0.261153 \
TCGA.31.1944.0V.C1_.1
                         0.500313
                                   0.691955 0.142887
                                                       0.741099 0.130762
                                   0.616241 0.592075
                                                       0.161456 0.161456
TCGA.DK.A1A7.BLCA.C1_.1
                         0.535029
TCGA.EW.A10Z.BRCA.C1_.1
                         0.520022
                                   0.661331 0.488972
                                                       0.129630 0.147665
TCGA.E2.A15M.BRCA.C2 .1
                                   0.581101 0.458070
                                                       0.061834 0.061834
                         0.505676
TCGA.25.2396.0V.C2_.1
                         0.496169
                                   0.660765 0.182190
                                                      0.137118 0.174494
TCGA.FY.A3WA.THCA.C3 .1
                         0.488890
                                   0.656424 0.227736
                                                      0.227736 0.503648
TCGA.5L.AATO.BRCA.C3_.1
                                                       0.103449 0.133479
                         0.480981
                                   0.645153 0.550348
TCGA.EM.A2CO.THCA.C3_.1
                         0.479143
                                   0.658761 0.251717
                                                       0.231493 0.251717
TCGA.G9.7509.PRAD.C3_.1
                         0.519053
                                   0.629964 0.254507
                                                       0.274949 0.221177
TCGA.BK.A4ZD.UCEC.C4_.1
                         0.526226
                                   0.673062 0.400839 0.230479 0.230479
TCGA.26.5134.GBM.C4_.1
                         0.533901
                                   0.654626 0.153145 0.153145 0.153145
TCGA.DD.AACX.LIHC.C4_.1
                         0.521093
                                   0.618170 0.254250
                                                      0.754658 0.254250
                                   0.634882 0.199747 0.199747 0.199747
TCGA.4G.AAZO.CHOL.C4_.1
                         0.521786
TCGA.CZ.5454.KIRC.C4_.1
                                   0.613291 0.215119
                                                       0.419721
                         0.441574
                                                                 0.145300
                                                      0.205295 0.255208
TCGA.E1.A7YM.LGG.C5_.1
                         0.493780
                                   0.637238 0.205295
TCGA.DU.5871.LGG.C5_.1
                         0.445841
                                   0.616982 0.239331
                                                      0.221897
                                                                0.271622
                         0.509657
                                   0.667191 0.258388
                                                       0.245990 0.352207
TCGA.F6.A803.LGG.C5_.1
TCGA.S9.A6WE.LGG.C5_.1
                         0.434459
                                   0.640533 0.285710 0.230978 0.265094
TCGA.HW.7486.LGG.C5_.1
                                   0.616956 0.234051 0.203934 0.307448
                         0.466008
TCGA.P5.A5EV.LGG.C5_.1
                         0.446377
                                   0.631684 0.208168 0.208168 0.226906
TCGA.WY.A85D.LGG.C5_.1
                         0.435418
                                   0.615406 0.234147
                                                       0.234147 0.254682
TCGA.CS.4938.LGG.C5_.1
                                   0.611320 0.305500
                                                      0.223255 0.241685
                         0.454508
TCGA.E1.A7YU.LGG.C5_.1
                                                       0.224542 0.271461
                         0.469480
                                   0.627374 0.295937
TCGA.TM.A7C4.LGG.C5_.1
                         0.490772
                                   0.626892  0.303506  0.222642  0.374109
                                   0.622553 0.289119 0.175140 0.348325
TCGA.HT.7483.LGG.C5_.1
                         0.483866
TCGA.OR.A5J8.ACC.C6_.1
                         0.500395
                                   0.670649 0.370831 0.150130 0.169537
                                   0.644050 0.290445
                                                      0.155997 0.127740
TCGA.D7.A748.STAD.C6_.1
                         0.459230
TCGA.DX.AB2L.SARC.C6_.1
                         0.493623
                                   0.663616
                                            0.287781
                                                       0.356373
                                                                0.215465
TCGA.BH.AOH5.BRCA.C6_.1
                         0.461398
                                   0.635343 0.356803
                                                       0.066221
                                                                 0.128751
```

TCGA.D8.A141.BRCA.C6_.1 0.636768 0.470924 0.090656 0.090656 0.475919 TCGA.A7.AODB.BRCA.C6_.1 0.150174 0.495301 0.635466 0.469915 0.150174 TCGA.FB.A4P5.PAAD.C6_.1 0.447937 0.666365 0.373320 0.066713 0.066713 TCGA.FB.AAQ1.PAAD.C6_.1 0.472689 0.653401 0.307704 0.332028 0.125693 TCGA.A8.A08Z.BRCA.C6_.1 0.506346 0.636528 0.490175 0.121022 0.121022 TCGA.AR.AOTT.BRCA.C6_.1 0.497730 0.628467 0.509683 0.060906 0.137421 TCGA.EL.A3GP.THCA.C6_.1 0.452201 0.624234 0.378650 0.130648 0.196287 TCGA.DX.AB2Z.SARC.C6_.1 0.529220 0.654313 0.312090 0.135493 0.135493 TCGA.05.5715.LUAD.C6 .1 0.479822 0.633190 0.211564 0.124307 0.124307 0.166204 0.166204 TCGA.XF.AAN8.BLCA.C6_.1 0.430004 0.677198 0.331032 TCGA.05.5715.LUAD.C6_.2 0.479822 0.633190 0.211564 0.124307 0.124307 0.676210 0.559915 0.098843 0.098843 TCGA.3U.A98H.MESO.C6_.1 0.451374 TCGA.E7.A7DU.BLCA.C6_.1 0.539230 0.669733 0.549867 0.241214 0.241214 TCGA.E7.A7DU.BLCA.C6_.2 0.539230 0.669733 0.549867 0.241214 0.241214 TCGA.A7.AODB.BRCA.C6_.2 0.495301 0.635466 0.469915 0.150174 0.150174 TCGA.FB.AAQ1.PAAD.C6_.2 0.472689 0.653401 0.307704 0.332028 0.125693 TCGA.DX.A1KU.SARC.C6_.1 0.666805 0.486879 0.485532 0.163456 0.216325 TCGA.3U.A98I.MESO.C6_.1 0.493496 0.659347 0.204457 0.146536 0.182592

Subgroup

TCGA.EB.A5FP.SKCM.C1_.1 C1 C1 TCGA.31.1944.0V.C1_.1 TCGA.DK.A1A7.BLCA.C1_.1 C1 TCGA.EW.A10Z.BRCA.C1 .1 C1 TCGA.E2.A15M.BRCA.C2_.1 C2 TCGA.25.2396.0V.C2_.1 C2 TCGA.FY.A3WA.THCA.C3_.1 C3 TCGA.5L.AATO.BRCA.C3_.1 C3 TCGA.EM.A2CO.THCA.C3_.1 C3 TCGA.G9.7509.PRAD.C3_.1 C3 C4 TCGA.BK.A4ZD.UCEC.C4_.1 TCGA.26.5134.GBM.C4_.1 C4 C4 TCGA.DD.AACX.LIHC.C4_.1 TCGA.4G.AAZO.CHOL.C4_.1 C4 TCGA.CZ.5454.KIRC.C4_.1 C4 TCGA.E1.A7YM.LGG.C5_.1 C5 TCGA.DU.5871.LGG.C5 .1 C5 TCGA.F6.A803.LGG.C5_.1 C5 TCGA.S9.A6WE.LGG.C5 .1 C5 TCGA.HW.7486.LGG.C5_.1 C5 TCGA.P5.A5EV.LGG.C5_.1 C5 TCGA.WY.A85D.LGG.C5_.1 C5 TCGA.CS.4938.LGG.C5_.1 C5 TCGA.E1.A7YU.LGG.C5_.1 C5 TCGA.TM.A7C4.LGG.C5_.1 C5 TCGA.HT.7483.LGG.C5_.1 C5 TCGA.OR.A5J8.ACC.C6_.1 C6

```
C6
TCGA.D7.A748.STAD.C6_.1
TCGA.DX.AB2L.SARC.C6 .1
                                C6
TCGA.BH.AOH5.BRCA.C6_.1
                                C6
TCGA.D8.A141.BRCA.C6_.1
                                C6
TCGA.A7.AODB.BRCA.C6_.1
                                C6
TCGA.FB.A4P5.PAAD.C6_.1
                                C6
TCGA.FB.AAQ1.PAAD.C6_.1
                                C6
TCGA.A8.A08Z.BRCA.C6_.1
                                C6
TCGA.AR.AOTT.BRCA.C6_.1
                                C6
TCGA.EL.A3GP.THCA.C6_.1
                                C6
TCGA.DX.AB2Z.SARC.C6_.1
                                C6
TCGA.05.5715.LUAD.C6_.1
                                C6
TCGA.XF.AAN8.BLCA.C6_.1
                                C6
TCGA.05.5715.LUAD.C6_.2
                                C6
TCGA.3U.A98H.MESO.C6_.1
                                C6
TCGA.E7.A7DU.BLCA.C6_.1
                                C6
TCGA.E7.A7DU.BLCA.C6_.2
                                C6
TCGA.A7.AODB.BRCA.C6_.2
                                C6
TCGA.FB.AAQ1.PAAD.C6_.2
                                C6
TCGA.DX.A1KU.SARC.C6_.1
                                C6
TCGA.3U.A98I.MESO.C6_.1
                                C6
```

[48 rows x 441 columns]

All of this are duplicated data. Means this 48 rows has appear two times in the dataset. After checking, there are some duplicated data

```
[]: #delete duplicated data
Dataset_1 = Dataset_1.drop_duplicates()
```

```
[]: # check the data after drop duplicated data
Dataset_1
```

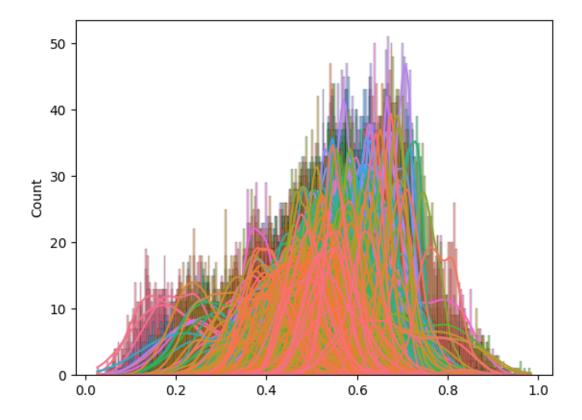
```
[]:
                            ACTL6A_S5
                                       ADAM9_S2
                                                 ADAMTS1_S5 ADCY7_S3 AIMP2_S5
     TCGA.HF.7136.STAD.C1_
                             0.592349
                                       0.628634
                                                   0.570785
                                                             0.536637
                                                                       0.509823
     TCGA.EW.A10Z.BRCA.C1_
                             0.616708
                                       0.589806
                                                   0.546915
                                                             0.522103
                                                                       0.523893
     TCGA.EY.A1GL.UCEC.C1_
                             0.591583
                                       0.601375
                                                   0.530573
                                                             0.470164
                                                                       0.573793
     TCGA.EB.A5FP.SKCM.C1_
                             0.604189
                                       0.586198
                                                   0.566644
                                                             0.523076
                                                                       0.575625
     TCGA.D1.A16D.UCEC.C1_
                             0.545903
                                       0.632497
                                                   0.587917
                                                             0.533486
                                                                       0.540958
     TCGA.43.2581.LUSC.C6_
                             0.544662
                                                   0.575653
                                                             0.557788
                                       0.620647
                                                                       0.515838
     TCGA.SH.A7BC.MESO.C6_
                             0.527214
                                                   0.626745
                                                             0.563070 0.503132
                                       0.635277
     TCGA.EL.A3T9.THCA.C6_
                             0.538555
                                       0.600622
                                                   0.599145 0.549116 0.533807
     TCGA.A2.A4S1.BRCA.C6_
                                       0.599382
                             0.513619
                                                   0.589908
                                                             0.543182
                                                                       0.478895
     TCGA.AR.A2LJ.BRCA.C6
                             0.540358
                                       0.551918
                                                   0.526153
                                                             0.489545 0.518348
                            ALKBH7_S5
                                       ALOX5AP S3
                                                   AMPD3 S3
                                                             APITD1 S5
                                                                        APOC1 S3
                                                              0.418519
     TCGA.HF.7136.STAD.C1_
                             0.462218
                                         0.443087
                                                   0.482923
                                                                        0.483556
```

```
0.588167
TCGA.EW.A1OZ.BRCA.C1_
                         0.545416
                                     0.518862
                                                0.428246
                                                           0.447287
TCGA.EY.A1GL.UCEC.C1_
                         0.560062
                                     0.408029
                                                0.529847
                                                           0.516928
                                                                      0.500291
TCGA.EB.A5FP.SKCM.C1_
                         0.497918
                                     0.362422
                                                0.428469
                                                           0.544391
                                                                      0.580780
TCGA.D1.A16D.UCEC.C1_
                         0.556670
                                     0.518468
                                               0.510708
                                                           0.488154
                                                                      0.585870
                                                           0.408028
TCGA.43.2581.LUSC.C6_
                         0.488698
                                     0.592145
                                               0.510097
                                                                      0.572360
TCGA.SH.A7BC.MESO.C6_
                         0.523583
                                     0.550000
                                                0.501574
                                                           0.417098
                                                                      0.594076
TCGA.EL.A3T9.THCA.C6_
                         0.514959
                                     0.532856
                                                           0.474861
                                                                      0.471344
                                               0.477059
TCGA.A2.A4S1.BRCA.C6
                         0.507401
                                     0.570468
                                                0.483158
                                                           0.441637
                                                                      0.463836
TCGA.AR.A2LJ.BRCA.C6_
                         0.603053
                                     0.517177
                                                0.453269
                                                           0.484431
                                                                      0.650400
                                                           WSB2_S5
                                                                     ZWILCH_S5
                           WIPF1_S3
                                     WNT2B_S2
                                                WNT8B_S2
TCGA.HF.7136.STAD.C1_
                           0.557671
                                     0.348506
                                                0.210016
                                                          0.629423
                                                                      0.515653
TCGA.EW.A10Z.BRCA.C1_
                           0.543131
                                     0.271636
                                                0.215562
                                                          0.588503
                                                                      0.520022
TCGA.EY.A1GL.UCEC.C1_
                                                          0.626342
                           0.537821
                                     0.370267
                                                0.256229
                                                                      0.500481
TCGA.EB.A5FP.SKCM.C1_
                           0.635673
                                     0.360680
                                                0.261153
                                                          0.612561
                                                                      0.564331
TCGA.D1.A16D.UCEC.C1_
                           0.533510
                                     0.332906
                                                0.129106
                                                          0.609040
                                                                      0.482094
TCGA.43.2581.LUSC.C6_
                           0.584858
                                     0.256580
                                                0.154807
                                                          0.574657
                                                                      0.465805
TCGA.SH.A7BC.MESO.C6_
                           0.580386
                                     0.560368
                                               0.185317
                                                          0.567794
                                                                      0.471550
TCGA.EL.A3T9.THCA.C6_
                           0.587950
                                     0.286881
                                                0.189631
                                                          0.562508
                                                                      0.489268
TCGA.A2.A4S1.BRCA.C6
                           0.601901
                                     0.340524
                                                0.171785
                                                          0.541964
                                                                      0.450655
TCGA.AR.A2LJ.BRCA.C6_
                           0.563845
                                     0.215693
                                               0.201434
                                                          0.558991
                                                                      0.462621
                          ZYX_S2
                                   MMP3_S2
                                               PLG_S5
                                                        RGS8 S5
                                                                  Subgroup
TCGA.HF.7136.STAD.C1_
                        0.664831
                                  0.548405
                                             0.144132
                                                       0.156693
                                                                        C1
                                  0.488972
TCGA.EW.A10Z.BRCA.C1_
                        0.661331
                                             0.129630
                                                       0.147665
                                                                        C1
TCGA.EY.A1GL.UCEC.C1_
                        0.650543
                                  0.602704
                                             0.236607
                                                       0.236607
                                                                        C1
TCGA.EB.A5FP.SKCM.C1_
                        0.620690
                                  0.457935
                                             0.261153
                                                       0.261153
                                                                        C1
TCGA.D1.A16D.UCEC.C1_
                        0.670960
                                                                        C1
                                  0.389138
                                             0.282479
                                                       0.151172
                                  0.372903
                                             0.098287
                                                       0.098287
                                                                        C6
TCGA.43.2581.LUSC.C6_
                        0.654632
TCGA.SH.A7BC.MESO.C6
                        0.683370
                                  0.354513
                                             0.093081
                                                       0.093081
                                                                        C6
TCGA.EL.A3T9.THCA.C6_
                        0.645087
                                  0.247726
                                             0.172708
                                                       0.172708
                                                                        C6
TCGA.A2.A4S1.BRCA.C6_
                        0.643585
                                  0.259902
                                             0.171785
                                                       0.171785
                                                                        C6
TCGA.AR.A2LJ.BRCA.C6_
                        0.676615
                                  0.476988
                                             0.133939
                                                       0.133939
                                                                        C6
```

[540 rows x 441 columns]

finding outliers Plot Dataset Histogram and Kernel Density Estimation for observation but cannot get too much details because this is a high dimensional with so many features I prefer to avoiding to find the outlier by observation, just have a general situation of the data distribution to have a preliminary judgement.

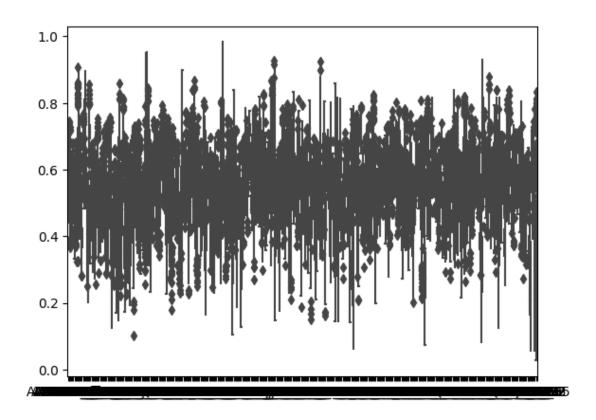
```
[]: sns.histplot(Dataset_1,kde=True, legend=False) plt.show()
```



Outliers are usually located in the tails of the distribution

sns.boxplot(data=Dataset_1)#for quartile method

[]: <Axes: >



It can clearly see that there are a lot of outliers.

Choosing quartile method to find the specific outliers in the data

[]: Dataset_1.describe() []: ADAMTS1 S5 ACTL6A S5 ADAM9 S2 ADCY7 S3 AIMP2 S5 ALKBH7 S5 540.000000 540.000000 540.000000 540.000000 540.000000 540.000000 0.562063 0.530075 0.532300 0.550593 mean 0.617497 0.549052 std 0.031346 0.046260 0.058148 0.039704 0.037663 0.045730 min 0.454512 0.481747 0.367899 0.420165 0.394824 0.406076 25% 0.519779 0.541103 0.594717 0.509507 0.501417 0.505232 50% 0.559485 0.618027 0.544527 0.531558 0.535666 0.552652 75% 0.581467 0.644837 0.586762 0.559147 0.560231 0.582331 0.710251 0.746323 0.729066 0.678374 0.636284 0.679299 maxALOX5AP_S3 AMPD3_S3 APITD1_S5 APOC1_S3 WDR77_S5 540.000000 540.000000 540.000000 540.000000 540.000000 count 0.478304 0.550695 mean 0.482367 0.494148 0.571891 std 0.053319 0.044860 0.036284 0.087900 0.030780 min 0.331671 0.368469 0.322530 0.324714 0.469474 25% 0.514803 0.444551 0.465861 0.452666 0.527979 50% 0.484568 0.492815 0.478269 0.570587 0.551934

```
75%
         0.520911
                      0.517119
                                  0.501981
                                               0.619868 ...
                                                               0.572067
         0.616650
                      0.682606
                                  0.569738
                                               0.908518
                                                               0.648555
max
         WIPF1_S3
                      WNT2B_S2
                                  WNT8B_S2
                                                WSB2_S5
                                                           ZWILCH_S5
                                                                          ZYX_S2
       540.000000 540.000000
                                540.000000
                                             540.000000
                                                         540.000000
                                                                      540.000000 \
count
         0.567491
                      0.356629
                                  0.210863
                                               0.607607
                                                            0.494693
                                                                        0.643181
mean
                                  0.063109
                                               0.034481
                                                                        0.026520
std
         0.036571
                      0.074973
                                                            0.035625
min
         0.445756
                      0.175897
                                  0.055078
                                               0.491753
                                                            0.393490
                                                                        0.542554
25%
         0.541440
                      0.304264
                                  0.164997
                                               0.581120
                                                            0.468695
                                                                        0.626757
50%
         0.571641
                      0.351196
                                  0.209848
                                               0.603842
                                                            0.493034
                                                                        0.641369
75%
         0.595177
                      0.399560
                                  0.253092
                                               0.633591
                                                            0.519085
                                                                        0.660907
         0.666154
                      0.611041
                                  0.455048
                                               0.704738
                                                            0.613592
                                                                        0.745479
max
          MMP3_S2
                        PLG_S5
                                   RGS8_S5
       540.000000 540.000000
                                540.000000
count
mean
         0.320501
                      0.220009
                                  0.191605
std
         0.130704
                      0.148883
                                  0.078200
min
         0.056857
                      0.026909
                                  0.046179
25%
         0.220523
                      0.138133
                                  0.134756
50%
         0.286077
                      0.186938
                                  0.178872
75%
                                  0.237335
         0.418848
                      0.232155
         0.782070
                                  0.540641
max
                      0.833178
```

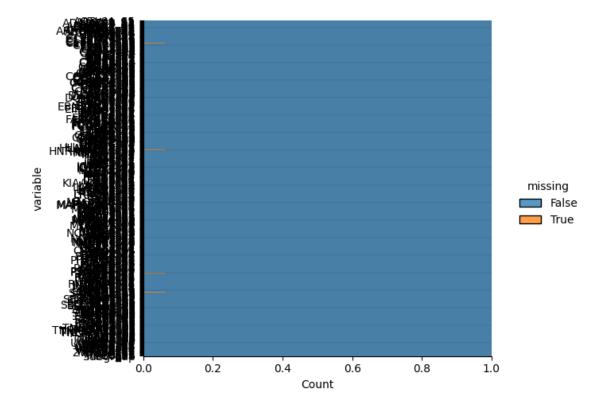
[8 rows x 440 columns]

Check the missing data situation before droped outliers

```
[]: # show the missing data before delet the outliers
plt.figure(figsize=(10,6))
sns.displot(
    data=Dataset_1.isna().melt(value_name="missing"),
    y="variable",
    hue="missing",
    multiple="fill",
    aspect=1.25
)
```

[]: <seaborn.axisgrid.FacetGrid at 0x29415a6c0d0>

<Figure size 1000x600 with 0 Axes>



Before drop the outliers the missing columns distribut like this

FInd the outliers location by Quartile Algorithm: upper quartile and lower quartile limits

```
[]: outliers = find_outliers_IQR(Dataset_1[Dataset_1.columns[0:-1]]) #get outliers_outliers_outliers_outliers_outliers_outliers_outliers_outliers_outliers
```

C:\Users\murui\AppData\Local\Temp\ipykernel_38176\714981418.py:6:
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/indexing.html#returning-a-view-versus-a-copy
 df[((df<(q1-1.5*IQR)) | (df>(q3+1.5*IQR)))] =1 #easy to sum how many outliers
C:\Users\murui\AppData\Local\Temp\ipykernel_38176\714981418.py:6:
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/indexing.html#returning-a-view-versus-a-copy df[((df<(q1-1.5*IQR)) | (df>(q3+1.5*IQR)))] =1 #easy to sum how many outliers C:\Users\murui\AppData\Local\Temp\ipykernel_38176\714981418.py:7: 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/pandasdocs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
 df[~((df<(q1-1.5*IQR)) | (df>(q3+1.5*IQR)))]=0
C:\Users\murui\AppData\Local\Temp\ipykernel_38176\714981418.py:7:
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/indexing.html#returning-a-view-versus-a-copy df[~((df<(q1-1.5*IQR))) | (df>(q3+1.5*IQR)))]=0

[]:		ACTL6A_S5	ADAM9_S2	ADAMTS1_S5	ADCY7_S3	AIMP2_S5
	TCGA.HF.7136.STAD.C1_	0.0	0.0	0.0	0.0	0.0 \
	TCGA.EW.A10Z.BRCA.C1_	0.0	0.0	0.0	0.0	0.0
	TCGA.EY.A1GL.UCEC.C1_	0.0	0.0	0.0	0.0	0.0
	TCGA.EB.A5FP.SKCM.C1_	0.0	0.0	0.0	0.0	0.0
	TCGA.D1.A16D.UCEC.C1_	0.0	0.0	0.0	0.0	0.0
		•••			•••	
	TCGA.43.2581.LUSC.C6_	0.0	0.0	0.0	0.0	0.0
	TCGA.SH.A7BC.MESO.C6_	0.0	0.0	0.0	0.0	0.0
	TCGA.EL.A3T9.THCA.C6_	0.0	0.0	0.0	0.0	0.0
	TCGA.A2.A4S1.BRCA.C6_	0.0	0.0	0.0	0.0	0.0
	TCGA.AR.A2LJ.BRCA.C6_	0.0	0.0	0.0	0.0	0.0
		ALKBH7 S5	ALOX5AP S	3 AMPD3_S3	APITD1 S5	APOC1_S3
	TCGA.HF.7136.STAD.C1_	0.0	_	0.0	0.0	-
	TCGA.EW.A10Z.BRCA.C1_	0.0	0.0	0.0	0.0	0.0
	TCGA.EY.A1GL.UCEC.C1_	0.0	0.0	0.0	0.0	0.0
	TCGA.EB.A5FP.SKCM.C1_	0.0	0.0	0.0	0.0	0.0
	TCGA.D1.A16D.UCEC.C1_	0.0	0.0	0.0	0.0	0.0
	•••	•••	•••	•••	•••	
	TCGA.43.2581.LUSC.C6_	0.0	0.0	0.0	0.0	0.0
	TCGA.SH.A7BC.MESO.C6_	0.0	0.0	0.0	0.0	0.0

```
TCGA.EL.A3T9.THCA.C6_
                              0.0
                                           0.0
                                                      0.0
                                                                 0.0
                                                                            0.0
TCGA.A2.A4S1.BRCA.C6
                              0.0
                                           0.0
                                                      0.0
                                                                 0.0
                                                                            0.0
TCGA.AR.A2LJ.BRCA.C6
                              0.0
                                           0.0
                                                      0.0
                                                                 0.0
                                                                            0.0
                           WDR77_S5
                                     WIPF1_S3
                                                WNT2B_S2
                                                          WNT8B_S2 WSB2_S5
TCGA.HF.7136.STAD.C1_
                                0.0
                                                      0.0
                                                                0.0
                                                                          0.0 \
                                           0.0
                                                      0.0
                                                                0.0
                                                                          0.0
TCGA.EW.A10Z.BRCA.C1_ ...
                                0.0
                                           0.0
TCGA.EY.A1GL.UCEC.C1_ ...
                                0.0
                                           0.0
                                                      0.0
                                                                0.0
                                                                          0.0
TCGA.EB.A5FP.SKCM.C1 ...
                                0.0
                                           0.0
                                                      0.0
                                                                0.0
                                                                          0.0
TCGA.D1.A16D.UCEC.C1_ ...
                                                                          0.0
                                0.0
                                           0.0
                                                      0.0
                                                                0.0
                                                        •••
TCGA.43.2581.LUSC.C6_ ...
                                0.0
                                           0.0
                                                      0.0
                                                                0.0
                                                                          0.0
TCGA.SH.A7BC.MESO.C6_ ...
                                0.0
                                           0.0
                                                      1.0
                                                                0.0
                                                                          0.0
TCGA.EL.A3T9.THCA.C6_ ...
                                0.0
                                           0.0
                                                      0.0
                                                                0.0
                                                                          0.0
                                                                          0.0
TCGA.A2.A4S1.BRCA.C6_ ...
                                0.0
                                           0.0
                                                      0.0
                                                                0.0
TCGA.AR.A2LJ.BRCA.C6_ ...
                                0.0
                                           0.0
                                                      0.0
                                                                0.0
                                                                          0.0
                                           MMP3_S2 PLG_S5
                                                              RGS8 S5
                        ZWILCH_S5 ZYX_S2
TCGA.HF.7136.STAD.C1_
                              0.0
                                       0.0
                                                0.0
                                                         0.0
                                                                  0.0
                              0.0
                                       0.0
                                                0.0
                                                         0.0
                                                                  0.0
TCGA.EW.A10Z.BRCA.C1_
TCGA.EY.A1GL.UCEC.C1_
                              0.0
                                       0.0
                                                0.0
                                                         0.0
                                                                  0.0
                                       0.0
TCGA.EB.A5FP.SKCM.C1
                              0.0
                                                0.0
                                                         0.0
                                                                  0.0
TCGA.D1.A16D.UCEC.C1_
                              0.0
                                                0.0
                                       0.0
                                                         0.0
                                                                  0.0
                              0.0
                                       0.0
                                                0.0
                                                         0.0
                                                                  0.0
TCGA.43.2581.LUSC.C6
TCGA.SH.A7BC.MESO.C6
                              0.0
                                       0.0
                                                0.0
                                                         0.0
                                                                  0.0
TCGA.EL.A3T9.THCA.C6_
                              0.0
                                       0.0
                                                0.0
                                                         0.0
                                                                  0.0
TCGA.A2.A4S1.BRCA.C6_
                              0.0
                                       0.0
                                                0.0
                                                         0.0
                                                                  0.0
TCGA.AR.A2LJ.BRCA.C6_
                              0.0
                                       0.0
                                                0.0
                                                         0.0
                                                                  0.0
```

[540 rows x 440 columns]

Separate the original data from the cleaned areas and compare them later.

```
[]: cleaned_data = drop_outliers_IQR(Dataset_1[Dataset_1.columns[0:-1]]) cleaned_data
```

```
[]:
                                                ADAMTS1_S5
                           ACTL6A_S5
                                      ADAM9_S2
                                                            ADCY7_S3 AIMP2_S5
    TCGA.HF.7136.STAD.C1_
                            0.592349
                                      0.628634
                                                  0.570785
                                                            0.536637
                                                                      0.509823
    TCGA.EW.A10Z.BRCA.C1
                            0.616708
                                      0.589806
                                                  0.546915
                                                            0.522103 0.523893
    TCGA.EY.A1GL.UCEC.C1_
                                                  0.530573 0.470164 0.573793
                            0.591583
                                      0.601375
    TCGA.EB.A5FP.SKCM.C1
                            0.604189
                                      0.586198
                                                  0.566644 0.523076 0.575625
    TCGA.D1.A16D.UCEC.C1_
                            0.545903
                                      0.632497
                                                  0.587917
                                                            0.533486 0.540958
    TCGA.43.2581.LUSC.C6_
                            0.544662
                                      0.620647
                                                  0.575653
                                                            0.557788 0.515838
    TCGA.SH.A7BC.MESO.C6
                                                  0.626745 0.563070 0.503132
                            0.527214
                                      0.635277
    TCGA.EL.A3T9.THCA.C6_
                            0.538555
                                      0.600622
                                                  0.599145 0.549116 0.533807
    TCGA.A2.A4S1.BRCA.C6_
                            0.513619
                                      0.599382
                                                  0.589908
                                                            0.543182
                                                                      0.478895
    TCGA.AR.A2LJ.BRCA.C6
                            0.540358
                                      0.551918
                                                  0.526153 0.489545 0.518348
                            ALKBH7_S5
                                      ALOX5AP_S3 AMPD3_S3
                                                            APITD1_S5
                                                                       APOC1_S3
    TCGA.HF.7136.STAD.C1_
                            0.462218
                                        0.443087 0.482923
                                                             0.418519
                                                                       0.483556
    TCGA.EW.A10Z.BRCA.C1_
                            0.545416
                                        0.518862 0.428246
                                                             0.447287
                                                                       0.588167
    TCGA.EY.A1GL.UCEC.C1_
                                        0.408029 0.529847
                                                             0.516928
                            0.560062
                                                                       0.500291
    TCGA.EB.A5FP.SKCM.C1
                            0.497918
                                        0.362422 0.428469
                                                             0.544391
                                                                       0.580780
    TCGA.D1.A16D.UCEC.C1_
                                        0.518468 0.510708
                            0.556670
                                                             0.488154
                                                                       0.585870
                               •••
    TCGA.43.2581.LUSC.C6_
                            0.488698
                                        0.592145 0.510097
                                                             0.408028
                                                                       0.572360
    TCGA.SH.A7BC.MESO.C6
                            0.523583
                                        0.550000 0.501574
                                                             0.417098
                                                                       0.594076
    TCGA.EL.A3T9.THCA.C6_
                            0.514959
                                        0.532856 0.477059
                                                             0.474861
                                                                       0.471344
                            0.507401
    TCGA.A2.A4S1.BRCA.C6_
                                        0.570468 0.483158
                                                             0.441637
                                                                       0.463836
    TCGA.AR.A2LJ.BRCA.C6_
                                                             0.484431
                            0.603053
                                        0.517177 0.453269
                                                                       0.650400
                                        WIPF1_S3 WNT2B_S2
                                                            WNT8B_S2
                              WDR77_S5
                                                                       WSB2_S5
    TCGA.HF.7136.STAD.C1_ ...
                              0.591241
                                        0.557671 0.348506
                                                            0.210016
                                                                      0.629423 \
    TCGA.EW.A10Z.BRCA.C1_ ...
                              0.544296
                                        0.543131 0.271636
                                                            0.215562
                                                                      0.588503
    TCGA.EY.A1GL.UCEC.C1_ ... 0.564828
                                        0.537821 0.370267
                                                            0.256229
                                                                      0.626342
    TCGA.EB.A5FP.SKCM.C1_ ...
                              0.582566
                                        0.635673 0.360680
                                                            0.261153 0.612561
    TCGA.D1.A16D.UCEC.C1_ ...
                              0.592322
                                        0.533510 0.332906
                                                            0.129106 0.609040
    TCGA.43.2581.LUSC.C6_ ...
                              0.524690
                                        0.584858 0.256580
                                                            0.154807
                                                                      0.574657
    TCGA.SH.A7BC.MESO.C6 ... 0.520420 0.580386
                                                            0.185317
                                                       {\tt NaN}
                                                                      0.567794
    TCGA.EL.A3T9.THCA.C6_ ...
                              0.522743
                                        0.587950 0.286881
                                                            0.189631
                                                                      0.562508
    TCGA.A2.A4S1.BRCA.C6_ ...
                              0.524518
                                        0.601901 0.340524
                                                            0.171785
                                                                      0.541964
    TCGA.AR.A2LJ.BRCA.C6_
                              0.515673  0.563845  0.215693  0.201434  0.558991
                            ZWILCH_S5
                                        ZYX_S2
                                                 MMP3_S2
                                                            PLG_S5
                                                                     RGS8_S5
    TCGA.HF.7136.STAD.C1_
                            0.515653
                                      0.664831
                                                0.548405
                                                          0.144132
                                                                    0.156693
    TCGA.EW.A10Z.BRCA.C1_
                            0.520022
                                      0.661331
                                                0.488972
                                                          0.129630
                                                                    0.147665
    TCGA.EY.A1GL.UCEC.C1_
                            0.500481
                                      0.650543
                                                0.602704
                                                          0.236607
                                                                    0.236607
    TCGA.EB.A5FP.SKCM.C1_
                            0.564331
                                      0.620690
                                                0.457935
                                                          0.261153
                                                                    0.261153
    TCGA.D1.A16D.UCEC.C1_
                            0.482094
                                      0.670960
                                                0.389138
                                                          0.282479
                                                                    0.151172
    TCGA.43.2581.LUSC.C6_
                            0.465805
                                      0.654632 0.372903
                                                          0.098287
                                                                    0.098287
```

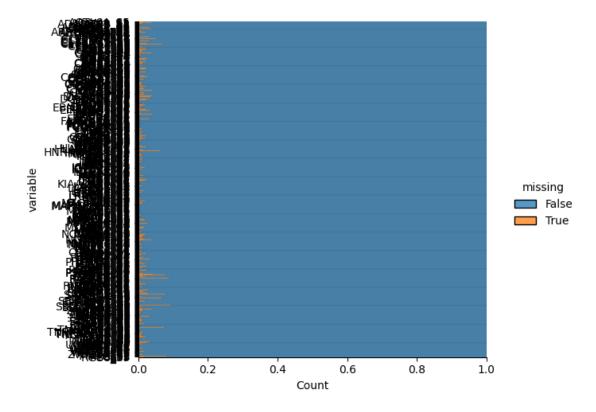
```
TCGA.SH.A7BC.MESO.C6
                       0.471550 0.683370 0.354513 0.093081
                                                              0.093081
                                                              0.172708
TCGA.EL.A3T9.THCA.C6_
                       0.489268 0.645087
                                          0.247726 0.172708
TCGA.A2.A4S1.BRCA.C6_
                       0.450655 0.643585
                                          0.259902
                                                    0.171785
                                                              0.171785
TCGA.AR.A2LJ.BRCA.C6_
                       0.462621 0.676615
                                         0.476988 0.133939
                                                              0.133939
```

[540 rows x 440 columns]

```
[]: #show the missing data afer cleaning
plt.figure(figsize=(10,6))
sns.displot(
    data=cleaned_data.isna().melt(value_name="missing"),
    y="variable",
    hue="missing",
    multiple="fill",
    aspect=1.25
)
```

[]: <seaborn.axisgrid.FacetGrid at 0x294158240d0>

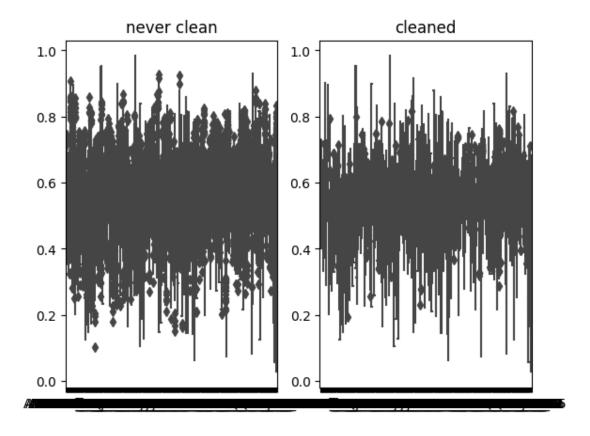
<Figure size 1000x600 with 0 Axes>



The outliers are removed to varying degrees for each feature.

```
[]: #compare in the plot
fig, axes = plt.subplots(1,2)
sns.boxplot(data=Dataset_1, ax=axes[0])#orginal data
sns.boxplot(data=cleaned_data, ax=axes[1])#without outliers
axes[0].set_title('never clean')
axes[1].set_title('cleaned')
```

[]: Text(0.5, 1.0, 'cleaned')



It shows after cleaning the data, outliers have gone down a lot. However, the retention of outliers is not decided for the time being because some outliers contain important data content. I don't think they should be calculated separately for each feature and deleted completely. The Quartile Algorithm is traditional, but I don't think it's perfect for high-dimensional arrays.

Due to the choice of the Normalization method being affected by outliers and PCA when doing the dimensional reducing, it will do more compared to the cleaned and original data. Also, I will compare the traditional method and some methods using machine learning, which I think is more suitable for high-dimensional arrays.

```
[]: # count the outliers
outliers.sum().sum()
```

[]: 2185.0

After Calculating, cleaned data drop 2185 data which is 0.92% original data.

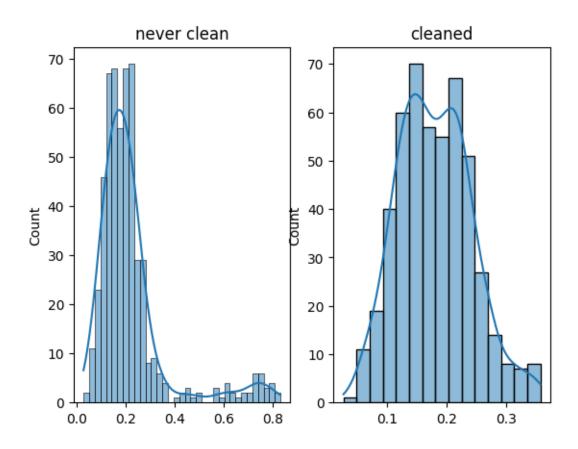
Choosing some feature to show the change between original data and cleaned data

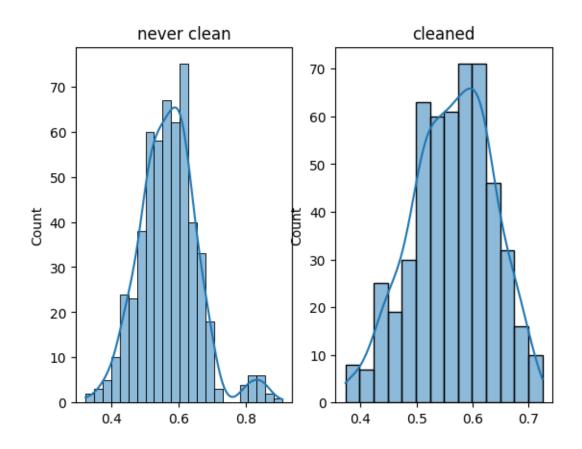
```
[]: #shows situation for count of the outliers in each features outliers.sum()
```

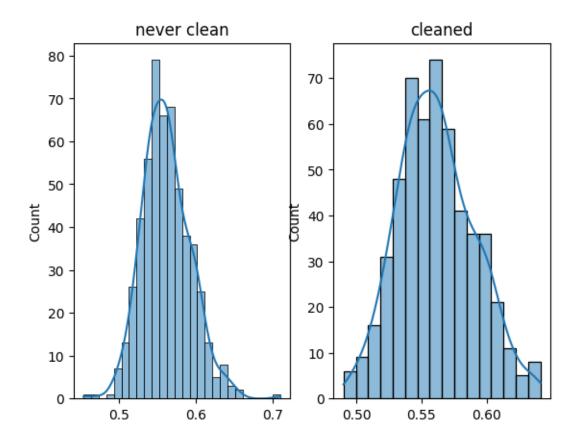
```
[]: ACTL6A_S5
                     8.0
     ADAM9 S2
                    21.0
     ADAMTS1_S5
                     6.0
     ADCY7_S3
                     1.0
     AIMP2_S5
                     1.0
     ZWILCH_S5
                     2.0
     ZYX_S2
                     8.0
     MMP3_S2
                     1.0
     PLG_S5
                    45.0
     RGS8_S5
                     9.0
     Length: 440, dtype: float64
```

Choose the 'PLG_S5' feature, 'APOC1_S3' feature and 'ACTL6A_S5' feature to plot the data distribution because it can be easier to observe in different situations: one is the feature has many outliers. Another one is the feature has seldom outliers. And compare original data and cleaned data.

```
[]: #plot for some features for have check
     fig, axes = plt.subplots(1,2)
     sns.histplot(Dataset_1[['PLG S5']],kde=True, legend=False, ax=axes[0])
     sns.histplot(cleaned_data[['PLG_S5']],kde=True, legend=False, ax=axes[1])
     axes[0].set title('never clean')
     axes[1].set_title('cleaned')
     fig, axes = plt.subplots(1,2)
     sns.histplot(Dataset_1[['APOC1_S3']],kde=True, legend=False, ax=axes[0])
     sns.histplot(cleaned data[['APOC1 S3']],kde=True, legend=False, ax=axes[1])
     axes[0].set title('never clean')
     axes[1].set_title('cleaned')
     fig, axes = plt.subplots(1,2)
     sns.histplot(Dataset_1[['ACTL6A_S5']],kde=True, legend=False, ax=axes[0])
     sns.histplot(cleaned_data[['ACTL6A_S5']],kde=True, legend=False, ax=axes[1])
     axes[0].set_title('never clean')
     axes[1].set_title('cleaned')
     plt.show()
```







Sometimes, the outliers include special significance. However, the PCA dimensionality reduction Algorithm is sensitive to outliers. Deleting the outliers benefits the stability of a model because of the equilibrium of a model. But dropping the outliers should be done with great care. Since IsolationForest Algorithms can only work without missing data, I will supplement this and reevaluate the decision to keep or remove outliers after imputing missing values.

Conclusion: Through the deletion of repeated values, outliers and machine learning algorithms to clean the data, I think the most challenging thing is how to clean high-dimensional arrays because high-dimensional arrays of features will be more or less correlation; the traditional cleaning methods are not suitable. How to identify the decision to retain the data: sometimes outliers are indeed identified, but the problem of maintaining the problem is still a headache.

b. Missing Data Imputation

check missing data

[]: # using isna() to check the missing data and summarise it
Dataset_1.isna().any()

[]: ACTL6A_S5 False
ADAM9_S2 False
ADAMTS1_S5 False

```
ZYX_S2
                   False
    MMP3_S2
                   False
    PLG_S5
                   False
    RGS8_S5
                   False
     Subgroup
                   False
    Length: 441, dtype: bool
[]: #shows the location of the missing data
     Dataset_1[Dataset_1.columns[Dataset_1.isna().any()]]
[]:
                            Clorf54 S3
                                         HN1L S5 PTPRC S3
                                                             SAMHD1 S3
                              0.364874
                                        0.611415
                                                  0.532904
                                                              0.530763
     TCGA.HF.7136.STAD.C1_
     TCGA.EW.A10Z.BRCA.C1_
                              0.421521
                                        0.641031
                                                  0.525117
                                                              0.533921
     TCGA.EY.A1GL.UCEC.C1_
                              0.457814
                                        0.637443
                                                  0.424625
                                                              0.486925
     TCGA.EB.A5FP.SKCM.C1_
                              0.427228
                                        0.642142
                                                              0.463744
                                                       {\tt NaN}
     TCGA.D1.A16D.UCEC.C1_
                                        0.700416 0.493172
                              0.398250
                                                              0.554316
                              0.351794
                                        0.599456
                                                       NaN
     TCGA.43.2581.LUSC.C6_
                                                              0.591878
     TCGA.SH.A7BC.MESO.C6_
                              0.425960
                                        0.614321
                                                  0.582419
                                                              0.588247
                              0.449813
     TCGA.EL.A3T9.THCA.C6
                                                  0.531815
                                                              0.544002
                                        0.602357
     TCGA.A2.A4S1.BRCA.C6_
                                   {\tt NaN}
                                        0.555404
                                                  0.533358
                                                              0.511731
     TCGA.AR.A2LJ.BRCA.C6
                              0.465609
                                        0.616445
                                                  0.529782
                                                              0.515932
     [540 rows x 4 columns]
[]: cleaned_data[cleaned_data.columns[cleaned_data.isna().any()]]
[]:
                            ACTL6A_S5
                                       ADAM9_S2
                                                 ADAMTS1_S5
                                                             ADCY7_S3 AIMP2_S5
     TCGA.HF.7136.STAD.C1
                             0.592349
                                       0.628634
                                                   0.570785
                                                              0.536637
                                                                        0.509823
     TCGA.EW.A10Z.BRCA.C1_
                             0.616708
                                       0.589806
                                                   0.546915
                                                             0.522103 0.523893
     TCGA.EY.A1GL.UCEC.C1_
                             0.591583
                                       0.601375
                                                   0.530573
                                                             0.470164
                                                                        0.573793
                                                             0.523076 0.575625
     TCGA.EB.A5FP.SKCM.C1_
                             0.604189
                                       0.586198
                                                   0.566644
     TCGA.D1.A16D.UCEC.C1_
                                                              0.533486 0.540958
                             0.545903
                                       0.632497
                                                   0.587917
                                                   0.575653
     TCGA.43.2581.LUSC.C6_
                             0.544662
                                       0.620647
                                                             0.557788 0.515838
     TCGA.SH.A7BC.MESO.C6_
                             0.527214
                                       0.635277
                                                   0.626745
                                                             0.563070
                                                                       0.503132
     TCGA.EL.A3T9.THCA.C6_
                             0.538555
                                       0.600622
                                                   0.599145
                                                              0.549116
                                                                        0.533807
     TCGA.A2.A4S1.BRCA.C6
                             0.513619
                                       0.599382
                                                   0.589908
                                                              0.543182
                                                                        0.478895
     TCGA.AR.A2LJ.BRCA.C6_
                             0.540358
                                       0.551918
                                                   0.526153
                                                             0.489545 0.518348
                            ALKBH7_S5
                                       AMPD3_S3
                                                 APITD1_S5
                                                             APOC1_S3
                                                                       ARHGAP1_S2
                             0.462218
                                       0.482923
                                                  0.418519
                                                             0.483556
                                                                         0.595520
     TCGA.HF.7136.STAD.C1
     TCGA.EW.A10Z.BRCA.C1_
                             0.545416
                                       0.428246
                                                  0.447287
                                                             0.588167
                                                                         0.634261
     TCGA.EY.A1GL.UCEC.C1_
                             0.560062
                                       0.529847
                                                  0.516928
                                                             0.500291
                                                                         0.648068
```

ADCY7_S3

AIMP2_S5

False

False

```
0.544391
                                                                      0.624863
    TCGA.EB.A5FP.SKCM.C1_
                            0.497918 0.428469
                                                          0.580780
    TCGA.D1.A16D.UCEC.C1_
                            0.556670
                                     0.510708
                                                0.488154
                                                          0.585870
                                                                      0.674815
    TCGA.43.2581.LUSC.C6_
                            0.488698
                                      0.510097
                                                0.408028
                                                          0.572360
                                                                      0.607820
    TCGA.SH.A7BC.MESO.C6_
                            0.523583 0.501574
                                                0.417098
                                                          0.594076
                                                                      0.608866
    TCGA.EL.A3T9.THCA.C6_
                                                0.474861
                            0.514959 0.477059
                                                          0.471344
                                                                      0.642155
    TCGA.A2.A4S1.BRCA.C6
                            0.507401
                                      0.483158
                                                0.441637
                                                          0.463836
                                                                      0.601681
    TCGA.AR.A2LJ.BRCA.C6_
                            0.603053 0.453269
                                                0.484431
                                                          0.650400
                                                                      0.649493
                           ... WDR77_S5 WIPF1_S3 WNT2B_S2 WNT8B_S2
                                                                      WSB2_S5
    TCGA.HF.7136.STAD.C1 ...
                              0.591241
                                       0.557671 0.348506 0.210016
                                                                     0.629423 \
    TCGA.EW.A10Z.BRCA.C1_ ... 0.544296 0.543131 0.271636 0.215562 0.588503
    TCGA.EY.A1GL.UCEC.C1_ ... 0.564828 0.537821 0.370267 0.256229 0.626342
    TCGA.EB.A5FP.SKCM.C1_ ... 0.582566 0.635673 0.360680 0.261153 0.612561
    TCGA.D1.A16D.UCEC.C1 ... 0.592322 0.533510 0.332906 0.129106 0.609040
    TCGA.43.2581.LUSC.C6_ ... 0.524690 0.584858 0.256580
                                                           0.154807
                                                                     0.574657
    TCGA.SH.A7BC.MESO.C6_ ... 0.520420 0.580386
                                                      \mathtt{NaN}
                                                           0.185317 0.567794
    TCGA.EL.A3T9.THCA.C6_ ... 0.522743 0.587950 0.286881 0.189631 0.562508
    TCGA.A2.A4S1.BRCA.C6_ ... 0.524518 0.601901 0.340524 0.171785 0.541964
    TCGA.AR.A2LJ.BRCA.C6_ ... 0.515673 0.563845 0.215693 0.201434 0.558991
                           ZWILCH_S5
                                        ZYX_S2
                                                MMP3_S2
                                                           PLG_S5
                                                                    RGS8_S5
    TCGA.HF.7136.STAD.C1
                            0.515653 0.664831
                                               0.548405 0.144132
                                                                   0.156693
    TCGA.EW.A10Z.BRCA.C1
                            0.520022 0.661331
                                               0.488972
                                                         0.129630
                                                                   0.147665
    TCGA.EY.A1GL.UCEC.C1
                            0.500481 0.650543
                                               0.602704 0.236607
                                                                   0.236607
    TCGA.EB.A5FP.SKCM.C1_
                            0.564331 0.620690
                                               0.457935 0.261153
                                                                   0.261153
    TCGA.D1.A16D.UCEC.C1
                            0.482094 0.670960 0.389138 0.282479
                                                                   0.151172
                            0.465805
                                      0.654632 0.372903 0.098287
    TCGA.43.2581.LUSC.C6_
                                                                   0.098287
    TCGA.SH.A7BC.MESO.C6_
                            0.471550
                                      0.683370 0.354513
                                                         0.093081
                                                                   0.093081
    TCGA.EL.A3T9.THCA.C6_
                            0.489268
                                      0.645087
                                               0.247726
                                                         0.172708
                                                                   0.172708
    TCGA.A2.A4S1.BRCA.C6_
                            0.450655
                                      0.643585
                                               0.259902
                                                         0.171785
                                                                   0.171785
    TCGA.AR.A2LJ.BRCA.C6_
                            0.462621
                                     0.676615 0.476988 0.133939
                                                                   0.133939
    [540 rows x 351 columns]
[]: |#sum() total of the missing data
     #show count of the missing data in list of features
     #Dataset_1.isnull().sum()
     #shows total missing data in all dataset -> a number
    Dataset_1.isnull().sum().sum()
```

[]: 140

[]: #sum the missing data after cleaning cleaned_data.isnull().sum().sum()

[]: 2326

dtype: int64 IL7R_S3 dtype: int64

There are 140 missing data in original dataset and 2327 missing data in cleaned dataset

Imputation The mice imputations are calculated as per logical reasoning (linear regression) with data and its relation to other features. It's commonly used in situations where data is missing at random, and it can help prevent biases and improve the performance of subsequent data analysis, such as outlier detection or machine learning. I will do IsolationForest Algorithms later this method is the best method to use.

```
[]: | # Apply mice imputation (Multiple Imputation by Chained Equation)
     mice_imputer = IterativeImputer()
     for data_c in Dataset_1.columns[Dataset_1.isna().any()]:
         Dataset_1[[data_c]] = mice_imputer.fit_transform(Dataset_1[[data_c]])
    C:\Users\murui\AppData\Local\Temp\ipykernel_38176\3014042716.py:5:
    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/indexing.html#returning-a-view-versus-a-copy
      Dataset_1[[data_c]] = mice_imputer.fit_transform(Dataset_1[[data_c]])
    \label{local-Temp-ipy-ernel_38176-3014042716.py:5:} C:\Users\murui\AppData\Local\Temp\ipy-kernel\_38176\3014042716.py:5:
    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/indexing.html#returning-a-view-versus-a-copy
      Dataset_1[[data_c]] = mice_imputer.fit_transform(Dataset_1[[data_c]])
    C:\Users\murui\AppData\Local\Temp\ipykernel_38176\3014042716.py:5:
    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/indexing.html#returning-a-view-versus-a-copy
      Dataset_1[[data_c]] = mice_imputer.fit_transform(Dataset_1[[data_c]])
    C:\Users\murui\AppData\Local\Temp\ipykernel 38176\3014042716.py:5:
    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/indexing.html#returning-a-view-versus-a-copy
      Dataset_1[[data_c]] = mice_imputer.fit_transform(Dataset_1[[data_c]])
[]: mice_imputer_c = IterativeImputer()
     for data_c in cleaned data.columns[cleaned_data.isna().any()]:
         cleaned_data[[data_c]] = mice_imputer_c.
      →fit_transform(cleaned_data[[data_c]])
    check the missing data after imputation
[]: Dataset_1.isnull().values.any()
[]: False
[]: cleaned_data.isnull().values.any()
[]: False
[]: Dataset_1.isnull().sum().sum()
[]: 0
[]: cleaned data.isnull().sum().sum()
[]: 0
    There is no missing data in dataset now
[]: Dataset 1
[]:
                            ACTL6A_S5 ADAM9_S2
                                                ADAMTS1_S5 ADCY7_S3 AIMP2_S5
     TCGA.HF.7136.STAD.C1_
                             0.592349
                                      0.628634
                                                   0.570785 0.536637
                                                                       0.509823
     TCGA.EW.A10Z.BRCA.C1_
                             0.616708 0.589806
                                                   0.546915 0.522103 0.523893
     TCGA.EY.A1GL.UCEC.C1_
                             0.591583 0.601375
                                                   0.530573 0.470164 0.573793
     TCGA.EB.A5FP.SKCM.C1_
                             0.604189
                                      0.586198
                                                   0.566644 0.523076 0.575625
     TCGA.D1.A16D.UCEC.C1_
                                                   0.587917 0.533486 0.540958
                             0.545903
                                      0.632497
     TCGA.43.2581.LUSC.C6_
                             0.544662 0.620647
                                                  0.575653 0.557788 0.515838
```

```
TCGA.SH.A7BC.MESO.C6
                       0.527214
                                 0.635277
                                             0.626745
                                                       0.563070 0.503132
TCGA.EL.A3T9.THCA.C6
                       0.538555
                                 0.600622
                                             0.599145
                                                       0.549116
                                                                 0.533807
TCGA.A2.A4S1.BRCA.C6_
                       0.513619
                                 0.599382
                                             0.589908
                                                       0.543182
                                                                 0.478895
TCGA.AR.A2LJ.BRCA.C6_
                       0.540358
                                 0.551918
                                             0.526153
                                                       0.489545
                                                                 0.518348
                      ALKBH7_S5
                                 ALOX5AP_S3 AMPD3_S3 APITD1_S5
                                                                  APOC1_S3
                       0.462218
                                   0.443087 0.482923
                                                        0.418519
TCGA.HF.7136.STAD.C1_
                                                                  0.483556 \
TCGA.EW.A10Z.BRCA.C1_
                       0.545416
                                   0.518862 0.428246
                                                        0.447287
                                                                  0.588167
TCGA.EY.A1GL.UCEC.C1
                       0.560062
                                   0.408029 0.529847
                                                        0.516928
                                                                  0.500291
TCGA.EB.A5FP.SKCM.C1_
                       0.497918
                                   0.362422 0.428469
                                                        0.544391
                                                                  0.580780
TCGA.D1.A16D.UCEC.C1
                       0.556670
                                   0.518468 0.510708
                                                        0.488154
                                                                  0.585870
TCGA.43.2581.LUSC.C6_
                       0.488698
                                   0.592145 0.510097
                                                        0.408028
                                                                  0.572360
TCGA.SH.A7BC.MESO.C6_
                       0.523583
                                                        0.417098
                                                                  0.594076
                                   0.550000 0.501574
TCGA.EL.A3T9.THCA.C6_
                       0.514959
                                   0.532856 0.477059
                                                        0.474861
                                                                  0.471344
TCGA.A2.A4S1.BRCA.C6_
                       0.507401
                                   0.570468 0.483158
                                                        0.441637
                                                                  0.463836
TCGA.AR.A2LJ.BRCA.C6_
                       0.603053
                                   0.517177 0.453269
                                                        0.484431
                                                                  0.650400
                         WIPF1_S3
                                   WNT2B_S2
                                             WNT8B_S2
                                                        WSB2_S5
                                                                 ZWILCH_S5
TCGA.HF.7136.STAD.C1_
                         0.557671
                                   0.348506 0.210016
                                                       0.629423
                                                                  0.515653
TCGA.EW.A10Z.BRCA.C1_
                         0.543131
                                   0.271636 0.215562
                                                       0.588503
                                                                  0.520022
TCGA.EY.A1GL.UCEC.C1_
                         0.537821 0.370267 0.256229
                                                       0.626342
                                                                  0.500481
TCGA.EB.A5FP.SKCM.C1_
                         0.635673
                                   0.360680 0.261153
                                                       0.612561
                                                                  0.564331
TCGA.D1.A16D.UCEC.C1 ...
                         0.533510
                                   0.332906 0.129106
                                                       0.609040
                                                                  0.482094
                            •••
TCGA.43.2581.LUSC.C6 ...
                         0.584858
                                   0.256580 0.154807
                                                       0.574657
                                                                  0.465805
TCGA.SH.A7BC.MESO.C6_
                         0.580386
                                   0.560368 0.185317
                                                       0.567794
                                                                  0.471550
TCGA.EL.A3T9.THCA.C6_ ...
                         0.587950
                                   0.286881 0.189631
                                                       0.562508
                                                                  0.489268
TCGA.A2.A4S1.BRCA.C6_ ...
                         0.601901
                                   0.340524 0.171785
                                                       0.541964
                                                                  0.450655
TCGA.AR.A2LJ.BRCA.C6_
                         0.563845
                                   0.215693 0.201434
                                                       0.558991
                                                                  0.462621
                        ZYX_S2
                                 MMP3_S2
                                            PLG_S5
                                                     RGS8_S5
                                                              Subgroup
TCGA.HF.7136.STAD.C1_
                      0.664831
                                0.548405
                                          0.144132
                                                    0.156693
                                                                    C1
TCGA.EW.A10Z.BRCA.C1_
                      0.661331
                                0.488972
                                          0.129630
                                                    0.147665
                                                                    C1
TCGA.EY.A1GL.UCEC.C1_
                      0.650543
                                0.602704
                                          0.236607
                                                    0.236607
                                                                    C1
TCGA.EB.A5FP.SKCM.C1_
                      0.620690
                                0.457935
                                                                    C1
                                          0.261153
                                                    0.261153
TCGA.D1.A16D.UCEC.C1
                      0.670960
                                0.389138 0.282479
                                                    0.151172
                                                                    C1
                                                                    C6
TCGA.43.2581.LUSC.C6
                      0.654632
                                0.372903
                                          0.098287
                                                    0.098287
TCGA.SH.A7BC.MESO.C6_
                      0.683370
                                0.354513 0.093081
                                                    0.093081
                                                                    C6
TCGA.EL.A3T9.THCA.C6
                      0.645087
                                0.247726
                                          0.172708
                                                    0.172708
                                                                    C6
TCGA.A2.A4S1.BRCA.C6_
                      0.643585
                                0.259902
                                          0.171785
                                                    0.171785
                                                                    C6
TCGA.AR.A2LJ.BRCA.C6
                      0.676615 0.476988 0.133939
                                                    0.133939
                                                                    C6
```

[540 rows x 441 columns]

[]: cleaned_data

```
[]:
                            ACTL6A_S5
                                      ADAM9_S2
                                                ADAMTS1_S5
                                                            ADCY7_S3 AIMP2_S5
    TCGA.HF.7136.STAD.C1_
                            0.592349
                                      0.628634
                                                  0.570785
                                                            0.536637
                                                                      0.509823
    TCGA.EW.A10Z.BRCA.C1
                            0.616708
                                      0.589806
                                                  0.546915
                                                            0.522103 0.523893
    TCGA.EY.A1GL.UCEC.C1_
                                                  0.530573 0.470164 0.573793
                            0.591583
                                      0.601375
    TCGA.EB.A5FP.SKCM.C1
                            0.604189
                                      0.586198
                                                  0.566644
                                                            0.523076
                                                                      0.575625
    TCGA.D1.A16D.UCEC.C1_
                            0.545903
                                      0.632497
                                                  0.587917
                                                            0.533486 0.540958
    TCGA.43.2581.LUSC.C6_
                            0.544662
                                      0.620647
                                                  0.575653
                                                            0.557788 0.515838
    TCGA.SH.A7BC.MESO.C6
                                                  0.626745 0.563070 0.503132
                            0.527214
                                      0.635277
    TCGA.EL.A3T9.THCA.C6_
                            0.538555
                                      0.600622
                                                  0.599145
                                                            0.549116 0.533807
    TCGA.A2.A4S1.BRCA.C6_
                            0.513619
                                      0.599382
                                                  0.589908
                                                            0.543182
                                                                      0.478895
    TCGA.AR.A2LJ.BRCA.C6
                            0.540358
                                      0.551918
                                                  0.526153
                                                            0.489545 0.518348
                            ALKBH7_S5
                                      ALOX5AP_S3 AMPD3_S3
                                                            APITD1_S5
                                                                       APOC1_S3
    TCGA.HF.7136.STAD.C1_
                            0.462218
                                         0.443087 0.482923
                                                             0.418519
                                                                       0.483556
    TCGA.EW.A10Z.BRCA.C1_
                            0.545416
                                         0.518862 0.428246
                                                             0.447287
                                                                       0.588167
    TCGA.EY.A1GL.UCEC.C1_
                                         0.408029 0.529847
                                                             0.516928
                            0.560062
                                                                       0.500291
    TCGA.EB.A5FP.SKCM.C1_
                            0.497918
                                         0.362422 0.428469
                                                             0.544391
                                                                       0.580780
    TCGA.D1.A16D.UCEC.C1_
                            0.556670
                                         0.518468 0.510708
                                                             0.488154
                                                                       0.585870
                               •••
    TCGA.43.2581.LUSC.C6_
                            0.488698
                                         0.592145 0.510097
                                                             0.408028
                                                                       0.572360
    TCGA.SH.A7BC.MESO.C6
                            0.523583
                                        0.550000 0.501574
                                                             0.417098
                                                                       0.594076
    TCGA.EL.A3T9.THCA.C6_
                            0.514959
                                         0.532856 0.477059
                                                             0.474861
                                                                       0.471344
    TCGA.A2.A4S1.BRCA.C6_
                            0.507401
                                        0.570468 0.483158
                                                             0.441637
                                                                        0.463836
    TCGA.AR.A2LJ.BRCA.C6_
                                                             0.484431
                            0.603053
                                        0.517177 0.453269
                                                                       0.650400
                              WDR77_S5
                                        WIPF1_S3 WNT2B_S2
                                                            WNT8B_S2
                                                                        WSB2_S5
    TCGA.HF.7136.STAD.C1_ ...
                              0.591241
                                         0.557671 0.348506
                                                            0.210016
                                                                      0.629423 \
    TCGA.EW.A10Z.BRCA.C1_ ...
                              0.544296
                                        0.543131 0.271636
                                                            0.215562
                                                                      0.588503
    TCGA.EY.A1GL.UCEC.C1_ ... 0.564828
                                        0.537821 0.370267
                                                            0.256229
                                                                      0.626342
    TCGA.EB.A5FP.SKCM.C1_ ...
                              0.582566
                                        0.635673 0.360680
                                                            0.261153 0.612561
    TCGA.D1.A16D.UCEC.C1_ ...
                                                            0.129106 0.609040
                              0.592322
                                        0.533510 0.332906
    TCGA.43.2581.LUSC.C6_ ...
                              0.524690
                                        0.584858 0.256580
                                                            0.154807
                                                                      0.574657
    TCGA.SH.A7BC.MESO.C6 ... 0.520420
                                                            0.185317
                                        0.580386 0.352507
                                                                      0.567794
    TCGA.EL.A3T9.THCA.C6_ ...
                              0.522743
                                        0.587950 0.286881
                                                            0.189631
                                                                      0.562508
    TCGA.A2.A4S1.BRCA.C6_ ...
                              0.524518
                                         0.601901 0.340524
                                                            0.171785
                                                                      0.541964
    TCGA.AR.A2LJ.BRCA.C6_
                              0.515673
                                                            0.201434 0.558991
                                        0.563845 0.215693
                            ZWILCH_S5
                                         ZYX_S2
                                                 MMP3_S2
                                                             PLG_S5
                                                                     RGS8_S5
    TCGA.HF.7136.STAD.C1_
                            0.515653
                                      0.664831
                                                0.548405
                                                          0.144132
                                                                    0.156693
    TCGA.EW.A10Z.BRCA.C1_
                                      0.661331
                                                0.488972
                                                          0.129630
                                                                     0.147665
                            0.520022
    TCGA.EY.A1GL.UCEC.C1_
                            0.500481
                                      0.650543
                                                0.602704
                                                          0.236607
                                                                     0.236607
    TCGA.EB.A5FP.SKCM.C1_
                            0.564331
                                      0.620690
                                                0.457935
                                                          0.261153
                                                                     0.261153
    TCGA.D1.A16D.UCEC.C1_
                            0.482094
                                      0.670960
                                                0.389138
                                                          0.282479
                                                                    0.151172
                            0.465805
    TCGA.43.2581.LUSC.C6_
                                      0.654632 0.372903
                                                          0.098287
                                                                    0.098287
```

```
TCGA.SH.A7BC.MESO.C6_ 0.471550 0.683370 0.354513 0.093081 0.093081 TCGA.EL.A3T9.THCA.C6_ 0.489268 0.645087 0.247726 0.172708 0.172708 TCGA.A2.A4S1.BRCA.C6_ 0.450655 0.643585 0.259902 0.171785 0.171785 TCGA.AR.A2LJ.BRCA.C6_ 0.462621 0.676615 0.476988 0.133939 0.133939 [540 rows x 440 columns]
```

Using IsolationForest Algortims to Estimate Outliers Using machine learning method to find the outliers which suit to high dimensional data

```
[]: data = Dataset_1
     # Separate features and labelling
     X = data.drop(['Subgroup'], axis=1) # 440 features
     y = data['Subgroup'] # subgroup
     # create Isolation Forest model and training
     model = IsolationForest(contamination=0.05, random state=42)
     model.fit(X)
     # Predict outliers
     y_pred = model.predict(X)
     outlier_indices = X.index[y_pred == -1]
     # let outliers to NaN
     X cleaned = X.copy()
     X_cleaned.loc[outlier_indices] = None
     cleaned data 2 = pd.concat([X cleaned, y], axis=1)
     cleaned_group_labels = cleaned_data_2['Subgroup']
     cleaned data 2 = cleaned data 2.drop(outlier indices)
     #cleaned_data.to_csv('cleaned_data.csv', index=False)
```

```
[]: outlier_indices.value_counts().sum()
```

[]: 27

```
[]: cleaned_data_2
```

```
[]:
                          ACTL6A_S5 ADAM9_S2
                                              ADAMTS1_S5 ADCY7_S3 AIMP2_S5
                           0.592349 0.628634
                                                0.570785 0.536637 0.509823 \
    TCGA.HF.7136.STAD.C1
    TCGA.EW.A10Z.BRCA.C1_
                           0.616708 0.589806
                                                0.546915 0.522103 0.523893
    TCGA.EY.A1GL.UCEC.C1_
                           0.591583 0.601375
                                                0.530573 0.470164 0.573793
    TCGA.D1.A16D.UCEC.C1_
                           0.545903 0.632497
                                                0.587917 0.533486 0.540958
    TCGA.R6.A8W8.ESCA.C1_
                           0.604241 0.683214
                                                0.518696 0.568172 0.529827
```

•••	•••	•••		•••		
TCGA.43.2581.LUSC.C6_	0.544662	0.620647	0.575653	0.557788	0.515838	
TCGA.SH.A7BC.MESO.C6_	0.527214	0.635277	0.626745	0.563070	0.503132	
TCGA.EL.A3T9.THCA.C6	0.538555	0.600622	0.599145	0.549116	0.533807	
TCGA.A2.A4S1.BRCA.C6_	0.513619	0.599382	0.589908	0.543182	0.478895	
TCGA.AR.A2LJ.BRCA.C6_	0.540358	0.551918	0.526153	0.489545	0.518348	
TOUR. RIC. RZES . DICOR . GO_	0.04000	0.001010	0.020100	0.400040	0.010040	
	ALKBH7_S5	ALOX5AP_S3	AMPD3_S3	APITD1_S5	APOC1_S3	
TCGA.HF.7136.STAD.C1_	0.462218	0.443087	0.482923	0.418519	0.483556	\
TCGA.EW.A10Z.BRCA.C1_	0.545416	0.518862	0.428246	0.447287	0.588167	`
TCGA.EY.A1GL.UCEC.C1_	0.560062	0.408029	0.529847	0.516928	0.500291	
TCGA.D1.A16D.UCEC.C1_	0.556670	0.518468	0.510708	0.488154		
_						
TCGA.R6.A8W8.ESCA.C1_	0.508240	0.425075	0.463861	0.503452	0.447875	
TCGA.43.2581.LUSC.C6_	 0.488698	 0.592145	0.510097	 0.408028	0.572360	
-						
TCGA.SH.A7BC.MESO.C6_	0.523583	0.550000	0.501574	0.417098	0.594076	
TCGA.EL.A3T9.THCA.C6_	0.514959	0.532856	0.477059	0.474861	0.471344	
TCGA.A2.A4S1.BRCA.C6_	0.507401	0.570468	0.483158	0.441637	0.463836	
TCGA.AR.A2LJ.BRCA.C6_	0.603053	0.517177	0.453269	0.484431	0.650400	
	WIPF1_S	3 WNT2B_S2	WNT8B_S2	WSB2_S5	ZWILCH_S5	
TOOL HE 7126 GTAD OI	_	_	_	0.629423	0.515653	`
TCGA.HF.7136.STAD.C1_	0.55767		0.210016			\
TCGA.EW.A1OZ.BRCA.C1_	0.54313		0.215562	0.588503	0.520022	
TCGA.EY.A1GL.UCEC.C1_	0.53782		0.256229	0.626342	0.500481	
TCGA.D1.A16D.UCEC.C1_	0.53351		0.129106	0.609040	0.482094	
TCGA.R6.A8W8.ESCA.C1_	0.52407	2 0.318327	0.246978	0.597891	0.568461	
TCGA.43.2581.LUSC.C6_	0.58485	 8 0.256580	0.154807	 0.574657	0.465805	
-						
TCGA.SH.A7BC.MESO.C6_	0.58038		0.185317	0.567794	0.471550	
TCGA.EL.A3T9.THCA.C6_	0.58795		0.189631	0.562508	0.489268	
TCGA.A2.A4S1.BRCA.C6_	0.60190		0.171785	0.541964	0.450655	
TCGA.AR.A2LJ.BRCA.C6_	0.56384	5 0.215693	0.201434	0.558991	0.462621	
	ZYX_S2	MMP3 S2	PLG S5 F	RGS8_S5 Sul	bgroup	
TCGA.HF.7136.STAD.C1_	0.664831		.144132 0.		C1	
TCGA.EW.A10Z.BRCA.C1_				147665	C1	
TCGA.EY.A1GL.UCEC.C1_				236607	C1	
TCGA.D1.A16D.UCEC.C1_				151172	C1	
-						
TCGA.R6.A8W8.ESCA.C1_		0.570034 0	.186503 0.	. 183873	C1	
TCGA.43.2581.LUSC.C6_	0.654632	0.372903 0	 .098287 0.	 .098287	C6	
TCGA.SH.A7BC.MESO.C6_				.093081	C6	
TCGA.EL.A3T9.THCA.C6_				172708	C6	
TCGA.A2.A4S1.BRCA.C6_				171785	C6	
-				.133939	C6	
TCGA.AR.A2LJ.BRCA.C6_	0.070015	0.4/0300 0	. 133939 0.	100303	CO	

[513 rows x 441 columns]

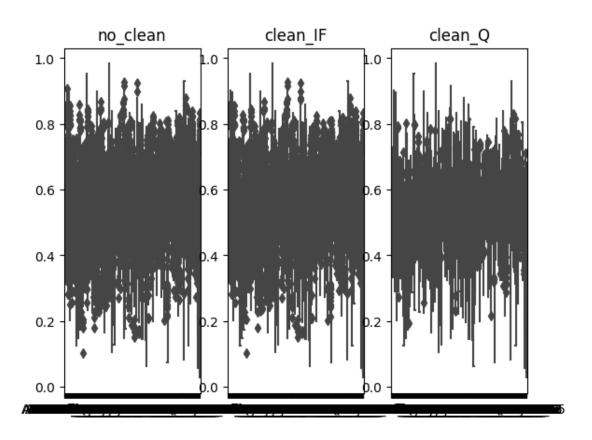
[]: cleaned_data

```
[]:
                            ACTL6A S5
                                      ADAM9_S2
                                                ADAMTS1_S5 ADCY7_S3 AIMP2_S5
    TCGA.HF.7136.STAD.C1_
                            0.592349
                                      0.628634
                                                  0.570785
                                                            0.536637
                                                                      0.509823 \
    TCGA.EW.A10Z.BRCA.C1
                            0.616708
                                      0.589806
                                                  0.546915
                                                            0.522103 0.523893
    TCGA.EY.A1GL.UCEC.C1_
                            0.591583
                                      0.601375
                                                  0.530573 0.470164 0.573793
    TCGA.EB.A5FP.SKCM.C1_
                            0.604189
                                      0.586198
                                                  0.566644
                                                            0.523076 0.575625
    TCGA.D1.A16D.UCEC.C1_
                            0.545903
                                      0.632497
                                                  0.587917
                                                            0.533486 0.540958
    TCGA.43.2581.LUSC.C6_
                            0.544662
                                      0.620647
                                                  0.575653
                                                            0.557788 0.515838
                            0.527214
                                                            0.563070 0.503132
    TCGA.SH.A7BC.MESO.C6_
                                      0.635277
                                                  0.626745
    TCGA.EL.A3T9.THCA.C6
                            0.538555
                                                  0.599145
                                                            0.549116 0.533807
                                      0.600622
    TCGA.A2.A4S1.BRCA.C6_
                            0.513619
                                      0.599382
                                                  0.589908
                                                            0.543182
                                                                      0.478895
    TCGA.AR.A2LJ.BRCA.C6_
                            0.540358
                                      0.551918
                                                  0.526153 0.489545 0.518348
                            ALKBH7_S5
                                      ALOX5AP_S3 AMPD3_S3
                                                            APITD1 S5
                                                                       APOC1 S3
    TCGA.HF.7136.STAD.C1_
                            0.462218
                                        0.443087 0.482923
                                                             0.418519
                                                                       0.483556
    TCGA.EW.A10Z.BRCA.C1_
                            0.545416
                                        0.518862 0.428246
                                                             0.447287
                                                                        0.588167
    TCGA.EY.A1GL.UCEC.C1_
                            0.560062
                                        0.408029 0.529847
                                                             0.516928
                                                                       0.500291
    TCGA.EB.A5FP.SKCM.C1
                            0.497918
                                        0.362422 0.428469
                                                             0.544391
                                                                       0.580780
    TCGA.D1.A16D.UCEC.C1_
                            0.556670
                                        0.518468 0.510708
                                                             0.488154
                                                                       0.585870
                               •••
                                                                  •••
    TCGA.43.2581.LUSC.C6_
                            0.488698
                                        0.592145 0.510097
                                                             0.408028
                                                                       0.572360
    TCGA.SH.A7BC.MESO.C6_
                                                             0.417098
                                                                       0.594076
                            0.523583
                                        0.550000 0.501574
    TCGA.EL.A3T9.THCA.C6_
                            0.514959
                                        0.532856 0.477059
                                                             0.474861
                                                                       0.471344
    TCGA.A2.A4S1.BRCA.C6_
                            0.507401
                                        0.570468 0.483158
                                                             0.441637
                                                                        0.463836
    TCGA.AR.A2LJ.BRCA.C6_
                                                             0.484431
                            0.603053
                                        0.517177 0.453269
                                                                       0.650400
                              WDR77_S5
                                        WIPF1_S3 WNT2B_S2
                                                            WNT8B_S2
                                                                        WSB2_S5
    TCGA.HF.7136.STAD.C1_
                              0.591241
                                        0.557671 0.348506
                                                            0.210016
                                                                      0.629423
    TCGA.EW.A10Z.BRCA.C1
                              0.544296
                                        0.543131 0.271636
                                                            0.215562 0.588503
    TCGA.EY.A1GL.UCEC.C1_
                              0.564828
                                        0.537821 0.370267
                                                            0.256229
                                                                      0.626342
    TCGA.EB.A5FP.SKCM.C1_
                              0.582566
                                        0.635673 0.360680
                                                            0.261153
                                                                      0.612561
    TCGA.D1.A16D.UCEC.C1_
                              0.592322
                                        0.533510 0.332906 0.129106 0.609040
                              0.524690
    TCGA.43.2581.LUSC.C6_
                                        0.584858 0.256580
                                                            0.154807 0.574657
    TCGA.SH.A7BC.MESO.C6_ ... 0.520420
                                                            0.185317
                                        0.580386 0.352507
                                                                      0.567794
    TCGA.EL.A3T9.THCA.C6_ ...
                              0.522743
                                        0.587950 0.286881
                                                            0.189631
                                                                      0.562508
    TCGA.A2.A4S1.BRCA.C6_ ...
                              0.524518
                                        0.601901
                                                  0.340524
                                                            0.171785
                                                                      0.541964
    TCGA.AR.A2LJ.BRCA.C6_
                              0.515673
                                        0.563845 0.215693
                                                            0.201434 0.558991
                            ZWILCH_S5
                                        ZYX_S2
                                                 MMP3_S2
                                                             PLG_S5
                                                                     RGS8_S5
    TCGA.HF.7136.STAD.C1_
                            0.515653
                                      0.664831
                                                0.548405
                                                          0.144132
                                                                    0.156693
                            0.520022
                                      0.661331
                                                0.488972
                                                          0.129630
                                                                    0.147665
    TCGA.EW.A1OZ.BRCA.C1_
    TCGA.EY.A1GL.UCEC.C1_
                            0.500481
                                      0.650543
                                                0.602704
                                                          0.236607
                                                                    0.236607
    TCGA.EB.A5FP.SKCM.C1_
                            0.564331
                                      0.620690
                                                0.457935
                                                          0.261153
                                                                    0.261153
    TCGA.D1.A16D.UCEC.C1_
                            0.482094
                                      0.670960
                                                0.389138
                                                          0.282479
                                                                    0.151172
```

```
TCGA.43.2581.LUSC.C6
                             0.465805
                                        0.654632 0.372903
                                                            0.098287
                                                                       0.098287
     TCGA.SH.A7BC.MESO.C6
                             0.471550
                                        0.683370
                                                  0.354513
                                                            0.093081
                                                                       0.093081
     TCGA.EL.A3T9.THCA.C6_
                             0.489268
                                        0.645087
                                                  0.247726
                                                            0.172708
                                                                       0.172708
     TCGA.A2.A4S1.BRCA.C6_
                             0.450655
                                                  0.259902
                                        0.643585
                                                            0.171785
                                                                       0.171785
     TCGA.AR.A2LJ.BRCA.C6_
                             0.462621
                                        0.676615
                                                  0.476988
                                                            0.133939
                                                                       0.133939
     [540 rows x 440 columns]
[]: cleaned_data_2[cleaned_data_2.columns[0:-1]].max().max()
[]: 0.983192666
[]: cleaned_data[cleaned_data.columns[0:-1]].max().max()
[]: 0.983192666
     cleaned_data_2[cleaned_data_2.columns[0:-1]].min().min()
[]: 0.026909471
    cleaned_data[cleaned_data.columns[0:-1]].min().min()
[]: 0.026909471
    It shows two type to clean data will not effect the min and max for the data
    Compare original data cleaned data by Quartile Algorithm and cleaned data by IsolationForest
    Algoriims
[]: #compare in the plot
     fig, axes = plt.subplots(1,3)
     sns.boxplot(data=Dataset 1, ax=axes[0])
     sns.boxplot(data=cleaned data 2, ax=axes[1])
     sns.boxplot(data=cleaned_data, ax=axes[2])
     axes[0].set_title('no_clean')
```

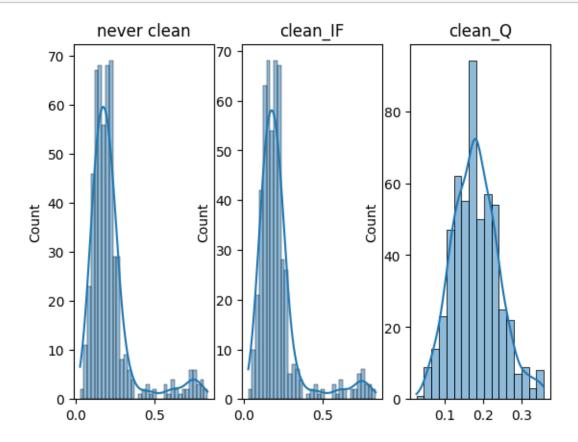
[]: Text(0.5, 1.0, 'clean_Q')

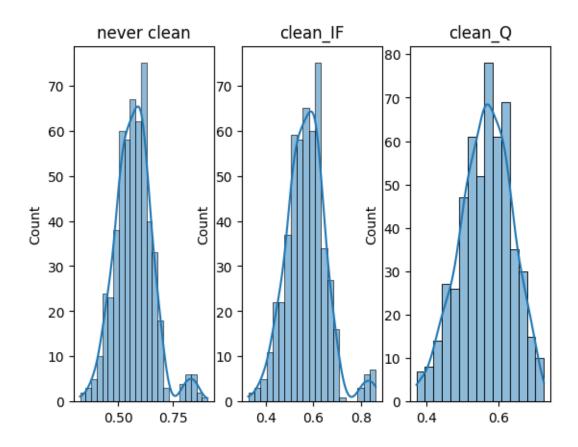
axes[1].set_title('clean_IF')
axes[2].set_title('clean_Q')

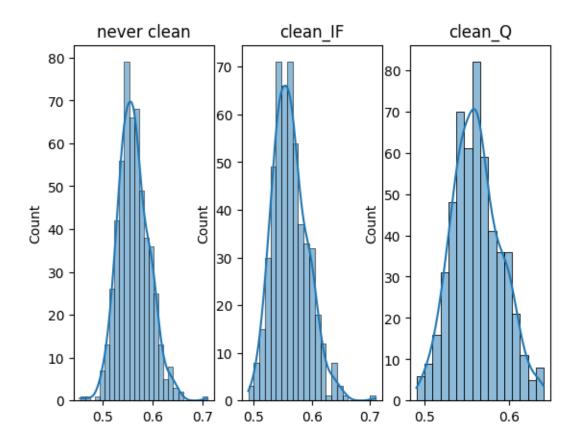


```
[]: #plot for some features for have check
     fig, axes = plt.subplots(1,3)
     sns.histplot(Dataset_1[['PLG_S5']],kde=True, legend=False, ax=axes[0])
     sns.histplot(cleaned_data_2[['PLG_S5']],kde=True, legend=False, ax=axes[1])
     sns.histplot(cleaned_data[['PLG_S5']],kde=True, legend=False, ax=axes[2])
     axes[0].set title('never clean')
     axes[1].set_title('clean_IF')
     axes[2].set_title('clean_Q')
     fig, axes = plt.subplots(1,3)
     sns.histplot(Dataset_1[['APOC1 S3']],kde=True, legend=False, ax=axes[0])
     sns.histplot(cleaned_data_2[['APOC1_S3']],kde=True, legend=False, ax=axes[1])
     sns.histplot(cleaned_data[['APOC1_S3']],kde=True, legend=False, ax=axes[2])
     axes[0].set_title('never clean')
     axes[1].set_title('clean_IF')
     axes[2].set_title('clean_Q')
     fig, axes = plt.subplots(1,3)
     sns.histplot(Dataset_1[['ACTL6A_S5']],kde=True, legend=False, ax=axes[0])
     sns.histplot(cleaned_data_2[['ACTL6A_S5']],kde=True, legend=False, ax=axes[1])
     sns.histplot(cleaned_data[['ACTL6A_S5']],kde=True, legend=False, ax=axes[2])
     axes[0].set_title('never clean')
     axes[1].set_title('clean_IF')
```

axes[2].set_title('clean_Q')
plt.show()







Because Isolation Forest Algorithm is inherently a method for detecting outliers and is well-suited for high-dimensional data, I believe the outliers it finds are more reasonable. In high-dimensional datasets, challenges can be related to what's known as the 'curse of dimensionality,' making traditional outlier detection methods less effective. Isolation Forest Algorithm, which predicts outliers through random sampling while considering all the features together, is more suitable than calcuate it one by one. It doesn't just look at a single feature to assess the range of each sample in that feature, as single-feature-based methods do.

Some points may appear as outliers when viewed in the context of a single feature, but when considering all the features collectively, they don't exhibit apparent outlier behaviour. I believe that this is why visualisations of the Isolation Forest's result may sometimes make some points seem like outliers. The reason is that these visualisations show the data distribution by breaking it down feature by feature, even in high-dimensional data with 440

Also, outliers may contain useful information, and removing outliers should be done carefully rather than across the board, so I think the isolated forest cleaned data is more in line with eliminating the data that needs to be released rather than across the board, like traditional quartile algorithms.

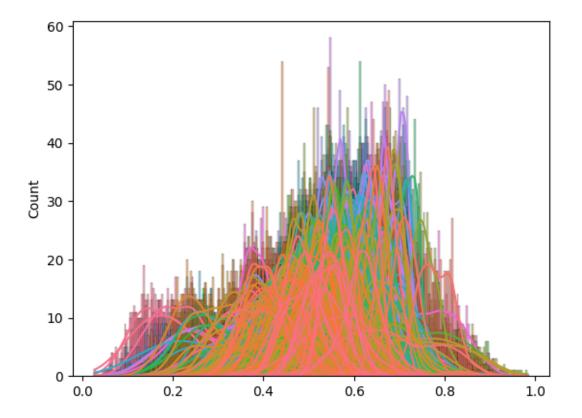
I chose to remove the outliers because they have a significant impact on models like PCA, which is a dimensionality reduction model, and they can lead to model instability and affect the performance of machine learning algorithms.

Conclusion: Again, it's a matter of dimensionality, and high-dimensional arrays make many tradi-

tional methods less applicable.

c. Normalisation I cleaned the outliers by isolated forest algorithms because that is more suitable for high-dimensional arrays. I observed that the maximum and minimum values did not change in both cleaning methods.

```
[]: #formal the data cause the subgroup are object cannot calculate
     features = Dataset 1.columns[0:-1]
     x = cleaned_data_2.loc[:,features].values
     y = Dataset_1.loc[:,['Subgroup']].values
[]: x
[]: array([[0.59234916, 0.62863443, 0.57078532, ..., 0.54840526, 0.14413165,
             0.15669266],
            [0.61670755, 0.58980588, 0.54691471, ..., 0.48897231, 0.12963003,
             0.14766489],
            [0.59158323, 0.60137506, 0.53057323, ..., 0.60270384, 0.23660706,
             0.23660706],
            [0.53855485, 0.60062186, 0.5991449, ..., 0.24772623, 0.17270843,
             0.17270843],
            [0.51361922, 0.59938179, 0.58990848, ..., 0.25990241, 0.1717848,
             0.1717848 ],
            [0.54035758, 0.55191784, 0.52615256, ..., 0.47698793, 0.13393862,
             0.13393862]])
[]: #check data type
     x.dtype
[]: dtype('float64')
[]: Dataset_max = np.amax(x)
     Dataset_max
[]: 0.983192666
[]: Dataset_min = np.amin(x)
     Dataset_min
[]: 0.026909471
    All data between 0 to 1
    plot the data for observation
[]: sns.histplot(x,kde=True,legend=False)
     plt.show()
```



Checking distribution:

Data does not follow a normal distribution

C:\Users\murui\AppData\Roaming\Python\Python311\sitepackages\scipy\stats_morestats.py:1816: UserWarning: p-value may not be
accurate for N > 5000.
 warnings.warn("p-value may not be accurate for N > 5000.")

Because the data does not follow a normal distribution, we will do the NMF which is only operate positive data and I have drop the outliers, I choose MinMaxScaler rather than StandardScaler

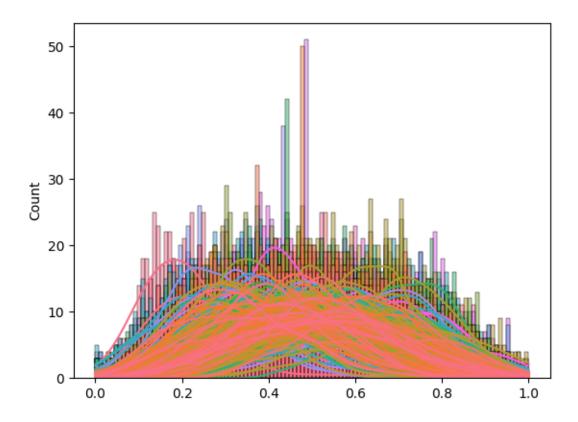
```
[]: #apply MinMax
scaler = MinMaxScaler()
X_scaled = scaler.fit_transform(x)
```

```
[]: X_scaled
[]: array([[0.46420631, 0.55301778, 0.55043053, ..., 0.67779844, 0.14538856,
            0.22350296],
            [0.5749009, 0.40554712, 0.48263009, ..., 0.5958461, 0.12740246,
            0.20524521],
            [0.4607256, 0.44948682, 0.43621486, ..., 0.75267098, 0.26008414,
            0.38512169],
            [0.21974274, 0.44662618, 0.63098116, ..., 0.26319088, 0.18083183,
            0.25589323],
            [0.10642494, 0.4419164, 0.60474664, ..., 0.27998066, 0.17968626,
            0.25402527],
            [0.22793511, 0.26164852, 0.42365869, ..., 0.57932079, 0.13274633,
            0.17748523]])
[]: np.amax(X_scaled)
[]: 1.0000000000000004
[]: np.amin(X_scaled)
[]: 0.0
[]: X_scaled.shape
[]: (513, 440)
    Formatting data with index and column to facilitate later use of standardised data
[ ]: Dataset_sd = pd.DataFrame(data=X_scaled,
                               columns=cleaned_data_2.columns[0:-1],
                               index=cleaned_data_2.index)
     Dataset_sd = pd.concat([Dataset_sd,cleaned_data_2[['Subgroup']]], axis=1)
     Dataset_sd
[]:
                                                ADAMTS1_S5 ADCY7_S3 AIMP2_S5
                            ACTL6A_S5 ADAM9_S2
                             0.464206 0.553018
                                                   0.550431 0.422275 0.401367 \
     TCGA.HF.7136.STAD.C1_
                             0.574901 0.405547
                                                   0.482630 0.363034 0.470152
     TCGA.EW.A10Z.BRCA.C1_
     TCGA.EY.A1GL.UCEC.C1
                             0.460726 0.449487
                                                   0.436215 0.151328 0.714113
     TCGA.D1.A16D.UCEC.C1_
                             0.253135
                                      0.567689
                                                   0.599091 0.409430 0.553581
     TCGA.R6.A8W8.ESCA.C1_
                             0.518248
                                      0.760312
                                                   0.402481 0.550812 0.499165
     TCGA.43.2581.LUSC.C6_
                             0.247497
                                      0.522681
                                                   0.564256 0.508487 0.430773
     TCGA.SH.A7BC.MESO.C6_
                             0.168205 0.578246
                                                   0.709375 0.530017 0.368653
     TCGA.EL.A3T9.THCA.C6_
                                                   0.630981 0.473138 0.518621
                             0.219743 0.446626
     TCGA.A2.A4S1.BRCA.C6
                             0.106425 0.441916
                                                   0.604747 0.448950 0.250162
     TCGA.AR.A2LJ.BRCA.C6
                             0.227935 0.261649
                                                   0.423659 0.230325 0.443044
```

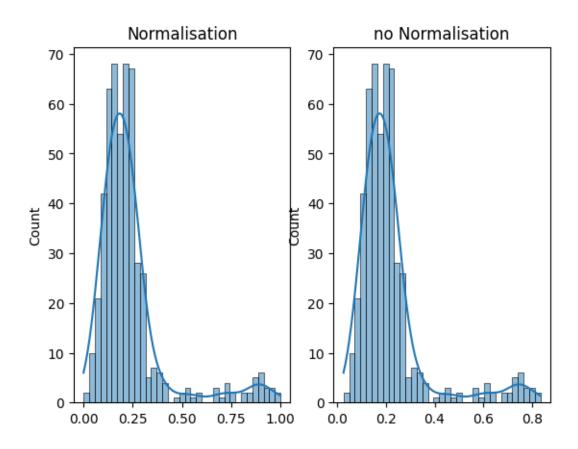
```
ALOX5AP_S3
                                                        APITD1_S5
                                              AMPD3_S3
                                                                   APOC1_S3
                       ALKBH7_S5
TCGA.HF.7136.STAD.C1_
                        0.176712
                                    0.390964 0.364345
                                                         0.395560
                                                                   0.295254
                                                         0.514111
TCGA.EW.A10Z.BRCA.C1_
                        0.514156
                                    0.656861 0.190290
                                                                   0.489703
TCGA.EY.A1GL.UCEC.C1_
                        0.573561
                                    0.267944 0.513717
                                                         0.801093
                                                                   0.326360
TCGA.D1.A16D.UCEC.C1_
                        0.559803
                                    0.655478 0.452793
                                                         0.682517
                                                                   0.485432
TCGA.R6.A8W8.ESCA.C1_
                                                         0.745557
                                                                   0.228929
                        0.363376
                                    0.327758 0.303664
                           •••
                                                              •••
TCGA.43.2581.LUSC.C6
                                                         0.352329
                        0.284113
                                    0.914014 0.450848
                                                                   0.460321
TCGA.SH.A7BC.MESO.C6_
                        0.425604
                                    0.766126 0.423715
                                                         0.389704
                                                                   0.500686
TCGA.EL.A3T9.THCA.C6_
                        0.390625
                                    0.705965 0.345678
                                                         0.627741
                                                                   0.272554
TCGA.A2.A4S1.BRCA.C6_
                        0.359972
                                    0.837949 0.365091
                                                         0.490826
                                                                   0.258597
TCGA.AR.A2LJ.BRCA.C6_
                        0.747928
                                    0.650948 0.269944
                                                         0.667177
                                                                   0.605381
                         WIPF1_S3
                                    WNT2B_S2 WNT8B_S2
                                                         WSB2_S5
                                                                  ZWILCH_S5
TCGA.HF.7136.STAD.C1_
                          0.553260
                                    0.396224 0.387375
                                                        0.646382
                                                                   0.555027
TCGA.EW.A10Z.BRCA.C1_ ...
                                    0.219441 0.401239
                          0.481381
                                                        0.454258
                                                                   0.574876
TCGA.EY.A1GL.UCEC.C1_ ...
                         0.455133
                                    0.446272 0.502915
                                                        0.631917
                                                                   0.486097
                         0.433820
                                    0.360347 0.185082
TCGA.D1.A16D.UCEC.C1_ ...
                                                        0.550679
                                                                   0.402559
TCGA.R6.A8W8.ESCA.C1_ ...
                          0.387164
                                   0.326819 0.479786
                                                        0.498336
                                                                   0.794955
TCGA.43.2581.LUSC.C6_ ...
                                   0.184814 0.249341
                                                        0.389247
                                                                   0.328550
                          0.687661
TCGA.SH.A7BC.MESO.C6_
                          0.665557
                                    0.883463 0.325622
                                                        0.357024
                                                                   0.354655
TCGA.EL.A3T9.THCA.C6 ...
                          0.702948 0.254499 0.336407
                                                        0.332205
                                                                   0.435153
TCGA.A2.A4S1.BRCA.C6_
                          0.771916
                                    0.377868 0.291789
                                                        0.235748
                                                                   0.259721
TCGA.AR.A2LJ.BRCA.C6_ ... 0.583781 0.090782 0.365918
                                                        0.315691
                                                                   0.314086
                         ZYX_S2
                                  MMP3_S2
                                             PLG_S5
                                                      RGS8_S5
                                                               Subgroup
TCGA.HF.7136.STAD.C1_
                       0.510994
                                0.677798
                                          0.145389
                                                     0.223503
                                                                     C1
                       0.489773
                                                                     C1
TCGA.EW.A1OZ.BRCA.C1
                                0.595846
                                          0.127402
                                                     0.205245
TCGA.EY.A1GL.UCEC.C1_
                       0.424361
                                 0.752671
                                          0.260084
                                                     0.385122
                                                                     C1
                                                                     C1
TCGA.D1.A16D.UCEC.C1_
                       0.548159
                                 0.458184
                                           0.316978
                                                     0.212338
TCGA.R6.A8W8.ESCA.C1_
                       0.126130
                                 0.707623
                                          0.197941
                                                     0.278473
                                                                     C1
                       0.449154
                                0.435797 0.088529
                                                                     C6
TCGA.43.2581.LUSC.C6_
                                                     0.105384
TCGA.SH.A7BC.MESO.C6_
                       0.623405
                                 0.410439
                                           0.082071
                                                     0.094855
                                                                     C6
TCGA.EL.A3T9.THCA.C6
                       0.391279
                                0.263191
                                          0.180832
                                                     0.255893
                                                                     C6
TCGA.A2.A4S1.BRCA.C6_
                       0.382173
                                 0.279981
                                          0.179686
                                                     0.254025
                                                                     C6
TCGA.AR.A2LJ.BRCA.C6
                                                                     C6
                       0.582450
                                0.579321
                                          0.132746
                                                     0.177485
```

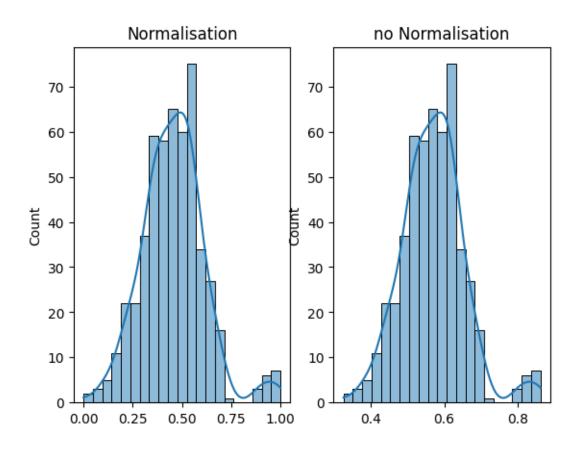
[513 rows x 441 columns]

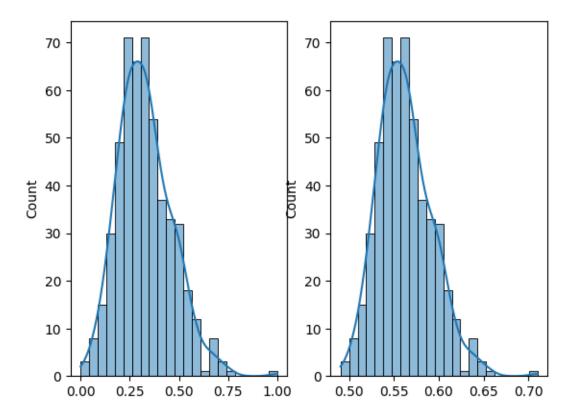
```
[]: sns.histplot(X_scaled,kde=True,legend=False)
plt.show()
```



```
[]: #plot for some features for have check
     fig, axes = plt.subplots(1,2)
     sns.histplot(Dataset_sd[['PLG_S5']],kde=True, legend=False, ax=axes[0])
     sns.histplot(cleaned_data_2[['PLG_S5']],kde=True, legend=False, ax=axes[1])
     axes[0].set_title('Normalisation')
     axes[1].set title('no Normalisation')
     fig, axes = plt.subplots(1,2)
     sns.histplot(Dataset_sd[['APOC1_S3']],kde=True, legend=False, ax=axes[0])
     sns.histplot(cleaned_data_2[['APOC1_S3']],kde=True, legend=False, ax=axes[1])
     axes[0].set_title('Normalisation')
     axes[1].set_title('no Normalisation')
     fig, axes = plt.subplots(1,2)
     sns.histplot(Dataset_sd[['ACTL6A_S5']],kde=True, legend=False, ax=axes[0])
     sns.histplot(cleaned_data_2[['ACTL6A_S5']],kde=True, legend=False, ax=axes[1])
     plt.show()
     axes[0].set_title('Normalisation')
     axes[1].set_title('no Normalisation')
```







[]: Text(0.5, 1.0, 'no Normalisation')

Conclusion: Outliers strongly influence the choice of normalisation method, as some normalisation models are strongly influenced by outliers. I am concerned about the maximum and minimum values and the outliers, and the data range.

1.1.2 Non-negative Matrix Factorization(NMF)

a. Application of NMF Format the dataset firstly, because the data using by NMF need to transform standard dataset

```
[]: # get dataset from standared dataset and format it.

Dataset_nmf = Dataset_sd[Dataset_sd.columns[0:-1]].T

Dataset_nmf
```

```
[]:
                 TCGA.HF.7136.STAD.C1_
                                          TCGA.EW.A10Z.BRCA.C1_
     ACTL6A_S5
                               0.464206
                                                        0.574901
     ADAM9_S2
                               0.553018
                                                        0.405547
     ADAMTS1_S5
                               0.550431
                                                        0.482630
     ADCY7_S3
                                                        0.363034
                               0.422275
     AIMP2_S5
                               0.401367
                                                        0.470152
     ZWILCH_S5
                               0.555027
                                                        0.574876
```

```
ZYX_S2
                          0.510994
                                                  0.489773
MMP3_S2
                          0.677798
                                                  0.595846
PLG_S5
                          0.145389
                                                  0.127402
RGS8_S5
                          0.223503
                                                  0.205245
            TCGA.EY.A1GL.UCEC.C1
                                    TCGA.D1.A16D.UCEC.C1
                          0.460726
                                                  0.253135 \
ACTL6A S5
ADAM9_S2
                          0.449487
                                                  0.567689
ADAMTS1 S5
                          0.436215
                                                  0.599091
ADCY7 S3
                          0.151328
                                                  0.409430
AIMP2 S5
                          0.714113
                                                  0.553581
ZWILCH S5
                          0.486097
                                                  0.402559
ZYX_S2
                          0.424361
                                                  0.548159
MMP3 S2
                          0.752671
                                                  0.458184
PLG_S5
                          0.260084
                                                  0.316978
RGS8_S5
                          0.385122
                                                  0.212338
            TCGA.R6.A8W8.ESCA.C1_
                                    TCGA.CM.6676.COAD.C1_
ACTL6A_S5
                          0.518248
                                                  0.447402 \
ADAM9_S2
                          0.760312
                                                  0.462684
ADAMTS1 S5
                          0.402481
                                                  0.474015
ADCY7_S3
                          0.550812
                                                  0.516051
AIMP2 S5
                          0.499165
                                                  0.601612
ZWILCH S5
                          0.794955
                                                  0.575535
ZYX S2
                          0.126130
                                                  0.530853
MMP3_S2
                          0.707623
                                                  0.527010
PLG_S5
                          0.197941
                                                  0.184610
RGS8_S5
                          0.278473
                                                  0.262055
                                    TCGA.31.1944.0V.C1_
            TCGA.L5.A43C.ESCA.C1_
                                                          TCGA.D5.6920.COAD.C1_
ACTL6A_S5
                                                0.514568
                                                                        0.392942 \
                          0.121114
ADAM9_S2
                          0.584997
                                                0.472245
                                                                        0.623314
ADAMTS1_S5
                          0.646580
                                                0.514861
                                                                        0.502959
ADCY7_S3
                          0.337942
                                                0.333021
                                                                        0.324566
AIMP2 S5
                          0.208691
                                                0.409707
                                                                        0.534003
ZWILCH S5
                          0.496718
                                                0.485334
                                                                        0.576107
ZYX S2
                          0.280705
                                                0.675461
                                                                        0.335956
MMP3 S2
                          1.000000
                                                0.118628
                                                                        0.864037
PLG S5
                          0.084984
                                                0.885797
                                                                        0.131894
RGS8 S5
                          0.099603
                                                0.171061
                                                                        0.176096
                                       TCGA.55.7281.LUAD.C6_
            TCGA.K4.A3WS.BLCA.C1_
                          0.389479 ...
                                                     0.202406 \
ACTL6A_S5
ADAM9_S2
                          0.346830 ...
                                                     0.508479
```

ADAMTS1_S5	0.648235	0.487875
ADCY7_S3	0.299469	0.416073
AIMP2_S5	0.321041	
-	•••	•••
ZWILCH_S5	0.288294	
ZYX_S2	0.603726	0.354236
MMP3_S2	0.560052	0.377979
PLG_S5	0.094857	
RGS8_S5	0.115703	
rgso_ss	0.115703	0.140377
	TCCA OF SOAD LIEC CE	TCCA EV ADOS SARC CA
ACTICA CE	-	TCGA.FX.A2QS.SARC.C6_
ACTL6A_S5	0.580844	0.416179 \
ADAM9_S2	0.505128	0.380187
ADAMTS1_S5	0.663201	0.719852
ADCY7_S3	0.543013	0.364405
AIMP2_S5	0.280040	0.813834
•••	•••	•••
ZWILCH_S5	0.480491	0.794695
ZYX_S2	0.493984	0.091282
MMP3_S2	0.568345	0.252578
PLG_S5	0.167821	0.386939
RGS8_S5	0.042493	0.300423
	TCGA.CG.4462.STAD.C6	TCGA.IB.7889.PAAD.C6_
ACTL6A_S5	0.179242	0.203589 \
ADAM9_S2	0.769308	0.703449
ADAMTS1_S5	0.766986	0.477216
ADCY7_S3	0.565062	0.403333
AIMP2_S5	0.238249	0.401831
AIMFZ_55		
 71111 CU CE	 0. 272004	 0 072742
ZWILCH_S5	0.373904	0.273743
ZYX_S2	0.349063	0.402034
MMP3_S2	0.504051	0.310182
PLG_S5	0.118107	0.170704
RGS8_S5	0.179365	0.138091
	TCGA.43.2581.LUSC.C6_	TCGA.SH.A7BC.MESO.C6_
ACTL6A_S5	0.247497	0.168205 \
ADAM9_S2	0.522681	0.578246
ADAMTS1_S5	0.564256	0.709375
ADCY7_S3	0.508487	0.530017
AIMP2_S5	0.430773	0.368653
•••	•••	•••
ZWILCH_S5	0.328550	0.354655
ZYX_S2	0.449154	0.623405
MMP3_S2	0.435797	0.410439
PLG_S5	0.088529	0.082071
	3.000020	0.002011

```
RGS8_S5
                               0.105384
                                                       0.094855
                 TCGA.EL.A3T9.THCA.C6
                                         TCGA.A2.A4S1.BRCA.C6_
     ACTL6A_S5
                               0.219743
                                                       0.106425 \
     ADAM9_S2
                               0.446626
                                                       0.441916
     ADAMTS1_S5
                               0.630981
                                                       0.604747
     ADCY7_S3
                               0.473138
                                                       0.448950
     AIMP2_S5
                               0.518621
                                                       0.250162
     ZWILCH_S5
                               0.435153
                                                       0.259721
     ZYX_S2
                               0.391279
                                                       0.382173
     MMP3_S2
                               0.263191
                                                       0.279981
    PLG S5
                               0.180832
                                                       0.179686
     RGS8_S5
                               0.255893
                                                       0.254025
                 TCGA.AR.A2LJ.BRCA.C6_
     ACTL6A_S5
                               0.227935
     ADAM9_S2
                               0.261649
     ADAMTS1_S5
                               0.423659
     ADCY7_S3
                               0.230325
     AIMP2_S5
                               0.443044
     ZWILCH_S5
                               0.314086
     ZYX S2
                               0.582450
    MMP3 S2
                               0.579321
     PLG S5
                               0.132746
     RGS8_S5
                               0.177485
     [440 rows x 513 columns]
[]: # Dataset without subgroup column:
     X_scaled_nmf = Dataset_nmf[Dataset_nmf.columns[0:-1]]
     X scaled nmf
[]:
                 TCGA.HF.7136.STAD.C1_
                                         TCGA.EW.A10Z.BRCA.C1_
     ACTL6A_S5
                               0.464206
                                                       0.574901 \
     ADAM9_S2
                               0.553018
                                                       0.405547
     ADAMTS1_S5
                               0.550431
                                                       0.482630
     ADCY7_S3
                               0.422275
                                                       0.363034
     AIMP2_S5
                               0.401367
                                                       0.470152
     ZWILCH S5
                               0.555027
                                                       0.574876
     ZYX_S2
                               0.510994
                                                       0.489773
    MMP3 S2
                               0.677798
                                                       0.595846
     PLG_S5
                               0.145389
                                                       0.127402
     RGS8_S5
                               0.223503
                                                       0.205245
```

```
TCGA.EY.A1GL.UCEC.C1_
                                    TCGA.D1.A16D.UCEC.C1_
ACTL6A_S5
                          0.460726
                                                  0.253135
ADAM9_S2
                          0.449487
                                                  0.567689
ADAMTS1_S5
                          0.436215
                                                  0.599091
ADCY7_S3
                                                  0.409430
                          0.151328
AIMP2_S5
                          0.714113
                                                  0.553581
ZWILCH_S5
                          0.486097
                                                  0.402559
ZYX S2
                          0.424361
                                                  0.548159
MMP3 S2
                          0.752671
                                                  0.458184
PLG S5
                          0.260084
                                                  0.316978
RGS8_S5
                          0.385122
                                                  0.212338
            TCGA.R6.A8W8.ESCA.C1_
                                    TCGA.CM.6676.COAD.C1_
ACTL6A S5
                          0.518248
                                                  0.447402 \
ADAM9_S2
                          0.760312
                                                  0.462684
ADAMTS1_S5
                          0.402481
                                                  0.474015
ADCY7_S3
                          0.550812
                                                  0.516051
AIMP2_S5
                          0.499165
                                                  0.601612
                          0.794955
ZWILCH_S5
                                                  0.575535
ZYX S2
                          0.126130
                                                  0.530853
MMP3_S2
                          0.707623
                                                  0.527010
PLG S5
                          0.197941
                                                  0.184610
RGS8 S5
                          0.278473
                                                  0.262055
            TCGA.L5.A43C.ESCA.C1
                                    TCGA.31.1944.0V.C1_ TCGA.D5.6920.COAD.C1_
ACTL6A S5
                                                0.514568
                                                                        0.392942 \
                          0.121114
ADAM9_S2
                          0.584997
                                                0.472245
                                                                        0.623314
ADAMTS1 S5
                          0.646580
                                                0.514861
                                                                        0.502959
ADCY7_S3
                          0.337942
                                                0.333021
                                                                        0.324566
AIMP2_S5
                          0.208691
                                                0.409707
                                                                        0.534003
ZWILCH_S5
                          0.496718
                                                0.485334
                                                                        0.576107
ZYX_S2
                          0.280705
                                                0.675461
                                                                        0.335956
MMP3_S2
                          1.000000
                                                0.118628
                                                                        0.864037
PLG S5
                          0.084984
                                                0.885797
                                                                        0.131894
RGS8_S5
                          0.099603
                                                0.171061
                                                                        0.176096
            TCGA.K4.A3WS.BLCA.C1
                                       TCGA.XV.AAZV.SKCM.C6
ACTL6A S5
                          0.389479
                                                     0.127865
ADAM9 S2
                          0.346830 ...
                                                     0.317735
ADAMTS1 S5
                          0.648235 ...
                                                     0.660852
ADCY7_S3
                          0.299469 ...
                                                     0.324093
AIMP2_S5
                                                     0.464209
                          0.321041 ...
                          0.288294 ...
ZWILCH_S5
                                                     0.410685
```

ZYX_S2 MMP3_S2 PLG_S5 RGS8_S5	0.603726 0.560052 0.094857 0.115703	0.480864 0.138028	
ACTL6A_S5 ADAM9_S2 ADAMTS1_S5 ADCY7_S3 AIMP2_S5	TCGA.55.7281.LUAD.C6_ 0.202406 0.508479 0.487875 0.416073 0.275477	TCGA.85.8049.LUSC.C6_ 0.580844 \ 0.505128 0.663201 0.543013 0.280040	
ZWILCH_S5 ZYX_S2 MMP3_S2 PLG_S5 RGS8_S5	0.230800 0.354236 0.377979 0.109989 0.140377	0.480491 0.493984 0.568345 0.167821 0.042493	
ACTL6A_S5 ADAM9_S2 ADAMTS1_S5 ADCY7_S3 AIMP2_S5	TCGA.FX.A2QS.SARC.C6_ 0.416179 0.380187 0.719852 0.364405 0.813834	TCGA.CG.4462.STAD.C6_ 0.179242 \ 0.769308 0.766986 0.565062 0.238249	
ZWILCH_S5 ZYX_S2 MMP3_S2 PLG_S5 RGS8_S5	0.794695 0.091282 0.252578 0.386939 0.300423	 0.373904 0.349063 0.504051 0.118107 0.179365	
ACTL6A_S5 ADAM9_S2 ADAMTS1_S5 ADCY7_S3 AIMP2_S5 ZWILCH_S5 ZYX_S2 MMP3_S2 DIC_S5	0.203589 0.703449 0.477216 0.403333 0.401831 0.273743 0.402034 0.310182	TCGA.43.2581.LUSC.C6_	
PLG_S5 RGS8_S5 ACTL6A_S5 ADAM9_S2	0.170704 0.138091 TCGA.SH.A7BC.MESO.C6_ 0.168205 0.578246	0.088529 0.105384 TCGA.EL.A3T9.THCA.C6_ 0.219743 \ 0.446626	

```
ADAMTS1_S5
                         0.709375
                                                 0.630981
ADCY7_S3
                         0.530017
                                                 0.473138
AIMP2_S5
                         0.368653
                                                 0.518621
ZWILCH_S5
                         0.354655
                                                 0.435153
ZYX_S2
                         0.623405
                                                 0.391279
MMP3_S2
                         0.410439
                                                 0.263191
PLG_S5
                         0.082071
                                                 0.180832
                                                 0.255893
RGS8 S5
                         0.094855
            TCGA.A2.A4S1.BRCA.C6
ACTL6A_S5
                         0.106425
ADAM9_S2
                         0.441916
ADAMTS1_S5
                         0.604747
ADCY7_S3
                         0.448950
AIMP2_S5
                         0.250162
ZWILCH_S5
                         0.259721
ZYX_S2
                         0.382173
MMP3_S2
                         0.279981
PLG_S5
                         0.179686
                         0.254025
RGS8_S5
```

[440 rows x 512 columns]

plot cophenetic coefficients because the best n_component parameter need to confirmed by cophenetic coefficients

```
[]: #define the data for nmf
X = X_scaled_nmf
# Define the range of rank (k) values to test
rank_values = range(1, 11)
# Initialize a list to store cophenetic coefficients
cophenetic_coeffs = []

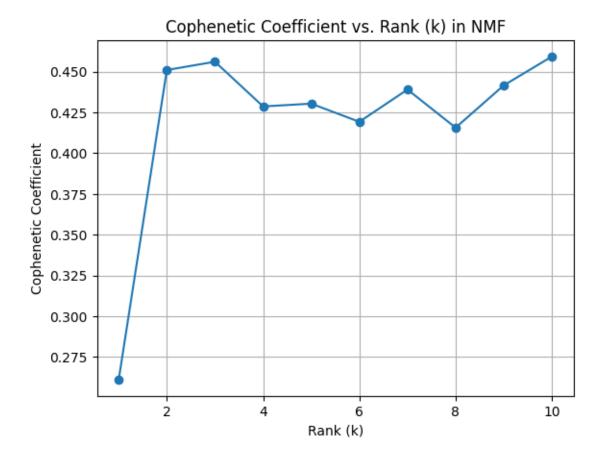
for k in rank_values:
    # Create an NMF model with the current rank (k)
    model = NMF(n_components=k, init='nndsvd', random_state=0) #because all_u
    data are positive so don't need to random

# Fit the NMF model to your data
W = model.fit_transform(X)
H = model.components_
# Get the linkage matrix for hierarchical clustering
linkage_matrix = linkage(W, method='ward')
```

```
# Calculate cophenetic coefficient
    coph_coeff, coph_dists = cophenet(linkage_matrix, pdist(X))
    # Append the cophenetic coefficient to the list
    cophenetic_coeffs.append(coph_coeff)
# Plot the cophenetic coefficients against rank (k)
plt.plot(rank_values, cophenetic_coeffs, marker='o')
plt.title('Cophenetic Coefficient vs. Rank (k) in NMF')
plt.xlabel('Rank (k)')
plt.ylabel('Cophenetic Coefficient')
plt.grid(True)
plt.show()
C:\Users\murui\AppData\Roaming\Python\Python311\site-
packages\sklearn\decomposition\ nmf.py:1710: ConvergenceWarning: Maximum number
of iterations 200 reached. Increase it to improve convergence.
  warnings.warn(
C:\Users\murui\AppData\Roaming\Python\Python311\site-
packages\sklearn\decomposition\_nmf.py:1710: ConvergenceWarning: Maximum number
of iterations 200 reached. Increase it to improve convergence.
  warnings.warn(
C:\Users\murui\AppData\Roaming\Python\Python311\site-
packages\sklearn\decomposition\_nmf.py:1710: ConvergenceWarning: Maximum number
of iterations 200 reached. Increase it to improve convergence.
  warnings.warn(
C:\Users\murui\AppData\Roaming\Python\Python311\site-
packages\sklearn\decomposition\_nmf.py:1710: ConvergenceWarning: Maximum number
of iterations 200 reached. Increase it to improve convergence.
  warnings.warn(
C:\Users\murui\AppData\Roaming\Python\Python311\site-
packages\sklearn\decomposition\ nmf.py:1710: ConvergenceWarning: Maximum number
of iterations 200 reached. Increase it to improve convergence.
 warnings.warn(
C:\Users\murui\AppData\Roaming\Python\Python311\site-
packages\sklearn\decomposition\_nmf.py:1710: ConvergenceWarning: Maximum number
of iterations 200 reached. Increase it to improve convergence.
  warnings.warn(
C:\Users\murui\AppData\Roaming\Python\Python311\site-
packages\sklearn\decomposition\ nmf.py:1710: ConvergenceWarning: Maximum number
of iterations 200 reached. Increase it to improve convergence.
  warnings.warn(
C:\Users\murui\AppData\Roaming\Python\Python311\site-
packages\sklearn\decomposition\ nmf.py:1710: ConvergenceWarning: Maximum number
of iterations 200 reached. Increase it to improve convergence.
  warnings.warn(
C:\Users\murui\AppData\Roaming\Python\Python311\site-
packages\sklearn\decomposition\_nmf.py:1710: ConvergenceWarning: Maximum number
```

of iterations 200 reached. Increase it to improve convergence. warnings.warn(

C:\Users\murui\AppData\Roaming\Python\Python311\sitepackages\sklearn\decomposition_nmf.py:1710: ConvergenceWarning: Maximum number
of iterations 200 reached. Increase it to improve convergence.
warnings.warn(



shows rank = 3 and rank = 10 are good rank for NMF

```
[]: n_components_1 = 3
n_components_2 = 10
```

```
[]: #fit and transform the machine learning model by dataset with two values for parameter n_components

model = NMF(n_components_1, init='nndsvd', random_state=0)#5 is the best rank...

W = model.fit_transform(Dataset_nmf) #nmf features

H = model.components_
```

C:\Users\murui\AppData\Roaming\Python\Python311\site-packages\sklearn\decomposition_nmf.py:1710: ConvergenceWarning: Maximum number of iterations 200 reached. Increase it to improve convergence.

```
warnings.warn(
```

```
[]: model2 = NMF(n_components 2, init='nndsvd', random_state=0) #5 is the best rank..
    W2 = model2.fit_transform(Dataset_nmf) #nmf features
    H2 = model2.components_
    C:\Users\murui\AppData\Roaming\Python\Python311\site-
    packages\sklearn\decomposition\ nmf.py:1710: ConvergenceWarning: Maximum number
    of iterations 200 reached. Increase it to improve convergence.
      warnings.warn(
    Check reconstruction err attribute, because it represents the fitted mass of the NMF model. The
    smaller the value, the better the model is fitted.
[]: print('error_value for rank = 3: ', model.reconstruction_err_, ' vs ', |
     Great - 'error_value for rank = 10: ', model2.reconstruction_err_)
    error_value for rank = 3: 63.920348014243686 vs error_value for rank = 10:
    51.31911989982033
[]: H.shape
[]: (3, 513)
[]: compontents_df = pd.DataFrame(H,
                                 columns=Dataset nmf.columns)
    compontents_df_2 = compontents_df.T
    compontents_df_2 = pd.concat([compontents_df.T,Dataset_sd[['Subgroup']]],axis=1)
    compontents_df_2 = compontents_df_2.T
    compontents_df
[]:
       0.670273
                                         0.536199
                                                               0.738639
                   0.374405
                                         0.436802
                                                               0.249843
    1
    2
                   0.043526
                                         0.130171
                                                               0.122499
       TCGA.D1.A16D.UCEC.C1 TCGA.R6.A8W8.ESCA.C1 TCGA.CM.6676.COAD.C1
    0
                   0.570018
                                         0.773193
                                                               0.825512 \
    1
                   0.415064
                                         0.345064
                                                               0.205967
    2
                   0.136425
                                         0.000000
                                                               0.101441
       0.253430
                                                             0.700875
    0
                                       0.655150
                   0.707069
                                       0.354750
                                                             0.392410
    1
    2
                   0.074782
                                       0.107439
                                                             0.005845
       TCGA.K4.A3WS.BLCA.C1_ ... TCGA.55.7281.LUAD.C6_ TCGA.85.8049.LUSC.C6_
                   0.518160 ...
    0
                                            0.213521
                                                                 0.267566 \
```

```
2
                     0.000000
                                               0.160447
                                                                       0.000583
                               TCGA.CG.4462.STAD.C6_ TCGA.IB.7889.PAAD.C6_
        TCGA.FX.A2QS.SARC.C6
     0
                     0.366987
                                            0.079072
                                                                    0.272852 \
                     0.457509
                                            0.768106
                                                                    0.660736
     1
     2
                     0.285564
                                            0.200387
                                                                    0.123943
                               TCGA.SH.A7BC.MESO.C6
                                                       TCGA.EL.A3T9.THCA.C6
        TCGA.43.2581.LUSC.C6
     0
                     0.205031
                                            0.140498
                                                                    0.403977 \
                     0.700451
                                            0.660060
                                                                    0.513931
     1
     2
                     0.160314
                                            0.281538
                                                                    0.172972
        TCGA.A2.A4S1.BRCA.C6_ TCGA.AR.A2LJ.BRCA.C6_
     0
                     0.182884
                                            0.314995
     1
                     0.615291
                                            0.587001
     2
                     0.290966
                                            0.187873
     [3 rows x 513 columns]
[]: compontents_df_3 = pd.DataFrame(H2,
                                   columns=Dataset nmf.columns)
     compontents_df_4 = compontents_df_3.T
     compontents_df_4 = pd.concat([compontents_df_3.

¬T,Dataset_sd[['Subgroup']]],axis=1)
     compontents df 4 = compontents df 4.T
     compontents_df_3
[]:
        TCGA.HF.7136.STAD.C1
                               TCGA.EW.A10Z.BRCA.C1
                                                      TCGA.EY.A1GL.UCEC.C1
     0
                     0.214136
                                            0.422697
                                                                    0.305488 \
     1
                     0.140067
                                            0.287877
                                                                    0.016342
     2
                     0.024846
                                            0.000000
                                                                    0.043107
     3
                     0.000000
                                            0.334069
                                                                    0.406192
     4
                     0.514916
                                            0.108418
                                                                    0.190731
     5
                     0.378831
                                            0.415083
                                                                    0.213826
     6
                     0.015444
                                            0.189833
                                                                    0.000000
     7
                     0.326869
                                            0.000000
                                                                    0.410831
     8
                     0.089061
                                            0.000000
                                                                    0.200452
     9
                     0.293239
                                            0.221573
                                                                    0.334435
        TCGA.D1.A16D.UCEC.C1_ TCGA.R6.A8W8.ESCA.C1_ TCGA.CM.6676.COAD.C1_
     0
                     0.277269
                                            0.211139
                                                                    0.209205 \
     1
                     0.260257
                                            0.159873
                                                                    0.015294
     2
                     0.012522
                                            0.000000
                                                                    0.069041
     3
                     0.355979
                                            0.000000
                                                                    0.260131
     4
                     0.147809
                                            0.692668
                                                                    0.563621
     5
                     0.070757
                                            0.071210
                                                                    0.182870
```

0.697346

0.739991

1

0.531307 ...

```
6
                 0.074263
                                         0.183608
                                                                  0.00000
7
                 0.470911
                                         0.329749
                                                                  0.255936
8
                 0.120332
                                         0.141949
                                                                  0.239100
9
                 0.365959
                                         0.356479
                                                                  0.299661
   TCGA.L5.A43C.ESCA.C1_
                           TCGA.31.1944.0V.C1_
                                                  TCGA.D5.6920.COAD.C1_
0
                 0.000000
                                        0.275706
                                                                0.110916
1
                 0.488001
                                        0.196189
                                                                0.213669
2
                 0.000000
                                        0.000000
                                                                0.000000
3
                 0.050107
                                        0.530276
                                                                0.104389
4
                 0.266254
                                        0.186807
                                                                0.654390
5
                 0.366757
                                       0.213738
                                                                0.089264
6
                 0.026205
                                        0.090180
                                                                0.042874
7
                 0.222796
                                        0.270383
                                                                0.292043
8
                 0.156547
                                        0.055248
                                                                0.107852
9
                 0.465909
                                        0.239568
                                                                0.488739
                                                        TCGA.85.8049.LUSC.C6
   TCGA.K4.A3WS.BLCA.C1_
                               TCGA.55.7281.LUAD.C6_
0
                 0.081141
                                             0.009077
                                                                      0.000000
                 0.194430
                                             0.546109
1
                                                                      0.481025
2
                 0.000000
                                             0.013214
                                                                      0.00000
3
                 0.354174
                                             0.347402
                                                                      0.065720
4
                 0.175588
                                                                      0.218572
                                             0.038262
5
                                             0.164927
                 0.314985
                                                                      0.302884
6
                 0.178225
                                             0.107719
                                                                      0.099827
7
                 0.137576
                                             0.430531
                                                                      0.272135
                                             0.008742
8
                 0.065014
                                                                     0.000000
9
                 0.601135
                                             0.388456
                                                                     0.561803
                            TCGA.CG.4462.STAD.C6_
                                                    TCGA.IB.7889.PAAD.C6_
   TCGA.FX.A2QS.SARC.C6_
0
                                         0.000000
                 0.082434
                                                                  0.044881
1
                 0.241396
                                         0.584710
                                                                  0.472232
2
                 0.183095
                                         0.029964
                                                                  0.000000
3
                 0.076648
                                         0.000000
                                                                  0.281784
                 0.289766
4
                                         0.099579
                                                                  0.072575
5
                 0.609481
                                         0.413940
                                                                  0.073662
6
                 0.200752
                                         0.019641
                                                                  0.099120
7
                 0.00000
                                         0.271405
                                                                  0.320940
8
                 0.227771
                                         0.301777
                                                                  0.218083
9
                 0.000000
                                         0.359692
                                                                  0.608885
   TCGA.43.2581.LUSC.C6
                           TCGA.SH.A7BC.MESO.C6
                                                    TCGA.EL.A3T9.THCA.C6
0
                 0.053565
                                         0.000000
                                                                  0.169299
1
                 0.599988
                                         0.496395
                                                                  0.281465
2
                 0.00000
                                                                  0.050251
                                         0.131154
3
                 0.102888
                                         0.223301
                                                                  0.282730
4
                 0.236687
                                         0.036853
                                                                  0.021897
```

```
5
                     0.360834
                                            0.345360
                                                                    0.347544
     6
                     0.105352
                                            0.157319
                                                                    0.026095
     7
                     0.287293
                                            0.272190
                                                                    0.428403
     8
                     0.012661
                                            0.086827
                                                                    0.201864
     9
                     0.176441
                                            0.203119
                                                                    0.282571
        TCGA.A2.A4S1.BRCA.C6_
                               TCGA.AR.A2LJ.BRCA.C6_
                     0.000000
     0
                                            0.138789
     1
                     0.410616
                                            0.453305
     2
                     0.081151
                                            0.00000
     3
                     0.402765
                                            0.590644
     4
                     0.000000
                                            0.00000
     5
                     0.418344
                                            0.176426
     6
                     0.147863
                                            0.109185
     7
                     0.106149
                                            0.008776
     8
                     0.386798
                                            0.087923
     9
                     0.158013
                                            0.541271
     [10 rows x 513 columns]
    I shows appear some 0.000 data
[]: W.shape
[]: (440, 3)
[]: compontents_df_W = pd.DataFrame(W,
                                     index=Dataset_nmf.index)
     compontents_df_W = compontents_df_W.T
     compontents_df_W
[]:
        ACTL6A_S5 ADAM9_S2
                             ADAMTS1_S5 ADCY7_S3 AIMP2_S5 ALKBH7_S5
                                                                        ALOX5AP_S3
     0
         0.523795
                  0.386598
                               0.413939
                                         0.179554 0.683130
                                                               0.656076
                                                                           0.123648
     1
         0.118208 0.598067
                               0.594447
                                         0.465999
                                                   0.077371
                                                               0.191279
                                                                           0.856451
     2
         0.163163 0.392037
                                                                           0.489633
                               0.269655 0.451391 0.554604
                                                               0.525198
        AMPD3_S3 APITD1_S5
                             APOC1_S3
                                          WDR77_S5
                                                    WIPF1_S3
                                                               WNT2B_S2
                                                                         WNT8B_S2
     0 0.318118
                   0.748332
                             0.260790
                                          0.687595
                                                     0.160825
                                                               0.361301
                                                                         0.537607
     1 0.351218
                   0.380590
                             0.506687
                                          0.062096
                                                     0.870081
                                                               0.341793
                                                                         0.032127
     2 0.400525
                   0.512428
                             0.466239
                                          0.384655
                                                     0.628547
                                                              0.392321
                                                                         0.424888
         WSB2_S5
                  ZWILCH_S5
                               ZYX_S2
                                        MMP3_S2
                                                    PLG_S5
                                                             RGS8_S5
     0 0.533319
                             0.340690
                                                 0.331779
                   0.680243
                                       0.430017
                                                            0.321591
     1 0.252569
                   0.221784
                             0.447574
                                       0.394233
                                                  0.074312
                                                            0.000000
     2 0.665708
                   0.229681
                             0.207330
                                      0.089724
                                                 0.194502 0.464619
```

[3 rows x 440 columns]

```
[]:
     compontents_df_W2 = pd.DataFrame(W2,
                                       index=Dataset_nmf.index)
     compontents_df_W2 = compontents_df_W2.T
     compontents_df_W2
[]:
        ACTL6A_S5
                    ADAM9_S2
                              ADAMTS1_S5
                                           ADCY7_S3
                                                     AIMP2_S5
                                                                ALKBH7_S5
                                                                            ALOX5AP_S3
                                           0.000000
     0
         0.430239
                    0.379590
                                 0.146470
                                                      0.529449
                                                                  0.431899
                                                                              0.101489
         0.038995
                                 0.000000
                                           0.291349
                                                      0.071195
                                                                  0.037884
     1
                    0.337747
                                                                              0.840680
     2
         0.132580
                    0.401605
                                 0.291162
                                           0.544452
                                                     0.532018
                                                                 0.490208
                                                                              0.462853
     3
         0.148231
                    0.00000
                                 0.201518
                                           0.000000
                                                     0.397999
                                                                 0.620760
                                                                              0.214920
     4
         0.523253
                    0.252605
                                0.000000
                                           0.286569
                                                     0.514471
                                                                  0.175233
                                                                              0.007627
     5
         0.163038
                   0.373766
                                0.575184
                                           0.335221
                                                     0.061498
                                                                 0.000000
                                                                              0.287167
     6
         0.132902
                                0.074577
                                                                 0.000000
                   0.000000
                                           0.199110
                                                     0.000000
                                                                              0.079860
     7
         0.132385
                   0.654977
                                0.415638
                                           0.382127
                                                      0.159397
                                                                 0.131819
                                                                              0.480442
     8
         0.000000
                    0.000000
                                0.298541
                                           0.000000
                                                      0.220628
                                                                  0.306916
                                                                              0.00000
     9
         0.000000
                    0.183018
                                 0.403738
                                           0.077339
                                                      0.000000
                                                                  0.258730
                                                                              0.041755
                              APOC1_S3
                                                                 WNT2B_S2
        AMPD3_S3
                  APITD1_S5
                                            WDR77_S5
                                                       WIPF1_S3
                                                                            WNT8B_S2
        0.326058
     0
                    0.577687
                              0.252097
                                            0.471757
                                                       0.045296
                                                                 0.028522
                                                                            0.516410
                                                                                       \
        0.201924
                    0.145153
                              0.647377
                                            0.028383
                                                       0.598717
                                                                 0.000000
                                                                            0.000000
     1
     2
        0.422952
                    0.462383
                              0.380538
                                            0.359222
                                                       0.693346
                                                                 0.483211
                                                                            0.416484
     3
        0.081995
                    0.480424
                              0.311009
                                            0.456640
                                                       0.037858
                                                                 0.214072
                                                                            0.221557
     4
        0.042139
                    0.267296
                                            0.549039
                                                       0.080647
                              0.113498
                                                                 0.285511
                                                                            0.273995
     5
        0.031794
                    0.121129
                              0.000000
                                            0.000000
                                                       0.544400
                                                                 0.439029
                                                                            0.087329
                                                                            0.00000
     6
        0.097504
                    0.193008
                              0.114607
                                            0.000000
                                                       0.161817
                                                                 0.015076
     7
        0.551267
                    0.459787
                              0.000000
                                            0.224082
                                                       0.144927
                                                                 0.263215
                                                                            0.096001
     8
        0.009732
                    0.251184
                              0.268957
                                            0.051885
                                                       0.210917
                                                                 0.076694
                                                                            0.139759
        0.188054
                              0.000000
                    0.136978
                                            0.056312
                                                       0.391260
                                                                 0.290523
                                                                            0.118597
         WSB2_S5
                   ZWILCH_S5
                                ZYX_S2
                                          MMP3_S2
                                                      PLG_S5
                                                               RGS8_S5
        0.540310
     0
                    0.490225
                              0.000000
                                         0.116208
                                                    0.186179
                                                              0.317912
     1
        0.156235
                    0.054440
                              0.077668
                                         0.000000
                                                    0.000000
                                                              0.000000
     2
        0.695047
                    0.192911
                              0.217656
                                         0.134679
                                                    0.151318
                                                              0.498077
                                                              0.121079
     3
        0.169033
                    0.258734
                              0.441062
                                         0.078630
                                                    0.099786
     4
        0.263097
                    0.706149
                              0.153551
                                         0.467293
                                                    0.144149
                                                              0.100824
        0.105917
                    0.424607
                              0.412070
                                                    0.000000
     5
                                         0.587580
                                                              0.105456
     6
        0.101570
                    0.150573
                              0.000000
                                         0.124582
                                                    0.197832
                                                              0.000000
     7
        0.328916
                    0.056305
                              0.227068
                                         0.179336
                                                    0.000000
                                                              0.154254
     8
        0.163678
                    0.019450
                              0.128711
                                         0.000000
                                                    0.435797
                                                              0.152734
        0.151052
                    0.007205
                              0.205977
                                         0.253172
                                                   0.000000
                                                              0.000000
```

[10 rows x 440 columns]

I shows appear some 0.000 data

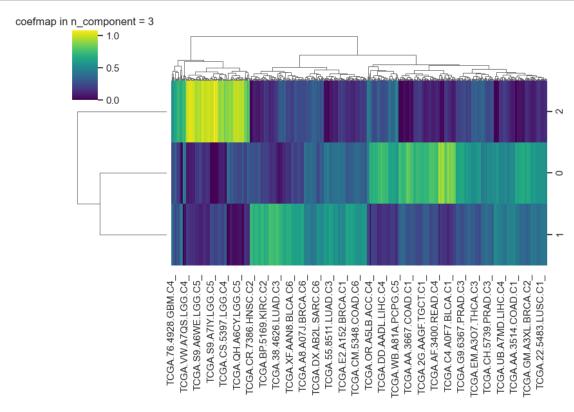
A large number of occurrences of 0 means that the proportion of weight is 0, which means that the meaning of the presence of this component is not significant because a lot of features contribute to 0 on this. In this case, those component is redundant.

b. Visualising Clustermap: help to understand the results of decomposition and patterns between data points. Helps provide insight into the structure of complex datasets

```
[]: sns.set(font_scale=1) # Adjust the font size if needed sns.clustermap(compontents_df, cmap='viridis', method='average', metric='euclidean', figsize=(8, 6))

plt.title('coefmap in n_component = 3')

# Show the plot
plt.show()
```

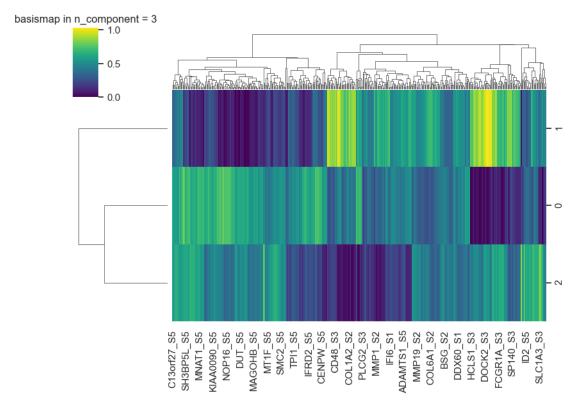


The light squares shows high relatship between horizontal coordinate and Vertical Coordinates. For example, the yellow square in the upper left corner shows high relationship between component 2 and the sample it Corresponding. And those sample have low relationship in component 0 and 1. For component 1 has a square which colour is lighter than others. Moreover, components 1 can find one square too. And looking at the top, shows some clusters and can see when sample in same cluster they have sample high relationship in same component.

Matrix W is represent the relationship bewteen the features and components. Because plot shows by clustermap

```
[]: sns.set(font_scale=1) # Adjust the font size if needed sns.clustermap(compontents_df_W, cmap='viridis', method='average',__ ometric='euclidean', figsize=(8, 6))
```

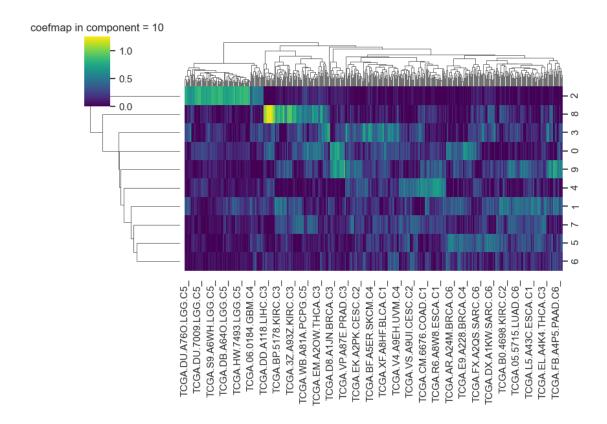
```
plt.title('basismap in n_component = 3')
# Show the plot
plt.show()
```



Martix W shows the relationship features and components. Same as before, light squares shows high relatship between horizontal coordinate and Vertical Coordinates.

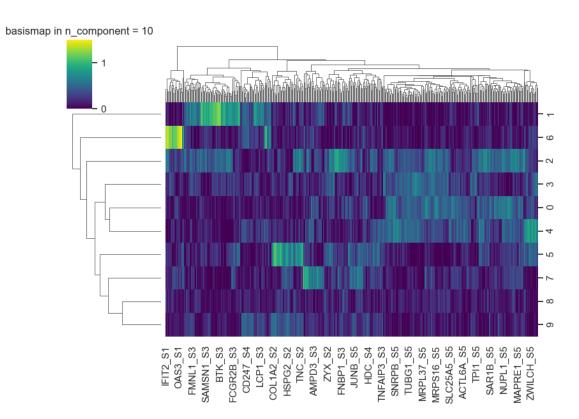
When rank = 3, the plot shows correlation and irrelevance very well, It is easy to observe the difference.

```
[]: sns.set(font_scale=1) # Adjust the font size if needed sns.clustermap(compontents_df_3, cmap='viridis', method='average', ometric='euclidean', figsize=(8, 6)) plt.title('coefmap in component = 10') # Show the plot plt.show()
```



The bottom 4 lines don't make much sense or clearly distinguish the relevancy.

```
[]: sns.set(font_scale=1) # Adjust the font size if needed sns.clustermap(compontents_df_W2, cmap='viridis', method='average', whether is a size if needed sns.clustermap(compontents_df_W2, cmap='viridis', method='average', whethere is a size if needed sns.clustermap(compontents_df_W2, cmap='viridis', method='average', where is a size if needed sns.clustermap(compontents_df_W2, cmap='viridis', method='average', where is a size if needed sns.clustermap(compontents_df_W2, cmap='viridis', method='average', where is a size if needed sns.clustermap(compontents_df_W2, cmap='viridis', method='average', where is a size if needed sns.clustermap(compontents_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(compontents_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(compontents_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(compontents_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(components_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(components_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(components_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(components_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(components_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(components_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(components_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(components_df_W2, cmap='viridis', method='average', where it is a size if needed sns.clustermap(components_df_W2, cmap='viridis', method='viridis', method='viridis
```



The bottom 2 lines don't make much sense or clearly distinguish the relevancy.

It seems rank = 3 is better than rank = 10 when doing the NMF. It is more obvious and effective. Because when rank = 10, some rows and columns seem don't need, and never display some useful information.

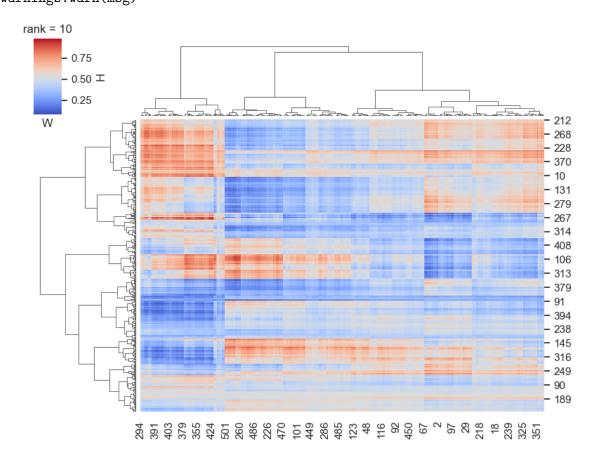
```
[]: # Create a sample dataset (replace this with your own data)
data = np.dot(W, H)

# Create a DataFrame for your NMF data
df = pd.DataFrame(data, columns=range(data.shape[1]))

# Create a clustermap
sns.clustermap(df, cmap='coolwarm', method='ward', figsize=(8, 6))
plt.title('rank = 10')
plt.xlabel("W")
plt.ylabel("H")
# Display the plot
plt.show()
```

C:\Users\murui\AppData\Roaming\Python\Python311\sitepackages\seaborn\matrix.py:560: UserWarning: Clustering large matrix with scipy.
Installing `fastcluster` may give better performance.
 warnings.warn(msg)

C:\Users\murui\AppData\Roaming\Python\Python311\sitepackages\seaborn\matrix.py:560: UserWarning: Clustering large matrix with scipy.
Installing `fastcluster` may give better performance.
 warnings.warn(msg)



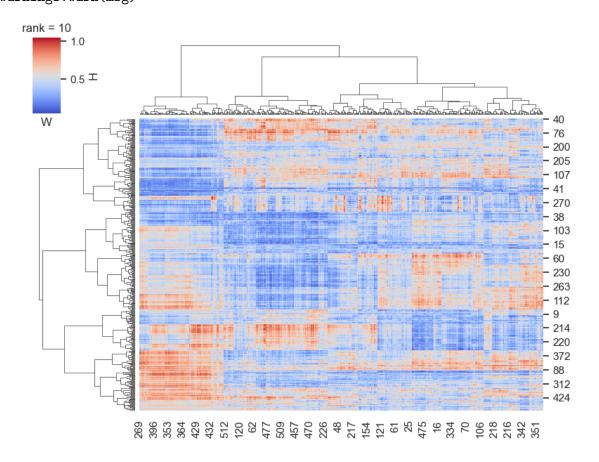
```
[]: # Create a sample dataset (replace this with your own data)
data = np.dot(W2, H2)

# Create a DataFrame for your NMF data
df = pd.DataFrame(data, columns=range(data.shape[1]))

# Create a clustermap
sns.clustermap(df, cmap='coolwarm', method='ward', figsize=(8, 6))
plt.title('rank = 10')
plt.xlabel("W")
plt.ylabel("H")
# Display the plot
plt.show()
```

C:\Users\murui\AppData\Roaming\Python\Python311\sitepackages\seaborn\matrix.py:560: UserWarning: Clustering large matrix with scipy.

Installing `fastcluster` may give better performance.
 warnings.warn(msg)
C:\Users\murui\AppData\Roaming\Python\Python311\sitepackages\seaborn\matrix.py:560: UserWarning: Clustering large matrix with scipy.
Installing `fastcluster` may give better performance.
 warnings.warn(msg)

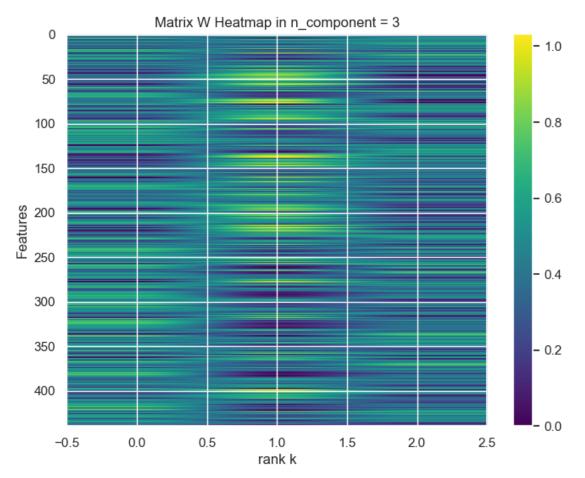


It can be seen that when they are reconstructed into a data set, the results obtained by the two ranks are almost the same, then the results are almost the same, I think it is more efficient and meaningful to choose the smaller rank value.

Feature Weight Heatmap: create a heatmap to visualize the feature weights in the factor matrix W. Each row in the heatmap represents a component, and each column represents a feature. The color intensity at the intersection of a component and feature shows the weight of that feature in the component.

```
[]: #for feature analysis
plt.figure(figsize=(8, 6))
plt.imshow(W, cmap='viridis', aspect='auto')
plt.colorbar()
plt.title("Matrix W Heatmap in n_component = 3")
```

```
plt.xlabel("rank k")
plt.ylabel("Features")
plt.show()
```



Matrix W is represent the how features are combined to reconstruct the original data.

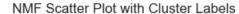
Cluster Visualization: Trying to find the cluster for subgroup

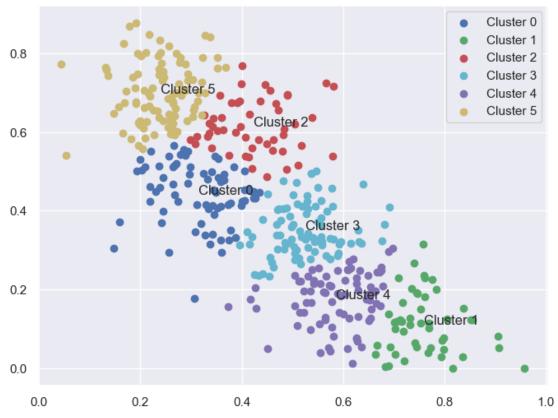
```
[]: X = X_scaled_nmf
# Apply NMF for dimensionality reduction
nmf = NMF(n_components=2)
X_nmf = nmf.fit_transform(X)

# Perform K-Means clustering into 6 clusters -> subgroup are 6
kmeans = KMeans(n_clusters=6)
labels = kmeans.fit_predict(X_nmf)

# Create a list of colors for plotting
```

```
colors = cycle(['b', 'g', 'r', 'c', 'm', 'y']) # You can extend this list for
 →more colors
# Visualize the scatter plot with different colors for each cluster
plt.figure(figsize=(8, 6))
for cluster num, color in zip(range(6), colors):
    cluster_points = X_nmf[labels == cluster_num]
    plt.scatter(cluster_points[:, 0], cluster_points[:, 1,], c=color,__
 ⇔label=f'Cluster {cluster_num}')
# Label clusters
for cluster in range(6):
    cluster_center = X_nmf[labels == cluster].mean(axis=0)
    plt.text(cluster_center[0], cluster_center[1], f'Cluster {cluster}',
 ofontsize=12)
plt.title("NMF Scatter Plot with Cluster Labels")
plt.legend()
plt.show()
C:\Users\murui\AppData\Roaming\Python\Python311\site-
packages\sklearn\decomposition\_nmf.py:1710: ConvergenceWarning: Maximum number
of iterations 200 reached. Increase it to improve convergence.
  warnings.warn(
C:\Users\murui\AppData\Roaming\Python\Python311\site-
packages\sklearn\cluster\_kmeans.py:1416: FutureWarning: The default value of
`n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init`
explicitly to suppress the warning
  super()._check_params_vs_input(X, default_n_init=10)
```





It can see that there is a linear relationship in the overall trend. But Cluster 1 is very recognisable.

```
[]: # Generate some example data
X= X_scaled_nmf

# Apply NMF for dimensionality reduction
nmf = NMF(n_components=3) # Use 3 components for 3D
X_nmf = nmf.fit_transform(X)

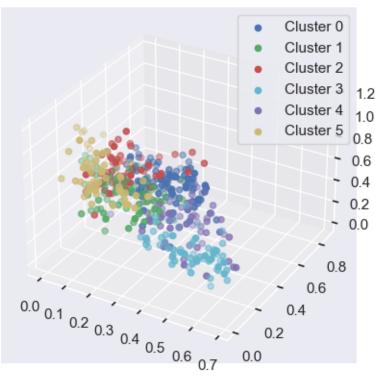
# Perform K-Means clustering into 6 clusters
kmeans = KMeans(n_clusters=6)
labels = kmeans.fit_predict(X_nmf)

# Create a list of colors for plotting
colors = cycle('bgrcmy') # You can extend this for more colors

# Visualize the 3D scatter plot with different colors for each cluster
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
```

C:\Users\murui\AppData\Roaming\Python\Python311\sitepackages\sklearn\decomposition_nmf.py:1710: ConvergenceWarning: Maximum number
of iterations 200 reached. Increase it to improve convergence.
 warnings.warn(
C:\Users\murui\AppData\Roaming\Python\Python311\sitepackages\sklearn\cluster_kmeans.py:1416: FutureWarning: The default value of
`n_init` will change from 10 to 'auto' in 1.4. Set the value of `n_init`
explicitly to suppress the warning
 super()._check_params_vs_input(X, default_n_init=10)

3D Scatter Plot with 6 Clusters



It looks two of the groups are very well separated, but the remaining four groups are together.

Conclusion: In terms of error, the error in reconstructing the data is a bit large. The success rate is only 50%, and it would be perfect if the error could be more minor. However, the generated W

and H have interpretable components, and the differences between the parts and the production clusters are also seen through visualisation.NMF for dataset targeting should be carried out for feature extraction and data dimensionality reduction. However, I think data degradation is to realise the extracted features. The aim is to efficiently analyse the main influencing components of the data set.

Visualisation provides a better view of clusters and their distribution, as well as trends in the data.

1.1.3 Principal Component Analysis(PCA)

a. Application of PCA

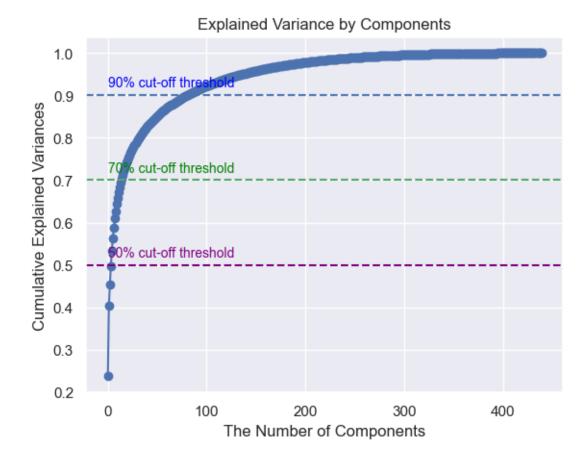
```
[]: #format dataset
    features = Dataset_1.columns[0:-1]
    x_pca = Dataset_sd.loc[:,features].values
    y pca = Dataset sd.loc[:,['Subgroup']].values
[]: pca = PCA(n components=0.9) # set pca function for 90% data
    Dataset_pca = pca.fit_transform(x_pca)
    Dataset_pca
[]: array([[-0.22086956, -1.57353236, 1.62778104, ..., 0.18280888,
            -0.03627199, 0.06702992],
           [-0.65072698, -0.77176889, 0.46795313, ..., 0.18633462,
             0.02753773, 0.15819418],
           [0.82876425, -1.7883118, -0.24780858, ..., -0.35957439,
             0.04768204, -0.36755787,
           [-1.30179571, -0.07552246, -0.13932056, ..., 0.07359615,
             0.14471046, -0.03762028,
           [-2.10909455, 1.16512941, -0.79659035, ..., 0.00502626,
            -0.27785708, 0.15322508],
           [-1.86684625, 0.39593328, -1.37928861, ..., -0.06436798,
             0.06116171, 0.04452186]])
[]: print(pca.explained_variance_ratio_.cumsum())
    [0.23706203 0.40262552 0.45346892 0.49663741 0.5327645 0.56335521
     0.68296563 0.69411493 0.70398508 0.71266598 0.72048057 0.72786919
     0.73464777 0.74094081 0.74713051 0.75312785 0.75881736 0.76415767
     0.76932186 0.77424919 0.77886561 0.78339976 0.78756513 0.79163156
     0.79563607 0.79937535 0.80293863 0.80638147 0.80973273 0.81303144
     0.81622553 0.81928301 0.82220704 0.82493434 0.82765238 0.83032314
     0.83289089 0.83536028 0.8378268 0.84023843 0.84264276 0.84497953
     0.8472294   0.84941442   0.85156252   0.8536918   0.85574011   0.85777526
     0.85975976 0.86171791 0.86358299 0.86543353 0.86725918 0.86904035
     0.87081097 0.87257487 0.87427877 0.87591737 0.8775382 0.87913788
     0.88073018 0.88229619 0.88383964 0.88537677 0.88684614 0.88830666
     0.88975582 0.89118181 0.89257139 0.89394927 0.89531181 0.89663958
```

0.89795251 0.89925148 0.90052438]

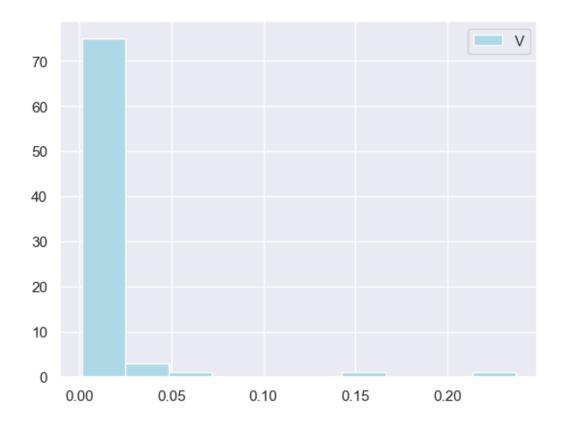
The motivation for performing PCA is to eliminate multicollinearity and perform feature selection to help build high-performance predictions while improving computational efficiency because the dimensionality of the

b. Plot and determining the number of retained components

```
[ ]: pca1 = PCA()
    pca1.fit_transform(x_pca)
     plt.plot(pca1.explained_variance_ratio_.cumsum(), marker='o',__
      ⇔linestyle='-')#plot variance_sum follow the principal
     plt.axhline(y=0.9, color='b', linestyle='--') # plot a line when y=1 cause this
      ⇒is when principal include 90% data
     plt.text(0.5, 0.92, '90% cut-off threshold', color = 'blue', fontsize=10)
     plt.axhline(y=0.7, color='g', linestyle='--') # plot a line when y=1 cause this
      →is when principal include 70% data
     plt.text(0.5, 0.72, '70% cut-off threshold', color = 'green', fontsize=10)
     plt.axhline(y=0.5, color='purple', linestyle='--') # plot a line when y=1 cause_
      →this is when principal include 50% data
     plt.text(0.5, 0.52, '50% cut-off threshold', color = 'purple', fontsize=10)
     plt.title('Explained Variance by Components')
     plt.xlabel("The Number of Components")
     plt.ylabel("Cumulative Explained Variances" )
     plt.show()
```



plot the relationship between explain variancess and components beacuase PCA is finding the biggest variance to build new coordinate system then can loss least data. So this is related to how many data will lose. Using explained_variance_ratio_ attribute from machine learning to check the precentage of the data hold by principal components. Can choose how many principal it need when I want 90% data or other precentage.



```
[]: df_pca_components = pca1.explained_variance_ratio_.cumsum() > 0.90
Number_of_components_percentage = 440 - df_pca_components.sum()
Number_of_components_percentage
```

[]: 80

It can be concluded that if we want to reduce Dimension that the downscaled data contains 90% of the original data, then 99 features are needed to do so. Bust first 4 feature can contains 50% data

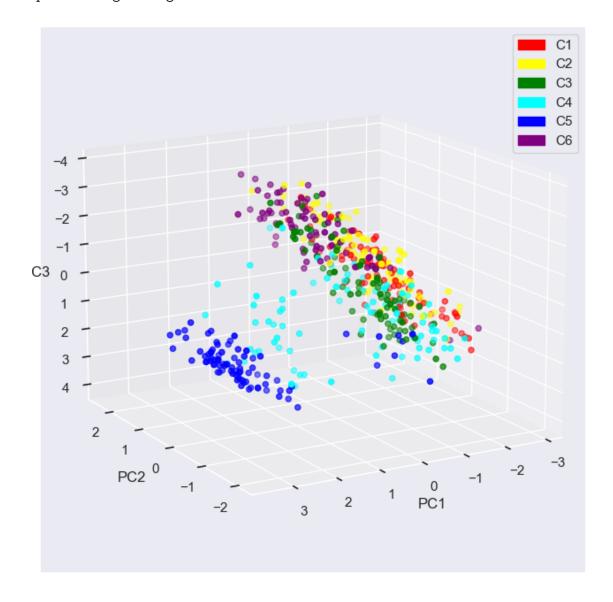
3D PCA Visualisation Due to 3D only need 3 feature, choose first 3 features to plot.

```
[]: PC1 PC2 PC3
TCGA.HF.7136.STAD.C1_ -0.220870 -1.573532 1.627781
TCGA.EW.A10Z.BRCA.C1_ -0.650727 -0.771769 0.467953
TCGA.EY.A1GL.UCEC.C1_ 0.828764 -1.788312 -0.247809
TCGA.D1.A16D.UCEC.C1_ -0.403537 -0.892226 -0.592516
TCGA.R6.A8W8.ESCA.C1_ 0.086907 -2.157220 1.319764
```

```
TCGA.43.2581.LUSC.C6_ -2.844417 0.868858 0.636143
    TCGA.SH.A7BC.MESO.C6_ -2.477495 1.364205 0.053401
    TCGA.EL.A3T9.THCA.C6_ -1.301796 -0.075522 -0.139321
    TCGA.A2.A4S1.BRCA.C6_ -2.109095 1.165129 -0.796590
    TCGA.AR.A2LJ.BRCA.C6_ -1.866846 0.395933 -1.379289
    [513 rows x 3 columns]
[]: Dataset_pca = pd.concat([Dataset_pca,Dataset_sd[['Subgroup']]], axis=1)
    Dataset_pca
[]:
                                PC1
                                          PC2
                                                    PC3 Subgroup
    TCGA.HF.7136.STAD.C1_ -0.220870 -1.573532 1.627781
                                                             C1
    TCGA.EW.A10Z.BRCA.C1_ -0.650727 -0.771769 0.467953
                                                             C1
    TCGA.EY.A1GL.UCEC.C1 0.828764 -1.788312 -0.247809
                                                             C1
    TCGA.D1.A16D.UCEC.C1_ -0.403537 -0.892226 -0.592516
                                                             C1
    TCGA.R6.A8W8.ESCA.C1 0.086907 -2.157220 1.319764
                                                             C1
    TCGA.43.2581.LUSC.C6_ -2.844417  0.868858  0.636143
                                                             C6
    TCGA.SH.A7BC.MESO.C6_ -2.477495 1.364205 0.053401
                                                             C6
    TCGA.EL.A3T9.THCA.C6_ -1.301796 -0.075522 -0.139321
                                                             C6
    TCGA.A2.A4S1.BRCA.C6_ -2.109095 1.165129 -0.796590
                                                             C6
    TCGA.AR.A2LJ.BRCA.C6_ -1.866846 0.395933 -1.379289
                                                             C6
    [513 rows x 4 columns]
[]: # plot 3D:
    fig = plt.figure(figsize=(8,8))
    ax = plt.axes(projection='3d')
     # Define colours
    color_map = {'C1': 'red', 'C2': 'yellow', 'C3':'green', 'C4':'cyan', 'C5':
     # Data for three-dimensional scattered points
    zdata = Dataset_pca['PC1']
    xdata = Dataset_pca['PC2']
    ydata = Dataset_pca['PC3']
    ax.set_xlabel('PC1')
    ax.set_ylabel('PC2')
    ax.set_zlabel('PC3')
    ax.view_init(-165, 120)
    ax.scatter3D(xdata, ydata, zdata, c=Dataset_pca['Subgroup'].map(color_map))
```

```
c1 = mpatches.Patch(color='red', label='C1')
c2 = mpatches.Patch(color='yellow', label='C2')
c3 = mpatches.Patch(color='green', label='C3')
c4 = mpatches.Patch(color='cyan', label='C4')
c5 = mpatches.Patch(color='blue', label='C5')
c6 = mpatches.Patch(color='purple', label='C6')
plt.legend(handles=[c1, c2, c3, c4, c5, c6])
```

[]: <matplotlib.legend.Legend at 0x29453b0c1d0>



It can be seen that the results are very similar to those of the previous NMF visualisation, in that

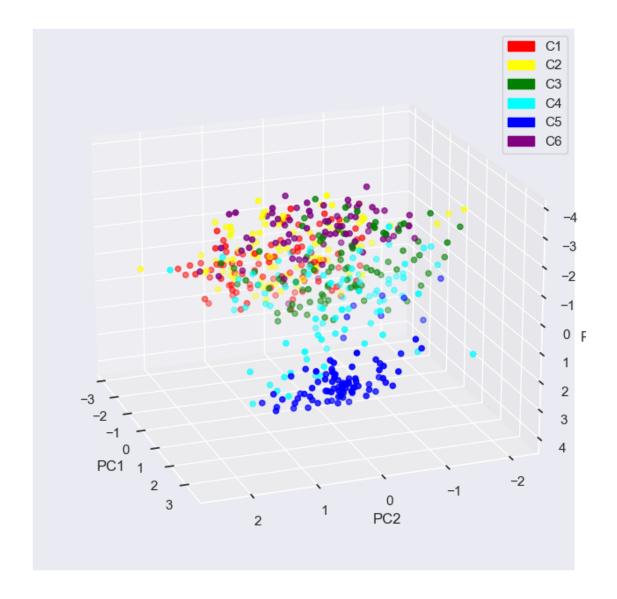
two of the groups are very clearly distinguishable, but the other four groups show a regular pattern of moving together in the same way from the top left corner to the bottom right corner. And in terms of general data trends, they are the same.

Closer points have higher similarity in structure and relationship and similar principal components.

Rotate the picture to observe

```
[]: fig = plt.figure(figsize=(8,8))
    ax = plt.axes(projection='3d')
     # Define colours
    color_map = {'C1': 'red', 'C2': 'yellow', 'C3': 'green', 'C4': 'cyan', 'C5': __
     # Data for three-dimensional scattered points
    zdata = Dataset_pca['PC1']
    xdata = Dataset_pca['PC2']
    ydata = Dataset_pca['PC3']
    ax.set_xlabel('PC1')
    ax.set_ylabel('PC2')
    ax.set_zlabel('PC3')
    ax.view_init(-160, 200)
    ax.scatter3D(xdata, ydata, zdata, c=Dataset_pca['Subgroup'].map(color_map))
    c1 = mpatches.Patch(color='red', label='C1')
    c2 = mpatches.Patch(color='yellow', label='C2')
    c3 = mpatches.Patch(color='green', label='C3')
    c4 = mpatches.Patch(color='cyan', label='C4')
    c5 = mpatches.Patch(color='blue', label='C5')
    c6 = mpatches.Patch(color='purple', label='C6')
    plt.legend(handles=[c1, c2, c3, c4, c5, c6])
```

[]: <matplotlib.legend.Legend at 0x29453b75490>



The four subgroups that look like they're together have the feeling of being one layer on top of another. And they all maintain a linear

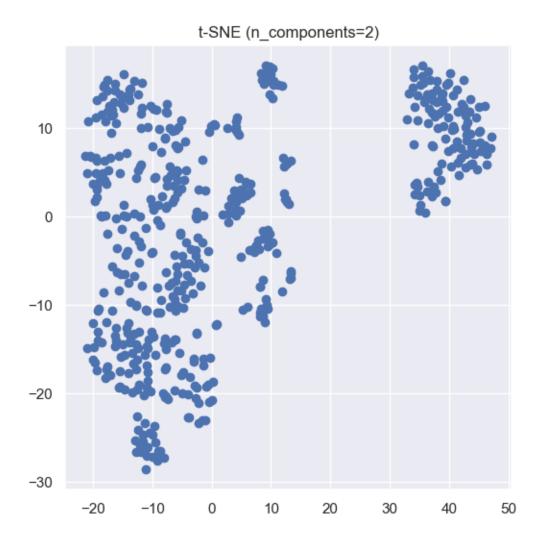
1.1.4 t-SNE Dimensionality Reduction

Prepare Data

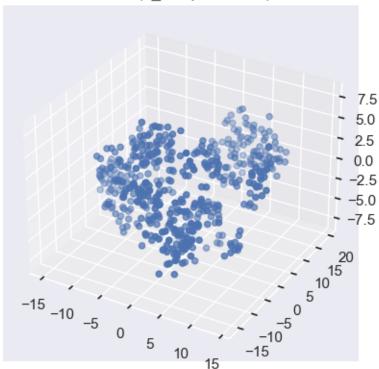
```
[]: features = Dataset_1.columns[0:-1]
x_tsne = Dataset_sd.loc[:,features].values
y_tsne = Dataset_sd.loc[:,['Subgroup']].values
```

a. Application of t-SNE Not sure if should draw 2D or 3D will better, check n_componments to see which is more appropriate in different situations.

```
[]: X = x_tsne
     \# Initialise t-SNE model, set different n_components values and visualise
     n_components_list = [2, 3] #
     perplexity = 30
     for n_components in n_components_list:
         tsne = TSNE(n_components=n_components, perplexity=perplexity)
         X_tsne = tsne.fit_transform(X)
         if n_components == 2:
            plt.figure(figsize=(6, 6))
            plt.scatter(X_tsne[:, 0], X_tsne[:, 1])
            plt.title(f't-SNE (n_components={n_components})')
            plt.show()
         elif n_components == 3:
            fig = plt.figure()
             ax = fig.add_subplot(111, projection='3d')
            ax.scatter(X_tsne[:, 0], X_tsne[:, 1], X_tsne[:, 2])
            ax.set_title(f't-SNE (n_components={n_components})')
            plt.show()
```



t-SNE (n_components=3)



The 2D image looks similar to the results obtained by the previous two downscaling methods. I decided to draw two pictures together

```
[]: tsne = TSNE(n_components=3, random_state=0)
    X_3d = tsne.fit_transform(x_tsne)
[]: tsne_1 = TSNE(n_components=2, random_state=0)
    X_2d = tsne_1.fit_transform(x_tsne)
[]: X_3d
[]: array([[ -1.6142616, -11.426699 , -5.145396],
           [-1.0413069, -1.5464859,
                                      -3.6518073],
           [ 4.791106 , -4.6398287,
                                      -1.5009079],
           [ -5.3804784, 0.6474102,
                                       3.2778208],
           [-8.747445, 2.0955217, -5.7901073],
           [ -4.704082 , -1.6342709, -2.8095233]], dtype=float32)
[]: Dataset_tsne = pd.DataFrame(data = X_3d,
                                columns=['feature1','feature2','feature3'],
                                index=Dataset_sd.index)
```

```
[]:
                            feature1
                                       feature2 feature3
                           -1.614262 -11.426699 -5.145396
    TCGA.HF.7136.STAD.C1_
    TCGA.EW.A10Z.BRCA.C1
                           -1.041307 -1.546486 -3.651807
    TCGA.EY.A1GL.UCEC.C1_
                            4.791106 -4.639829 -1.500908
    TCGA.D1.A16D.UCEC.C1
                            0.634710 -5.939110 -0.696586
    TCGA.R6.A8W8.ESCA.C1_
                            0.456902 -12.938315 -6.142682
    TCGA.43.2581.LUSC.C6_ -13.882877
                                      -0.772022 3.460467
    TCGA.SH.A7BC.MESO.C6 -9.458762 -0.729669 -4.345543
    TCGA.EL.A3T9.THCA.C6_ -5.380478
                                       0.647410 3.277821
    TCGA.A2.A4S1.BRCA.C6_ -8.747445
                                       2.095522 -5.790107
    TCGA.AR.A2LJ.BRCA.C6_ -4.704082 -1.634271 -2.809523
    [513 rows x 3 columns]
[]: Dataset_tsne1 = pd.DataFrame(data = X_2d,
                                 columns=['feature1','feature2'],
                                 index=Dataset_sd.index)
    Dataset_tsne1
[]:
                            feature1
                                       feature2
    TCGA.HF.7136.STAD.C1_
                            9.009348 -15.098787
    TCGA.EW.A10Z.BRCA.C1 -7.607230 -14.919571
    TCGA.EY.A1GL.UCEC.C1_
                            9.072879 -2.854402
    TCGA.D1.A16D.UCEC.C1_ -4.740012 -4.195903
    TCGA.R6.A8W8.ESCA.C1_
                            9.611462 -13.326759
    TCGA.43.2581.LUSC.C6_ -18.469227 -14.071336
    TCGA.SH.A7BC.MESO.C6_ -22.456432 -6.157858
    TCGA.EL.A3T9.THCA.C6_ -15.806913 -4.879653
    TCGA.A2.A4S1.BRCA.C6_ -21.192274 -1.086885
    TCGA.AR.A2LJ.BRCA.C6_ -19.546152 -6.487153
    [513 rows x 2 columns]
[]: Dataset_tsne = pd.concat([Dataset_tsne,Dataset_sd[['Subgroup']]], axis=1)
    Dataset_tsne
[]:
                                       feature2 feature3 Subgroup
                            feature1
                                                                C1
    TCGA.HF.7136.STAD.C1
                           -1.614262 -11.426699 -5.145396
                                                                C1
    TCGA.EW.A10Z.BRCA.C1_
                           -1.041307 -1.546486 -3.651807
    TCGA.EY.A1GL.UCEC.C1_
                            4.791106 -4.639829 -1.500908
                                                                C1
    TCGA.D1.A16D.UCEC.C1_
                            0.634710 -5.939110 -0.696586
                                                                C1
    TCGA.R6.A8W8.ESCA.C1_
                                                                C1
                            0.456902 -12.938315 -6.142682
```

Dataset_tsne

```
TCGA.43.2581.LUSC.C6_ -13.882877 -0.772022 3.460467 C6
TCGA.SH.A7BC.MESO.C6_ -9.458762 -0.729669 -4.345543 C6
TCGA.EL.A3T9.THCA.C6_ -5.380478 0.647410 3.277821 C6
TCGA.A2.A4S1.BRCA.C6_ -8.747445 2.095522 -5.790107 C6
TCGA.AR.A2LJ.BRCA.C6_ -4.704082 -1.634271 -2.809523 C6
```

[513 rows x 4 columns]

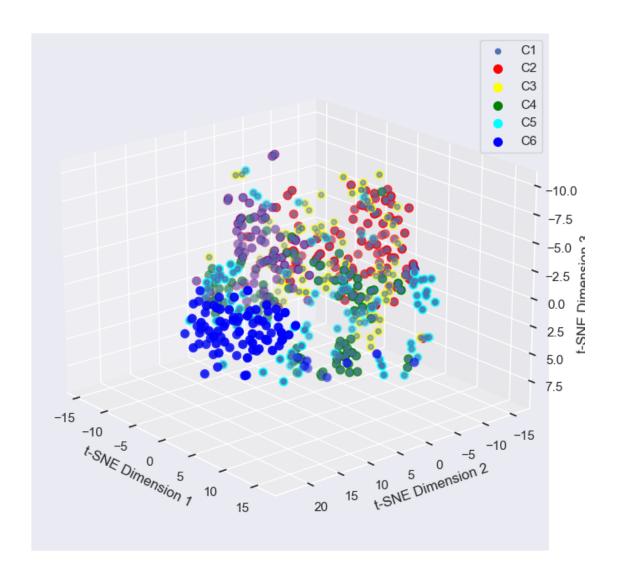
```
[ ]: Dataset_tsne1 = pd.concat([Dataset_tsne1,Dataset_sd[['Subgroup']]], axis=1)
    Dataset_tsne1
```

```
[]:
                            feature1
                                       feature2 Subgroup
    TCGA.HF.7136.STAD.C1_
                            9.009348 -15.098787
    TCGA.EW.A10Z.BRCA.C1 -7.607230 -14.919571
                                                      C1
    TCGA.EY.A1GL.UCEC.C1_
                            9.072879 -2.854402
                                                      C1
    TCGA.D1.A16D.UCEC.C1 -4.740012 -4.195903
                                                      C1
    TCGA.R6.A8W8.ESCA.C1_
                            9.611462 -13.326759
                                                      C1
    TCGA.43.2581.LUSC.C6_ -18.469227 -14.071336
                                                      C6
    TCGA.SH.A7BC.MESO.C6_ -22.456432 -6.157858
                                                      C6
    TCGA.EL.A3T9.THCA.C6_ -15.806913 -4.879653
                                                      C6
    TCGA.A2.A4S1.BRCA.C6_ -21.192274 -1.086885
                                                      C6
    TCGA.AR.A2LJ.BRCA.C6_ -19.546152 -6.487153
                                                      C6
```

[513 rows x 3 columns]

b. Visualising t-SNE Results

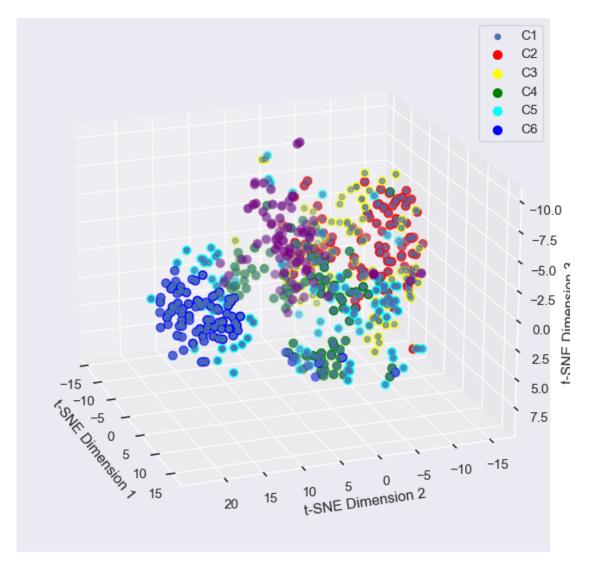
```
[]: fig = plt.figure(figsize=(8,8))
     ax = fig.add_subplot(111, projection='3d')
     ax.scatter(X_3d[:, 0], X_3d[:, 1], X_3d[:, 2], c='b', marker='o')
     ax.set_xlabel('t-SNE Dimension 1')
     ax.set ylabel('t-SNE Dimension 2')
     ax.set_zlabel('t-SNE Dimension 3')
     ax.view_init(-160, 220)
     targets = ['C1', 'C2', 'C3', 'C4', 'C5', 'C6']
     colors = ['red', 'yellow', 'green','cyan','blue','purple']
     for target, color in zip(targets,colors):
         indicesToKeep = Dataset_tsne['Subgroup'] == target
         ax.scatter(Dataset_tsne.loc[indicesToKeep, 'feature1']
                    , Dataset_tsne.loc[indicesToKeep, 'feature2']
                    , Dataset_tsne.loc[indicesToKeep, 'feature3']
                    , c = color
                    , s = 50)
     ax.legend(targets)
     ax.grid()
```



```
fig = plt.figure(figsize=(8,8))
ax = fig.add_subplot(111, projection='3d')

ax.scatter(X_3d[:, 0], X_3d[:, 1], X_3d[:, 2], c='b', marker='o')

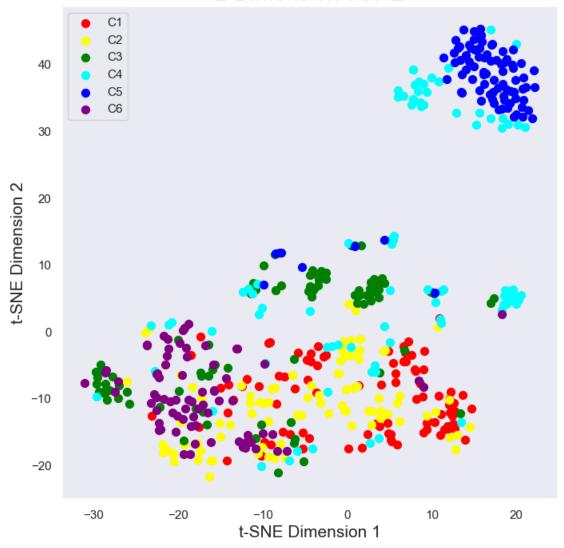
ax.set_xlabel('t-SNE Dimension 1')
ax.set_ylabel('t-SNE Dimension 2')
ax.set_zlabel('t-SNE Dimension 3')
ax.view_init(-160, 200)
targets = ['C1', 'C2', 'C3','C4','C5','C6']
colors = ['red', 'yellow', 'green','cyan','blue','purple']
for target, color in zip(targets,colors):
    indicesToKeep = Dataset_tsne['Subgroup'] == target
    ax.scatter(Dataset_tsne.loc[indicesToKeep, 'feature1']
```



t-SNE visualization results look similar to PCA dimensionality reduction, but not as crisp and clear as PCA. I thinks is beacuase t-SNE focuses on preserving local structures and capturing non-linear relationships in data. It is more care about interpreting patterns and clusters not the linear combinations.

```
[]: fig = plt.figure(figsize = (8,8)) #size of the plot
     ax = fig.add_subplot(1,1,1) #Add an Axes to the current figure or retrieve an_
     ⇔existing Axes.
     ax.set_xlabel('t-SNE Dimension 1', fontsize = 15)
     ax.set_ylabel('t-SNE Dimension 2', fontsize = 15)
     ax.set_title('2 Dimension t-SNE', fontsize=20)
     targets = ['C1', 'C2', 'C3', 'C4', 'C5', 'C6']
     colors = ['red', 'yellow', 'green','cyan','blue','purple']
     for target, color in zip(targets,colors):
         indicesToKeep = Dataset_tsne1['Subgroup'] == target
         ax.scatter(Dataset_tsne1.loc[indicesToKeep, 'feature1']
                    , Dataset_tsne1.loc[indicesToKeep, 'feature2']
                    , c = color
                    , s = 50)
     ax.legend(targets)#qroup point by targets
     ax.grid()
```

2 Dimension t-SNE



As far as the results are concerned, the effect of data reduction is not very bad, some subgroups are very successful and can be clearly distinguished from each other. There is always a subgroup that is very recognisable in both 3D and 2D. But for the other groups it is not so satisfactory, not completely clean and distinguishable. It means the similarity of the other subgroups may be higher because tight clusters are usually composed of similar observations. Similarly, groups that are far away from each other will be less similar.

Visualisation gives meaningful value to clusters of data that have unique characteristics and are clustered together. In addition, visualisation provides an understanding of the local structure of the data as a whole from point to point.

From some perspectives, the three diagrams are similar, but each one is a little different from the other. But with no exception, only one subgroup that is very recognisable.

1.2

1.3 conclusion

There have been three different dimensionality reduction methods to handle high-dimensional data, and each of these methods employs a distinct approach.

PCA, being a linear method, is more practical for finding linear combinations from data. It is suitable for tasks like removing redundant information, improving computational efficiency, and conducting feature selection. The purpose of PCA is to find new principal components, which are linear combinations of the original features.

On the other hand, t-SNE is a non-linear method that places a stronger emphasis on the distance relationships between similar data points, capturing local structures. Therefore, it is more suitable for visualizing the distribution of categories in high-dimensional data. The aim of t-SNE is to visualise high-dimensional arrays and maintain similarity information as much as possible, making it easier to understand the structure and relationships of the data.

However, NMF is a somewhat specialized method. It extracts hidden features through the factorization of non-negative matrices, resulting in sparse matrices during the process. NMF is best suited for describing the relative strengths of components within the data. When analyzing visualizations, the highlighted regions correspond to areas of pronounced correlation. The purpose of NMF is to find hidden components in high-dimensional data, helping to understand the underlying and patterns.