tp2

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1 Rapport TP1 - Méthode ACP

UP2 : Apprentissage Statistique - Analyse des données

Préparer par : ALLOUCH Omar - SROUR Mathieu

1.1 Imports

[186]:
```
import pandas as pd
import numpy as np
import plotly.express as px
import matplotlib.pyplot as plt
import seaborn as sns

from IPython.display import display

sns.set()
import warnings
warnings.filterwarnings("ignore")
```

1.2 Partie 1 : ACP : principes

1.2.1 Etape 1 - programmer l'ACP sur l'espace de variables

1. Chargement de données et pretraitement et indicateurs statistiques

[187]:
```
# Question 1
# Importing and preprocessing data
data = pd.read_csv('data_PDE20.csv', delimiter=';', decimal=',')
del data['Unnamed: 9']
del data['Num']
n = data.shape[0] # Nombre des individus
p = data.shape[1] # Nombre des variables

data
```

[187]:

	X1	X2	X3	X4	X5	X6	X7	X8
0	303.09	24.19	0.00	3.29	179.990	8.090	360.9000	120.330
1	281.88	38.59	4.29	1.06	192.000	10.500	353.5000	117.000

2	277.06	34.79	0.00	6.85	183.770	38.890	343.9500	114.650
3	276.38	32.43	4.14	2.04	190.790	38.530	341.1700	113.910
4	253.80	39.50	3.04	1.00	173.800	19.334	382.1100	127.373
5	243.56	34.39	2.79	3.43	166.670	27.590	391.1450	130.380
6	277.00	34.70	0.00	6.85	183.780	38.800	343.9400	114.650
7	294.80	28.29	1.85	1.83	182.290	10.290	360.2000	120.000
8	303.00	24.20	0.00	3.30	180.000	8.100	361.0000	120.340
9	269.38	36.89	2.99	1.03	197.700	12.590	359.4711	19.820
10	283.61	28.00	9.30	0.00	186.600	13.200	359.4180	119.806
11	290.32	23.20	0.80	2.34	172.400	39.400	353.6300	117.870
12	285.09	25.90	0.93	7.78	180.100	39.000	345.6900	115.230
13	265.48	40.39	0.95	5.14	184.390	38.830	348.5800	116.194
14	261.87	41.49	2.33	2.89	187.270	38.690	349.0620	116.345
15	274.38	29.79	6.69	0.00	183.580	38.890	349.9700	116.650
16	257.90	37.20	2.96	1.10	170.900	18.890	383.3000	127.769
17	238.20	29.80	2.60	0.80	166.705	14.140	410.1400	136.930
18	235.98	33.39	5.60	0.39	166.680	15.230	406.9700	135.650
19	247.77	36.69	5.03	1.79	166.680	27.090	386.2500	128.750
20	266.57	36.40	0.00	2.90	166.680	30.680	365.6000	121.880
21	264.79	24.19	1.19	5.60	166.680	39.690	391.9000	130.650
22	235.68	24.99	0.99	4.29	166.680	39.690	391.9700	130.650
23	239.58	47.89	0.40	4.19	166.680	39.690	376.0700	125.350
24	233.09	46.59	2.29	4.83	166.693	39.690	380.0800	126.690
25	241.37	34.50	5.15	0.39	166.683	39.690	383.7600	127.920

[188]:
```python
# Statistical indicators
# Mean
data_mean = data.mean().to_list()

# Variance
data_var = data.var().to_list()

# Standard Deviation
data_std = data.std().to_list()

# Covariance
data_cov = data.cov()

tab = pd.DataFrame({'Mean': data_mean, 'Variance': data_var,
                   'Std Deviation': data_std},
                   index=['X1', 'X2', 'X3', 'X4', 'X5', 'X6', 'X7', 'X8'])
display(tab)


print("\nThe list of covariance values for each variable:")
display(data_cov)
```

	Mean	Variance	Std Deviation
X1	265.447308	462.703068	21.510534
X2	33.399231	47.286335	6.876506
X3	2.550385	5.656148	2.378266
X4	2.888846	5.049235	2.247050
X5	176.776577	96.729128	9.835097
X6	27.892462	160.818919	12.681440
X7	368.452927	414.445129	20.357925
X8	118.953346	454.982368	21.330316

The list of covariance values for each variable:

	X1	X2	X3	X4	X5	X6 \
X1	462.703068	-77.286382	-9.677279	5.705937	135.476692	-82.971621
X2	-77.286382	47.286335	0.693332	-0.189765	-1.603496	17.318350
X3	-9.677279	0.693332	5.656148	-3.863496	2.998144	-6.514987
X4	5.705937	-0.189765	-3.863496	5.049235	-0.789097	14.981769
X5	135.476692	-1.603496	2.998144	-0.789097	96.729128	-26.443402
X6	-82.971621	17.318350	-6.514987	14.981769	-26.443402	160.818919
X7	-321.739760	4.084113	7.923145	-13.800739	-158.179147	-51.474476
X8	-123.682955	-12.819325	0.832045	2.877923	-136.929473	44.606713

	X7	X8
X1	-321.739760	-123.682955
X2	4.084113	-12.819325
X3	7.923145	0.832045
X4	-13.800739	2.877923
X5	-158.179147	-136.929473
X6	-51.474476	44.606713
X7	414.445129	174.751538
X8	174.751538	454.982368

2. Un script qui permet de faire successivement :

- La translation du nuage des individus dans l'espace initial R (centrer le nuage);
- De trouver les hyperplans pour lesquels l'inertie projetée est maximale.

[189]:
```
def data_center(data):
    data_center = data.copy()
    for i in range(1, data.shape[1]+1):
        data_center["X"+str(i)] = (data_center["X"+str(i)] - data.mean().
 ↪to_list()[i-1])
    return data_center

def data_reduce(data):
    data_red = data.copy()
    for i in range(1, data.shape[1]+1):
        data_red["X"+str(i)] = data["X"+str(i)] / data.std().to_list()[i-1]
```

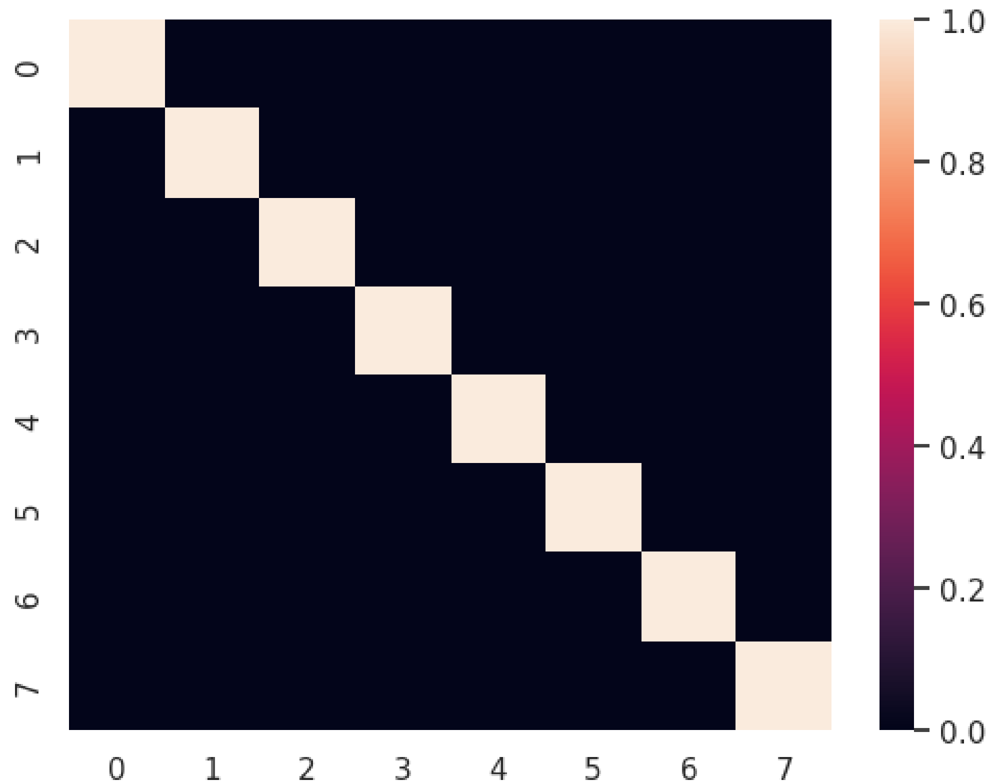
```
    return data_red


def processing_data(raw_data, normalize=False):
    data_centred = raw_data.copy()
    for col in raw_data.columns:
        data_centred[col] = (data_centred[col] - (sum(raw_data[col]) / raw_data.
↪shape[0])) \
                                / (np.std(raw_data[col], ddof=0) * normalize + 1 *␣
↪(1 - normalize))
    return data_centred

# Equal to the StandardScaler() function
data_centered = data_center(data)
data_centered_reduced = data_reduce(data_centered)

# Hyperplans
def hyperplans(data, k):
    eigenValues, eigenVectors = np.linalg.eig(data.cov())
    # Sorting the eigen values
    index = eigenValues.argsort()[::-1]
    eigenValues_sorted = eigenValues[index]
    eigenVectors_sorted = eigenVectors[:, index]
    return eigenValues_sorted[:k], eigenVectors_sorted[:, :k]
```

Nous pouvons vérifier maintenant que les valeurs propres forment une base orthonormales c'est à dire qu'ils sont pas corrélées.

[190]:
```
eigen_vector_basis = hyperplans(data, 8)[1]
print(pd.DataFrame(eigen_vector_basis))

sns.heatmap(np.dot(eigen_vector_basis,
            np.transpose(eigen_vector_basis)))
plt.show()
```

```
          0         1         2         3         4         5         6  \
0  0.605395 -0.460576  0.358994  0.296908  0.225960  0.006081 -0.391084
1 -0.050085  0.145526 -0.192659 -0.564511  0.604647 -0.010916 -0.503727
2 -0.010371  0.016962  0.023002 -0.101135 -0.308517  0.640599 -0.231258
3  0.009834 -0.024161 -0.068854  0.087402  0.140657 -0.623491  0.151071
4  0.280568  0.086156 -0.011420 -0.385747 -0.670406 -0.411831 -0.368618
5 -0.060801 -0.048967 -0.755556  0.511207 -0.079480 -0.018210 -0.390375
6 -0.591480  0.199047  0.503491  0.313874 -0.044240 -0.166773 -0.478158
7 -0.445556 -0.846392 -0.065095 -0.258176 -0.103244 -0.054638 -0.010129

          7
0 -0.017140
```

```
1 -0.032638
2 -0.655604
3 -0.745380
4  0.099998
5  0.051636
6  0.010281
7  0.021463
```

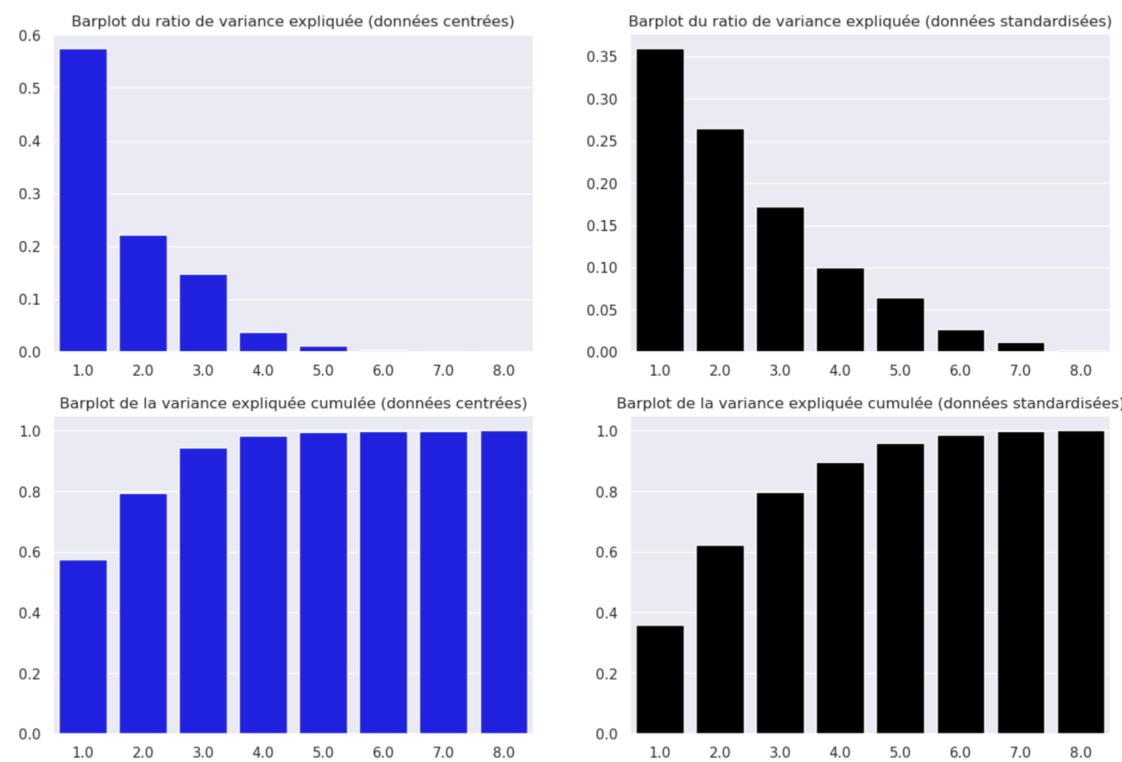


1.3 Partie 2 - Qualité de l'ACP

3. Bar plot pour choisir les axes principales

[191]:
```
eig_val_centred_data, eig_vect_centred_data = hyperplans(data_centered,␣
↪data_centered.shape[1])
eig_val_standard_data, eig_vect_standard_data =␣
↪hyperplans(data_centered_reduced, data_centered_reduced.shape[1])

fig = plt.figure(figsize= (15, 10))
ax1 = fig.add_subplot(221)
ax2 = fig.add_subplot(222)
ax3 = fig.add_subplot(223)
ax4 = fig.add_subplot(224)
```

```python
sns.barplot(x = np.linspace(start=1, stop=8, num=8),
            y = eig_val_centred_data / sum(eig_val_centred_data),
            color = 'blue', ax = ax1).set_title('Barplot du ratio de variance expliquée (données centrées)', fontsize=12)

sns.barplot(x = np.linspace(start=1, stop=8, num=8),
            y = eig_val_standard_data / sum(eig_val_standard_data),
            color = 'black', ax=ax2).set_title('Barplot du ratio de variance expliquée (données standardisées)', fontsize=12)

sns.barplot(x = np.linspace(start=1, stop=8, num=8),
            y = np.cumsum(eig_val_centred_data / sum(eig_val_centred_data)),
            color = 'blue', ax = ax3).set_title('Barplot de la variance expliquée cumulée (données centrées)', fontsize=12)

sns.barplot(x = np.linspace(start=1, stop=8, num=8),
            y = np.cumsum(eig_val_standard_data / sum(eig_val_standard_data)),
            color = 'black', ax = ax4).set_title('Barplot de la variance expliquée cumulée (données standardisées)', fontsize=12)

plt.show()
```

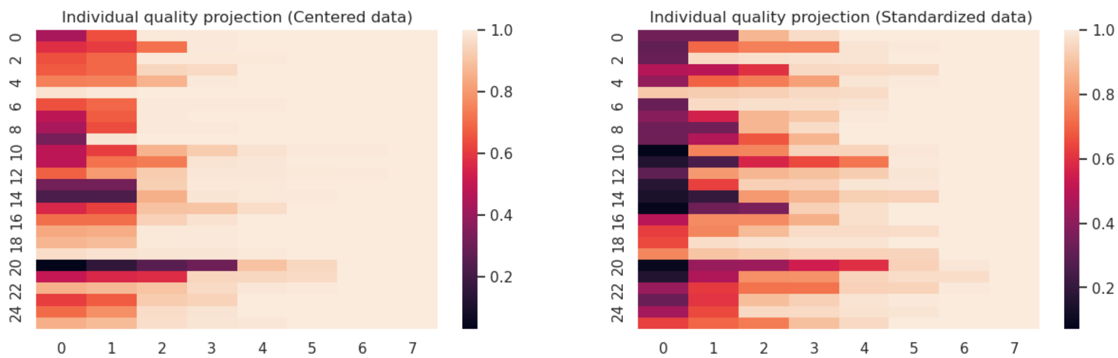


Les trois premières valeurs sont elles-mêmes les plus significatives, comme nous pouvons le constater pour les valeurs qui sont soit centrées (en bleu), soit bien réduites (en noir). Ainsi, selon l'ACP, nous pouvons réduire nos huit variables à trois.

4. Nouvelles coordonnées et matrice de qualité.

[192]:
```
def new_coord(data):
    '''
    On definit les nouvelles coordonnées suivant les hyperplans calculés avant
    '''
    _, eig_vect = hyperplans(data, data.shape[1])
    return np.dot(data, eig_vect)

def individual_quality_projection(coordinates_matrix):
    '''
    This function calculates the quality of each individual projection on 1, 2,␣
 ↪..., p hyperplans
    La formule de qualité peut être interprétée en faisant un simple calcul␣
 ↪matriciel
    '''
    individual_quality_projection_matrix = np.dot(np.
 ↪multiply(coordinates_matrix, coordinates_matrix),
                                                   np.triu(np.
 ↪ones((coordinates_matrix.shape[1],
                                                                             ␣
 ↪coordinates_matrix.shape[1]))))

    individual_quality_projection_matrix = np.
 ↪multiply(individual_quality_projection_matrix,
                                                         np.divide(1.0,␣
 ↪individual_quality_projection_matrix[:, -1:]))

    return individual_quality_projection_matrix


coord1 = new_coord(data_centered)
coord2 = new_coord(data_centered_reduced)

quality_centered = individual_quality_projection(coord1)
quality_reduced = individual_quality_projection(coord2)

fig = plt.figure(figsize= (15, 9))
ax1 = fig.add_subplot(221)
ax2 = fig.add_subplot(222)
sns.heatmap(quality_centered, ax = ax1).set_title('Individual quality␣
 ↪projection (Centered data)', fontsize=12)
```

```
sns.heatmap(quality_reduced, ax = ax2).set_title(' Individual quality projection (Standardized data)', fontsize=12)
plt.show()
```



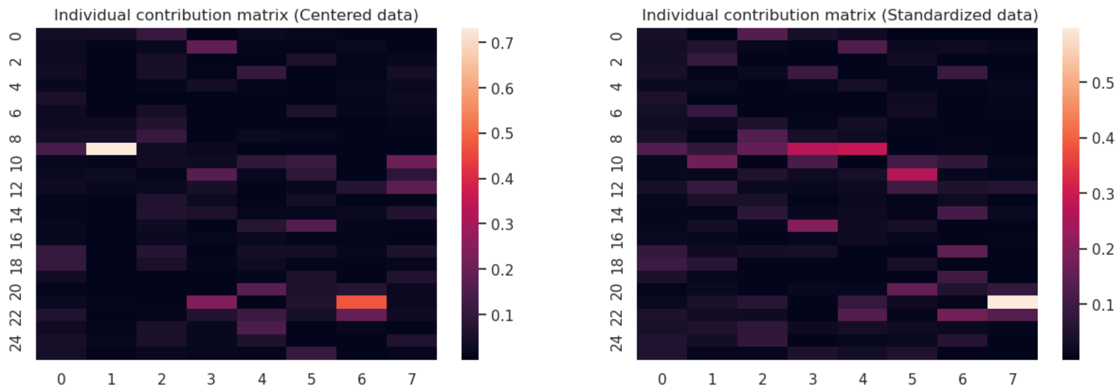
Une “carte thermique” est plus facile à comprendre. Et la nous constatons que les trois premiers sont aussi les plus significatifs. Et les nous constatons que la qualité est distribuée de manière plus uniforme que les vecteurs purs.

5. Contribution de l’individu

[193]:
```
def individual_contribution_matrix(coordinates_matrix):
    n = coordinates_matrix.shape[0]

    # Extract sorted eigen values
    eig_val, _ = hyperplans(pd.DataFrame(coordinates_matrix), coordinates_matrix.shape[1])
    denominator = eig_val * n

    individual_contribution_matrix = np.multiply(coordinates_matrix, coordinates_matrix)

    individual_contribution_matrix = np.multiply(individual_contribution_matrix, np.divide(1.0, denominator))

    return individual_contribution_matrix

individual_contribution_centered_data = individual_contribution_matrix(coord1)
individual_contribution_standardized_data = individual_contribution_matrix(coord2)
```

[194]:
```
fig = plt.figure(figsize= (15, 10))
ax1 = fig.add_subplot(221)
ax2 = fig.add_subplot(222)
```

```python
sns.heatmap(individual_contribution_centered_data, ax = ax1).set_title('Individual contribution matrix (Centered data)',fontsize=12)
sns.heatmap(individual_contribution_standardized_data, ax = ax2).set_title('Individual contribution matrix (Standardized data)', fontsize=12)
plt.show()
```



6. Comparaison avec ACP.

[195]:
```python
from sklearn.decomposition import PCA

pca_center = PCA()
pca_center.fit(data_centered)
pd.DataFrame(pca_center.components_.transpose())
```

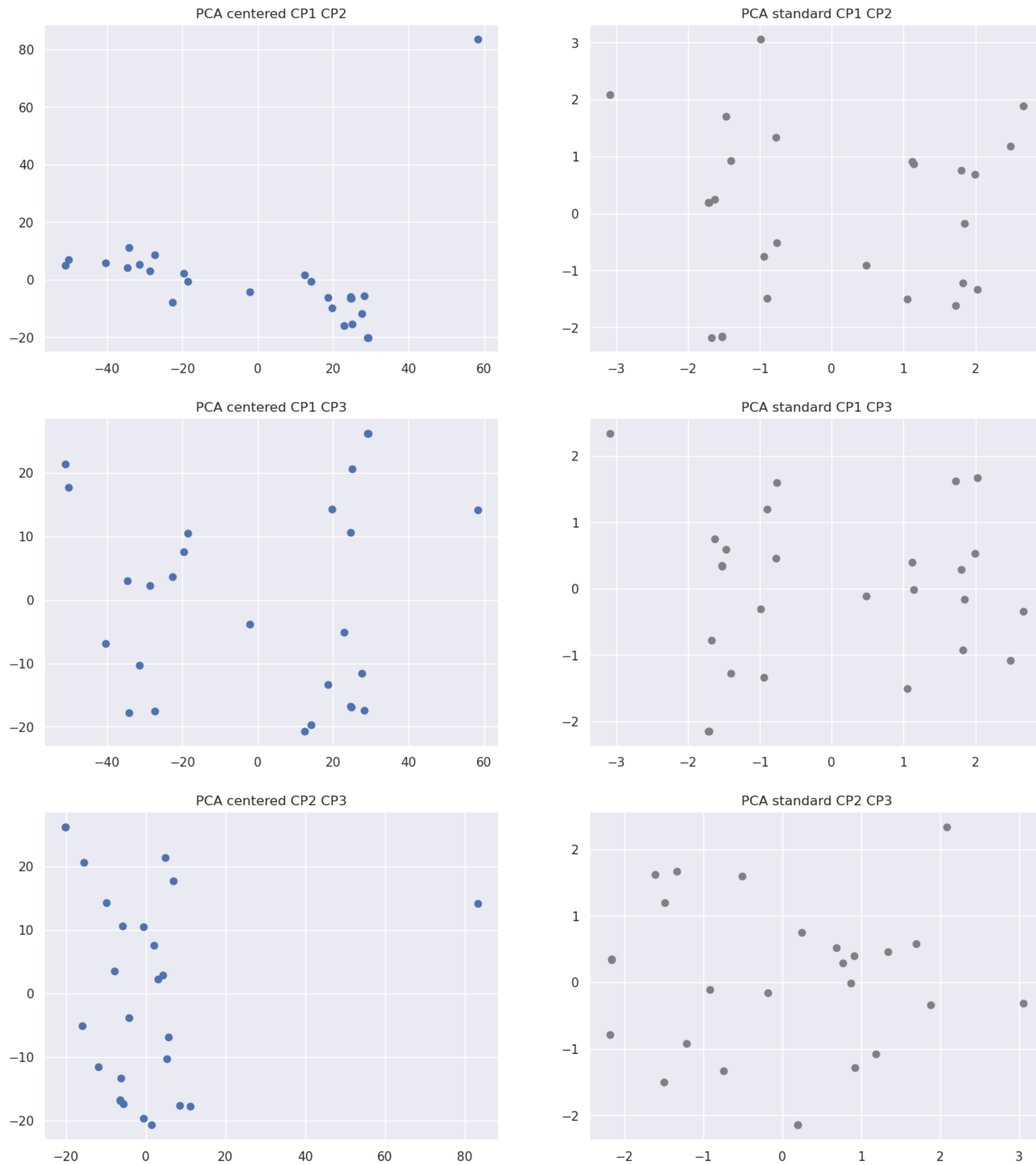
[195]:

	0	1	2	3	4	5	6	7
0	0.605395	-0.460576	0.358994	0.296908	0.225960	0.006081	0.391084	0.017140
1	-0.050085	0.145526	-0.192659	-0.564511	0.604647	-0.010916	0.503727	0.032638
2	-0.010371	0.016962	0.023002	-0.101135	-0.308517	0.640599	0.231258	0.655604
3	0.009834	-0.024161	-0.068854	0.087402	0.140657	-0.623491	-0.151071	0.745380
4	0.280568	0.086156	-0.011420	-0.385747	-0.670406	-0.411831	0.368618	-0.099998
5	-0.060801	-0.048967	-0.755556	0.511207	-0.079480	-0.018210	0.390375	-0.051636
6	-0.591480	0.199047	0.503491	0.313874	-0.044240	-0.166773	0.478158	-0.010281
7	-0.445556	-0.846392	-0.065095	-0.258176	-0.103244	-0.054638	0.010129	-0.021463

Same eigen vectors as the ones we got for the centered data as calculated previously.

7. Nuage des points.

[196]:
```
PCA_centered = new_coord(data_centered)
PCA_standard = new_coord(data_centered_reduced)

fig = plt.figure(figsize= (16, 18))
ax1 = fig.add_subplot(321)
ax2 = fig.add_subplot(322)
ax3 = fig.add_subplot(323)
ax4 = fig.add_subplot(324)
ax5 = fig.add_subplot(325)
ax6 = fig.add_subplot(326)

ax1.scatter(PCA_centered[:, 0], PCA_centered[:, 1])
ax1.set_title('PCA centered CP1 CP2')

ax3.scatter(PCA_centered[:, 0], PCA_centered[:, 2])
ax3.set_title('PCA centered CP1 CP3')

ax5.scatter(PCA_centered[:, 1], PCA_centered[:, 2])
ax5.set_title('PCA centered CP2 CP3')

ax2.scatter(PCA_standard[:, 0], PCA_standard[:, 1],  c='gray')
ax2.set_title('PCA standard CP1 CP2')

ax4.scatter(PCA_standard[:, 0], PCA_standard[:, 2],  c='gray')
ax4.set_title('PCA standard CP1 CP3')

ax6.scatter(PCA_standard[:, 1], PCA_standard[:, 2],  c='gray')
ax6.set_title('PCA standard CP2 CP3')

plt.show()
```



Nous pouvons regarder que nous avons des nuages des points différents entre les données centrées et les données réduites. Nous remarquons qu'il existe une relation entre les variables dans le cas PCA centralisés.

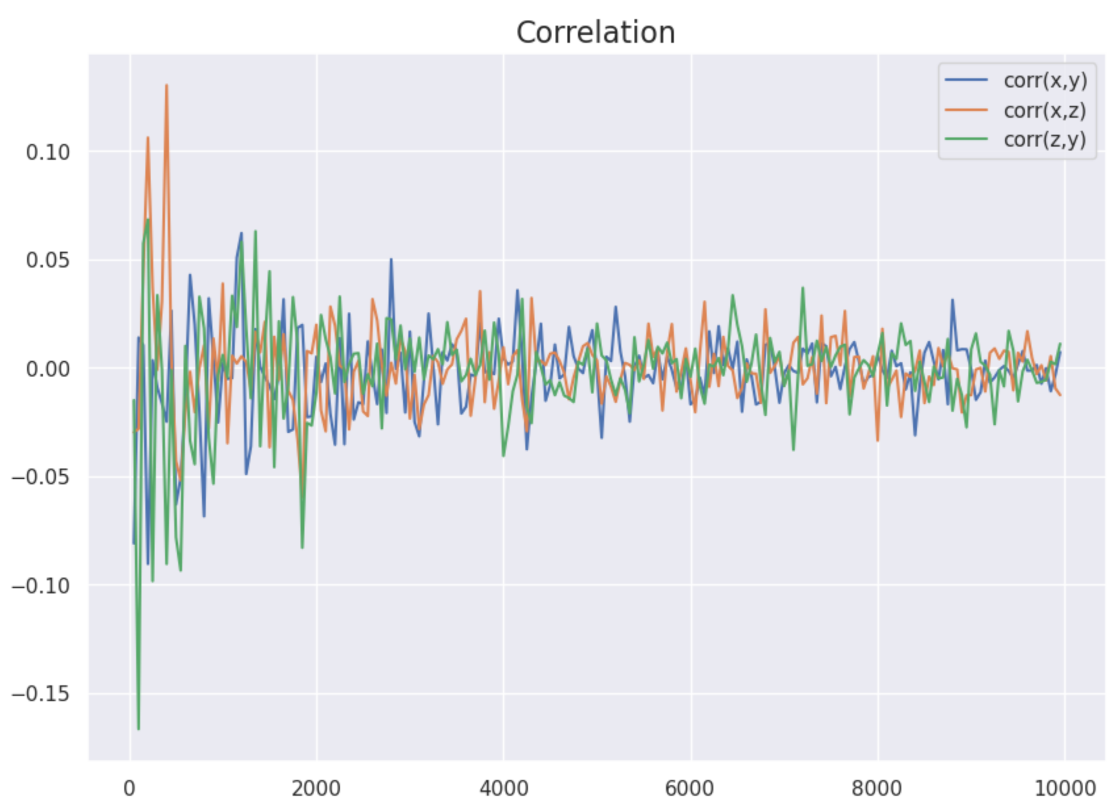
1.4 Partie 3 - Etude de la forme du nuage initiale et réduction de dimension

Nuage Isotropes

[197]:
```
V = np.random.normal(0, 1, (1000, 3))
V = pd.DataFrame(V)/np.linalg.norm(V)
```

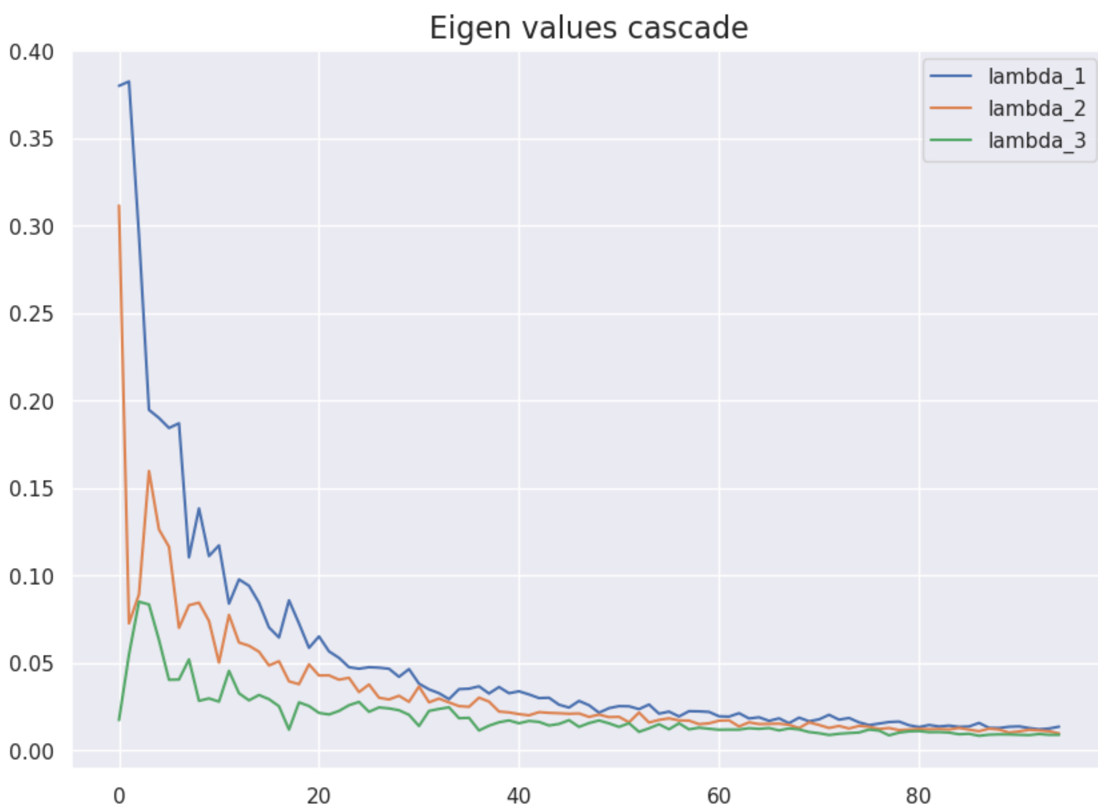
```
V.columns = ['x', 'y', 'z']

fig = px.scatter_3d(V , x='x', y='y', z='z', opacity=0.3)
fig.show()
```

[198]:
```
def generate_isotrope_cor(sample_size):
    V = np.random.normal(0, 1, (sample_size, 3))
    V = pd.DataFrame(V)/np.linalg.norm(V)
    cor_V = np.corrcoef(np.transpose(V))

    return [cor_V[0, 1], cor_V[0, 2], cor_V[1, 2]]

corr = np.asarray([generate_isotrope_cor(sample_size=k) for k in range(1,␣
 ↪10000, 50)])
corr = pd.DataFrame(corr)
corr.columns = ['corr(x,y)', 'corr(x,z)', 'corr(z,y)']

plt.figure(figsize = (10, 7))
plt.plot(range(1, 10000 , 50),corr)
plt.legend(['corr(x,y)', 'corr(x,z)', 'corr(z,y)'])
plt.title('Correlation', size=16)
plt.show()
```



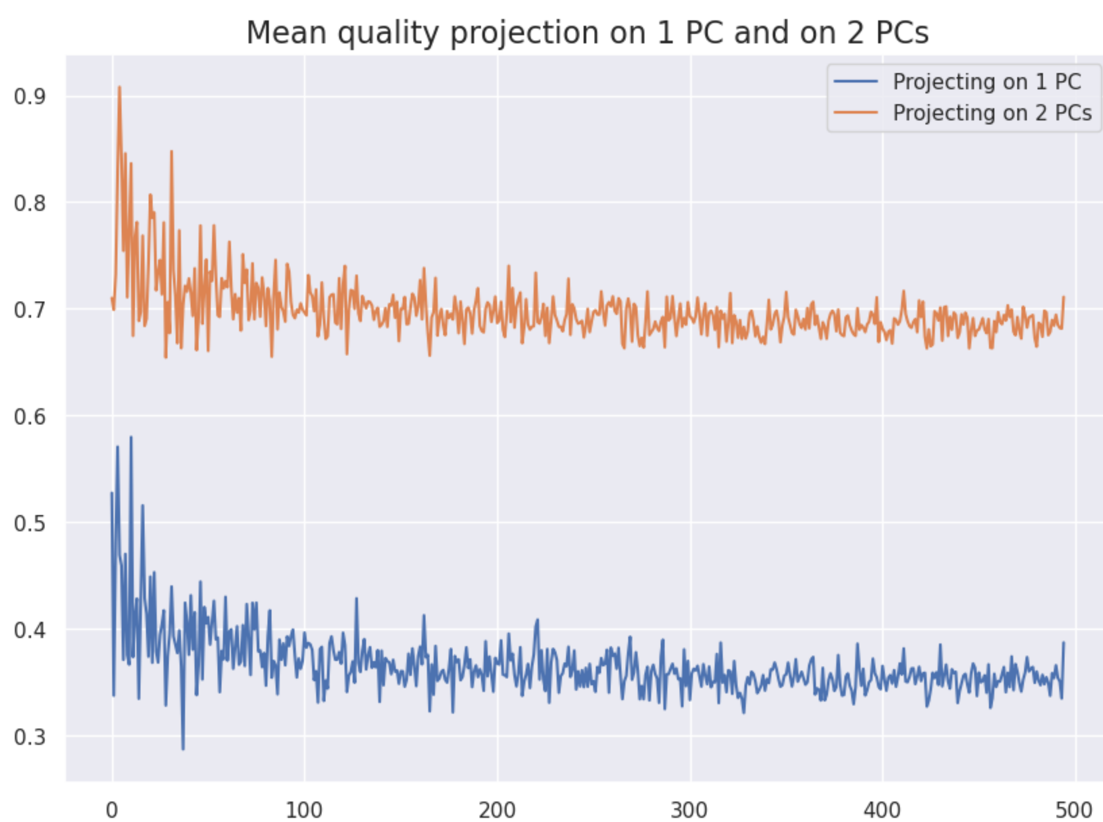
Nous voyons qu'avec l'augmentation de nombres d'observation, les 3 composants sont moins corrélés.

[199]:
```
def eigen_values_cascade(sample_size):
    V = np.random.normal(0, 1, (sample_size, 3))
    V = pd.DataFrame(V) / np.linalg.norm(V)
    V.columns = ['x', 'y', 'z']

    V_eigen_values = hyperplans(V, 3)[0]
    return V_eigen_values

eigen_cascade = np.asarray([eigen_values_cascade(k) for k in range(5, 100)])
eigen_cascade = pd.DataFrame(eigen_cascade)/np.linalg.norm(eigen_cascade)
eigen_cascade.columns = ['lambda_1', 'lambda_2', 'lambda_3']
plt.figure(figsize = (10, 7))
plt.plot(eigen_cascade)
plt.legend(['lambda_1', 'lambda_2', 'lambda_3'])
plt.title('Eigen values cascade', size=16)
plt.show()
```



Même remarque pour les valeurs propres

[200]:
```
def individual_quality_projection_stabilization(sample_size):
    V = np.random.normal(0, 1, (sample_size, 3))
    V = pd.DataFrame(V)/np.linalg.norm(V)
    V.columns = ['x', 'y', 'z']
    individual_quality_projection_matrix =␣
 ↪individual_quality_projection(new_coord(V))
    mean_projection_on_1 = np.mean(individual_quality_projection_matrix[:, 0])
    mean_projection_on_2 = np.mean(individual_quality_projection_matrix[:, 1])

    return [mean_projection_on_1, mean_projection_on_2]

quality = np.asarray([individual_quality_projection_stabilization(k) for k in␣
 ↪range(5, 500)])
quality = pd.DataFrame(quality)

plt.figure(figsize = (10, 7))
plt.plot(quality)
plt.title('Mean quality projection on 1 PC and on 2 PCs', size=16)
plt.legend(['Projecting on 1 PC', 'Projecting on 2 PCs'])
plt.show()
```



C'est claire que avec l'augmentation du nombre d'observation, la qualité moyenne se stabilize et atteint 33% pour une projection sur 1 seul axe et 66% pour une projection sur 2 axes.

Nuage *non Isotropes*

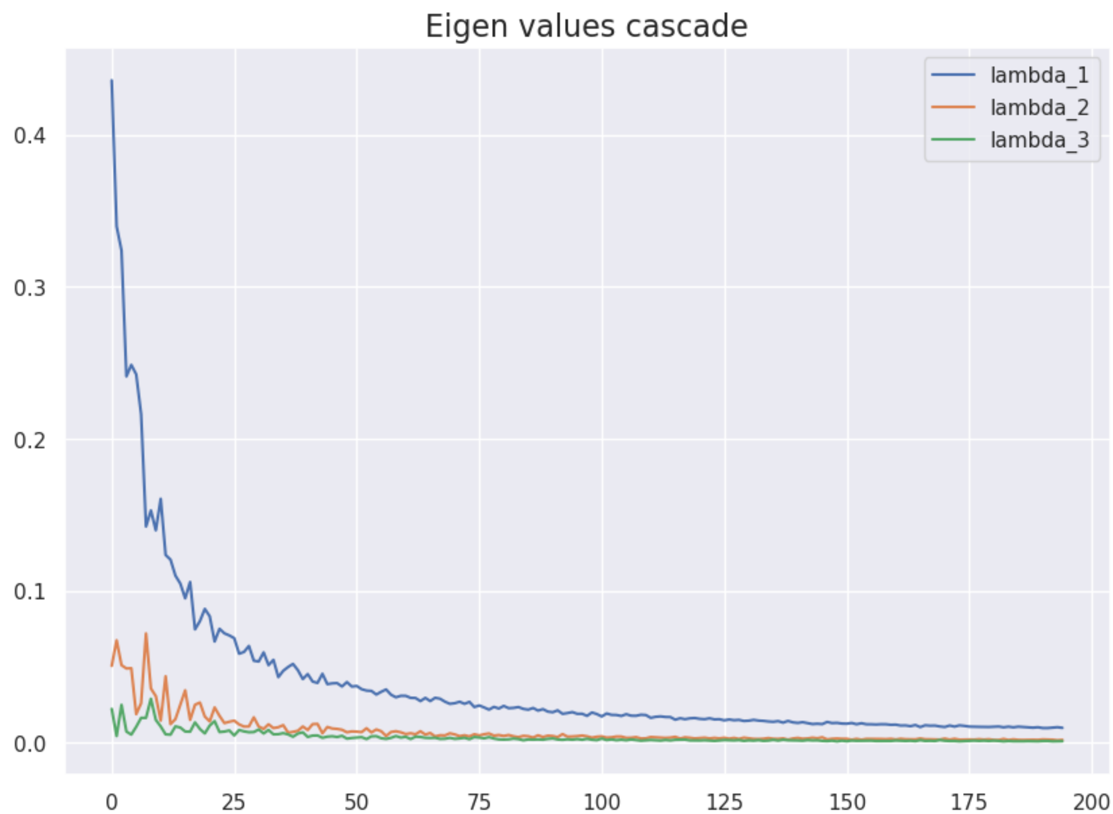
[201]:
```
V = np.random.normal(0, 1, (900, 3))
V = pd.DataFrame(V)

V.columns = ['x', 'y', 'z']
V['x'] = np.sort(V['x'])
V['z'] = V['z'] + np.arctan2(V['x'], V['y'])

V = pd.DataFrame(V)/np.linalg.norm(V)


fig = px.scatter_3d(V , x='x', y='y', z='z', opacity=0.3)
fig.show()
```

[202]:
```
def generate_non_isotrope_cor(sample_size):
    V = np.random.normal(0, 1, (sample_size, 3))
    V = pd.DataFrame(V)

    V.columns = ['x', 'y', 'z']
    V['x'] = np.sort(V['x'])
    V['z'] = V['z'] + np.arctan2(V['x'], V['y'])

    V = pd.DataFrame(V) / np.linalg.norm(V)

    cor_V = np.corrcoef(np.transpose(V))

    return [cor_V[0, 1], cor_V[0, 2], cor_V[1, 2]]

corr = np.asarray([generate_non_isotrope_cor(sample_size=k) for k in range(1,␣
↪10000 , 50)])
corr = pd.DataFrame(corr)
corr.columns = ['corr(x,y)', 'corr(x,z)', 'corr(z,y)']

plt.figure(figsize = (10, 7))
plt.plot(range(1, 10000, 50),corr)
plt.title('Correlation', size=16)
plt.legend(['corr(x,y)', 'corr(x,z)', 'corr(z,y)'])
plt.show()
```

Les corrélations sont très fortes toujours.

[203]:
```
def eigen_values_cascade(sample_size=3):
    V = np.random.normal(0, 1, (sample_size, 3))
    V = pd.DataFrame(V)

    V.columns = ['x', 'y', 'z']
    V['x'] = np.sort(V['x'])
    V['z'] = V['z'] + np.arctan2(V['x'], V['y'])

    V = pd.DataFrame(V) / np.linalg.norm(V)

    V_eigen_values = hyperplans(V, 3)[0]

    return V_eigen_values

eigen_cascade = np.asarray([eigen_values_cascade(k) for k in range(5, 200)])
eigen_cascade = pd.DataFrame(eigen_cascade)/np.linalg.norm(eigen_cascade)
eigen_cascade.columns = ['lambda_1', 'lambda_2', 'lambda_3']

plt.figure(figsize = (10, 7))
plt.plot(eigen_cascade)
```

```
plt.title('Eigen values cascade', size=16)
plt.legend(['lambda_1', 'lambda_2', 'lambda_3'])
plt.show()
```

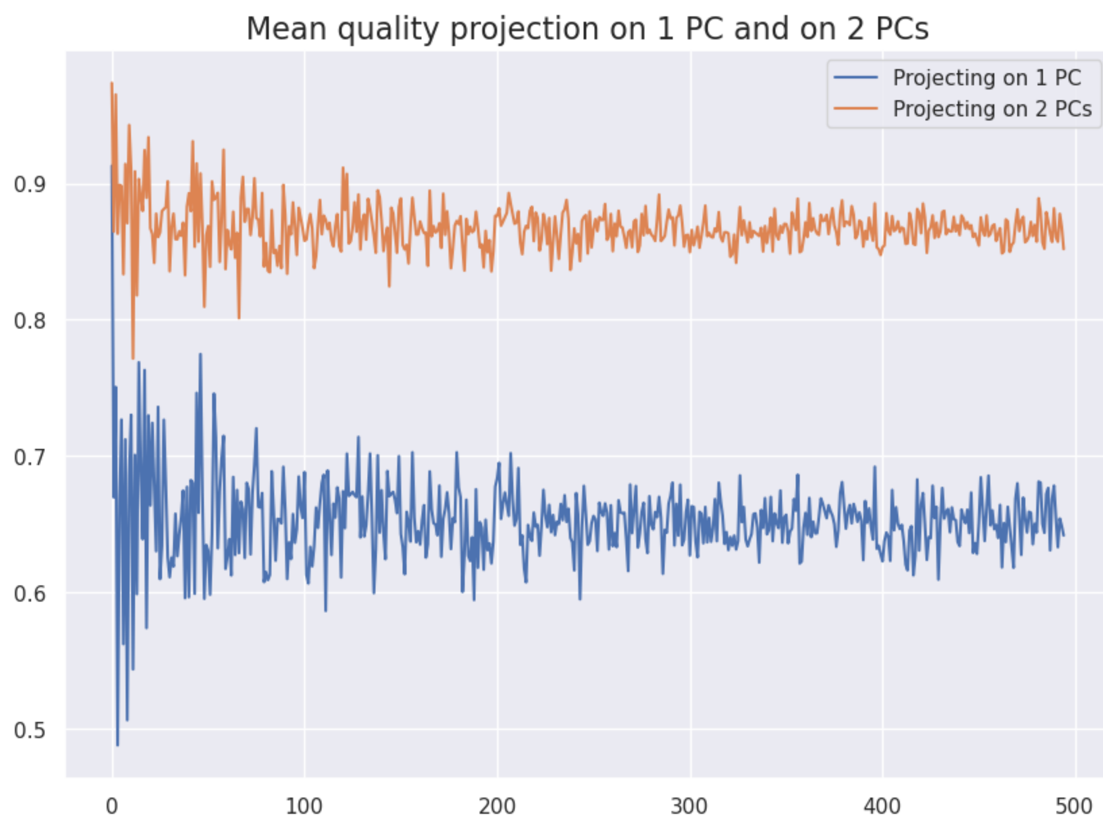


Lambda_2 et Lambda_3 sont presque nulles quand le nombre de points est grand à cause de la correlation entre les variables.

Seul lambda_1 a une valeur > 0 quand le nombre de points est grand.

[204]:
```
def individual_quality_projection_stabilization(sample_size=3):
    V = np.random.normal(0, 1, (sample_size, 3))
    V = pd.DataFrame(V)

    V.columns = ['x', 'y', 'z']
    V['x'] = np.sort(V['x'])
    V['z'] = V['z'] + np.arctan2(V['x'], V['y'])
    V = pd.DataFrame(V) / np.linalg.norm(V)

    mean_projection_PC1 = np.mean(individual_quality_projection(new_coord(V))[:
↪, 0])
    mean_projection_PC2 = np.mean(individual_quality_projection(new_coord(V))[:
↪, 1])
```

```
    return [mean_projection_PC1, mean_projection_PC2]

corr_stablization = np.asarray([individual_quality_projection_stabilization(k)␣
 ↪for k in range(5, 500)])
corr_stablization = pd.DataFrame(corr_stablization)
corr_stablization.columns = ['PC1', 'PC1_and2']

plt.figure(figsize = (10, 7))
plt.plot(corr_stablization)
plt.title('Mean quality projection on 1 PC and on 2 PCs', size=16)
plt.legend(['Projecting on 1 PC', 'Projecting on 2 PCs'])
plt.show()
```



Une projection sur 1 axe principal explique entre 60% et 70% de la variance.

Une projection sur 2 axes principal explique plus que 85% des informations.

Points extrémaux

[205]:
```
V = np.random.normal(0, 1, (900, 3))
V = pd.DataFrame(V)
```

```
V.columns = ['x', 'y', 'z']
V['x'] = np.sort(V['x'])
V['z'] = V['z'] + np.arctan2(V['x'], V['y'])
V = pd.DataFrame(V)/np.linalg.norm(V)

V_with_outliers = V.copy()
outliers = pd.DataFrame([[100, 0, 0]], columns=['x', 'y', 'z'])
V_with_outliers = V_with_outliers.add(outliers, fill_value=0)
V_with_outliers = V_with_outliers - V_with_outliers.mean()

fig = px.scatter_3d(V_with_outliers , x='x', y='y', z='z', opacity=0.3)
fig.show()
```

[206]:
```
eigen_values, eigen_vectors = hyperplans(V_with_outliers, 3)
first_principal_component = eigen_vectors[:, 0]
print("Eigen values: ", eigen_values)
print("First principal component: ", first_principal_component.round(3))
```

```
Eigen values:  [1.11018312e+01 7.84084122e-04 1.62120748e-04]
First principal component:  [ 1.  0. -0.]
```

[207]:
```
V_with_outliers_standardized = V_with_outliers.copy()
V_with_outliers_standardized = (V_with_outliers_standardized -
 ↪V_with_outliers_standardized.mean()) / V_with_outliers_standardized.std()
eigen_values, eigen_vectors = hyperplans(V_with_outliers_standardized, 3)
first_principal_component = eigen_vectors[:, 0]
print("Eigen values: ", eigen_values)
print("First principal component: ", first_principal_component.round(3))
```

```
Eigen values:  [1.02172155 0.99933969 0.97893875]
First principal component:  [ 0.701  0.242 -0.671]
```

Comme nous pouvons le voir, dans le cas de données centrées (et non centrées), la première composante primaire, qui représente la majorité de la variance, est entièrement orientée vers le point décentré [100, 0, 0], l'ACP est alors affecté par les valeurs aberrantes. Alors que dans le cas de données normées, l'effet est réduit: la première n'est plus tirée vers le point décentré, mais on a perdu les correlations, alors il faut penser à régler le problémes des points aberrants.

1.5 Partie 4. Etude de la forme du nuage initiale sur la réduction de dimension dans les deux espaces

Nuage Isotrope

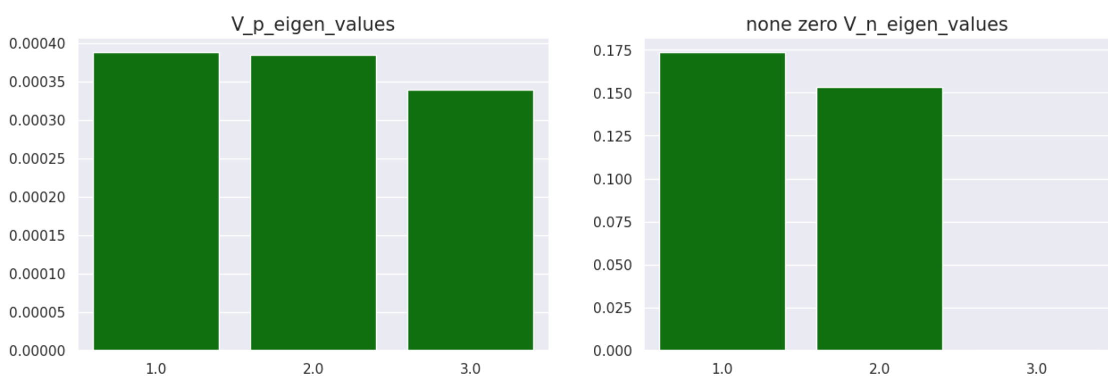
[271]:
```
V = np.random.normal(0, 1, (900, 3))
V = pd.DataFrame(V)/np.linalg.norm(V)

V_p = pd.DataFrame(V)
```

```python
V_n = pd.DataFrame(np.transpose(V))

V_p_eigen_values, V_p_eigen_vectors = hyperplans(V_p, k=3)
V_n_eigen_values, V_n_eigen_vectors = hyperplans(V_n, k=900)

print("The eigen values for the Rp problem are:")
print(V_p_eigen_values)
print("\n")
print("The eigen values (truncated as shape p) for the Rn problem are:")
print(V_n_eigen_values[0:3].astype(float))
```

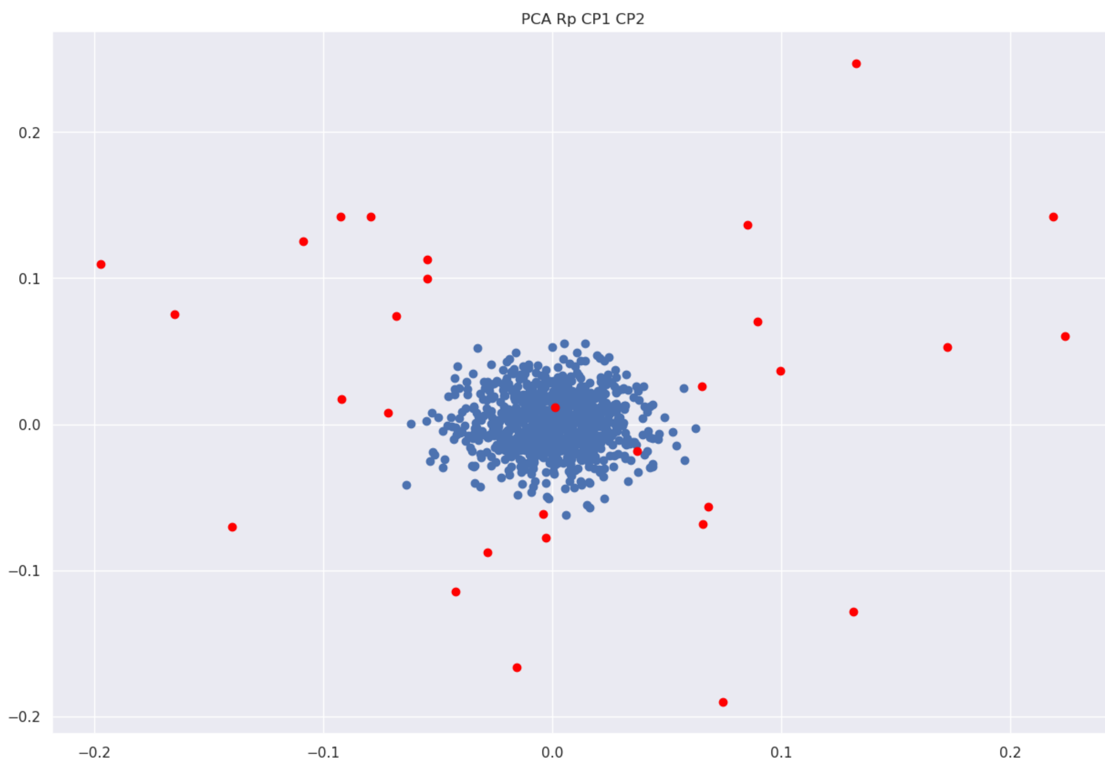
```
The eigen values for the Rp problem are:
[0.00038769 0.0003846  0.00033929]


The eigen values (truncated as shape p) for the Rn problem are:
[1.73351768e-01 1.53132266e-01 7.50053903e-18]
```

[272]:

```python
fig = plt.figure(figsize=(15, 10))
ax1 = fig.add_subplot(221)
ax2 = fig.add_subplot(222)

sns.barplot(x=np.linspace(start=1, stop=3, num=3),
            y=V_p_eigen_values,
            color='green',
            ax=ax1).set_title('V_p_eigen_values', fontsize=15)

sns.barplot(x=np.linspace(start=1, stop=3, num=3),
            y=V_n_eigen_values[:3],
            color = 'green', ax=ax2).set_title('none zero V_n_eigen_values ',␣
 ↪fontsize=15)
plt.show()
```



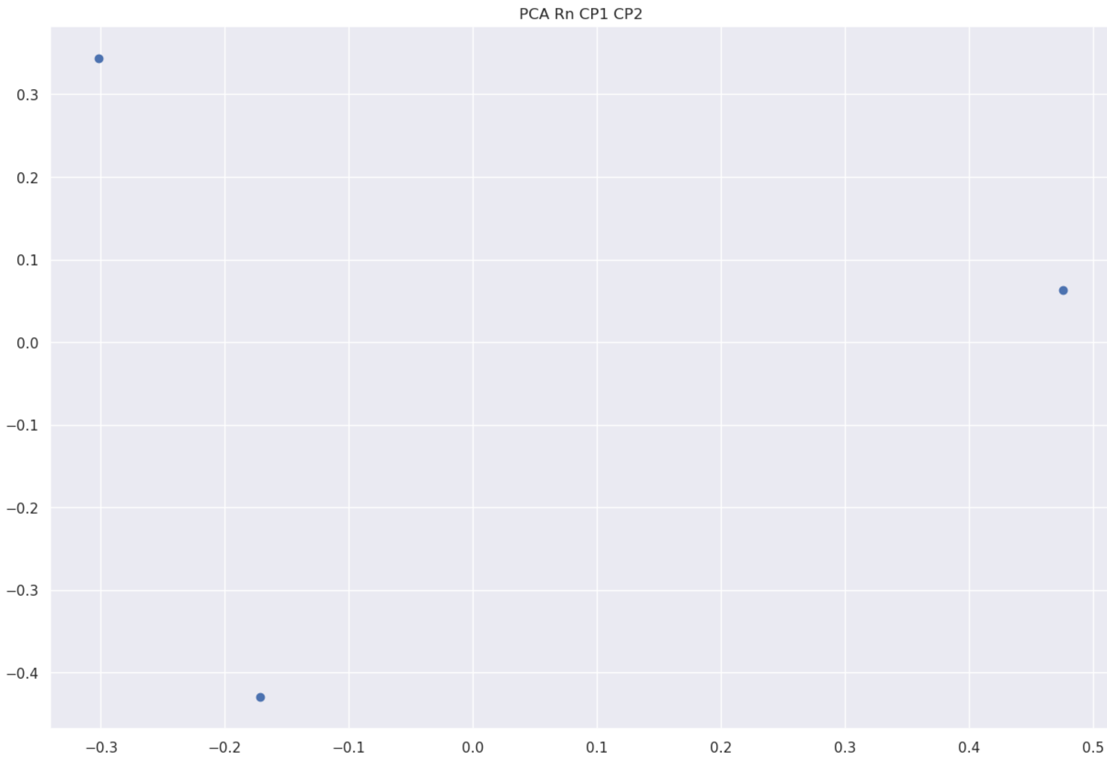
[273]:
```
X_p_new_coord_isotrope = np.dot(V_p, V_p_eigen_vectors)

new_V = np.random.normal(0, 1, (30, 3))
new_V = pd.DataFrame(new_V)/np.linalg.norm(new_V)

new_V_p = pd.DataFrame(new_V)
additional_point = np.dot(new_V_p, V_p_eigen_vectors)

fig = plt.figure(figsize= (15, 10))
ax1 = fig.add_subplot(111)
ax1.scatter(X_p_new_coord_isotrope[:, 0], X_p_new_coord_isotrope[:, 1])
ax1.scatter(additional_point[:30, 0], additional_point[:30, 1], c='red')
ax1.set_title('PCA Rp CP1 CP2')
plt.show()
```



Les points en rouges montrent les nouvelles observations.

[280]:
```
X_n_new_coord_isotrope = np.dot(V_n, V_n_eigen_vectors)

fig = plt.figure(figsize=(15, 10))
ax1 = fig.add_subplot(111)
ax1.scatter(X_n_new_coord_isotrope[:, 0], X_n_new_coord_isotrope[:, 1])
ax1.set_title('PCA Rn CP1 CP2')
```

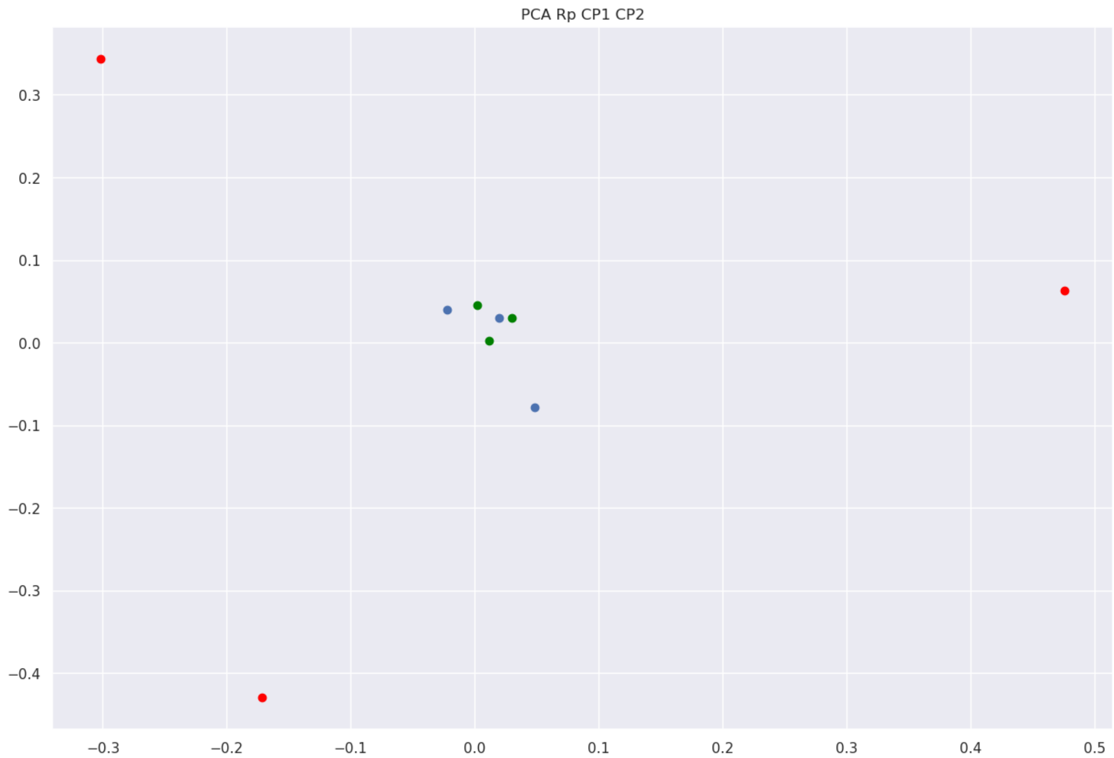
```
plt.show()
```



Formule de passage

[284]:
```
estimated_dual_vectors = np.zeros(V_n_eigen_vectors.shape)
for i in range(V_p_eigen_vectors.shape[0]):
    estimated_dual_vectors[i] = np.dot(V_p, np.transpose(V_p_eigen_vectors)[i])␣
 ↪/ np.sqrt(V_p_eigen_values[i])
print('The sum of absolute differences between the V_p_eigen_vectors and the␣
 ↪vectors calculated is:')
print(round(np.mean(abs(estimated_dual_vectors[:3]) - abs(V_n_eigen_vectors[:3].
 ↪astype(float))), 4))

estimated_projection = np.dot(V_n, estimated_dual_vectors)

fig = plt.figure(figsize= (15, 10))
ax1 = fig.add_subplot(111)
ax1.scatter(estimated_projection[:, 0], estimated_projection[:, 1])
ax1.scatter(X_n_new_coord_isotrope[:, 0], X_n_new_coord_isotrope[:, 1], c='red')
ax1.scatter(additional_point[:, 0], additional_point[:, 1], c='green')
ax1.set_title('PCA Rp CP1 CP2')
plt.show()
```

```
The sum of absolute differences between the V_p_eigen_vectors and the vectors
calculated is:
0.7961
```



Les points en blue sont projetés en utilisant les vecteurs estimés, ceux en rouges sont les originales, et ceux en vert sont les points additionnels.

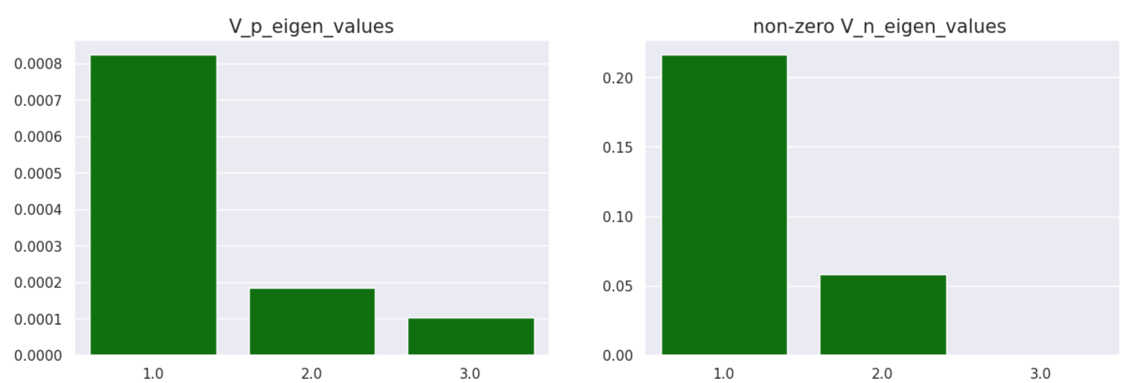
Nuage Non isotrope

[213]:
```python
V = np.random.normal(0, 1, (900, 3))
V = pd.DataFrame(V)

V.columns = ['x', 'y', 'z']
V['x'] = np.sort(V['x'])
V['z'] = V['z'] + np.arctan2(V['x'], V['y'])
V = pd.DataFrame(V)/np.linalg.norm(V)
V_p = pd.DataFrame(V)
V_n = pd.DataFrame(np.transpose(V_p))

V_p_eigen_values, V_p_eigen_vectors = hyperplans(V_p, k=3)
V_n_eigen_values, V_n_eigen_vectors = hyperplans(V_n, k=900)

print("The eigen values for the Rp problem are:")
print(V_p_eigen_values)
```

```
print("\n")
print("The eigen values (truncated as shape p) for the Rn problem are:")
print(V_n_eigen_values[0:3].astype(float))
```

```
The eigen values for the Rp problem are:
[0.00082343 0.00018593 0.00010277]


The eigen values (truncated as shape p) for the Rn problem are:
[2.16154621e-01 5.79760636e-02 8.77324541e-18]
```

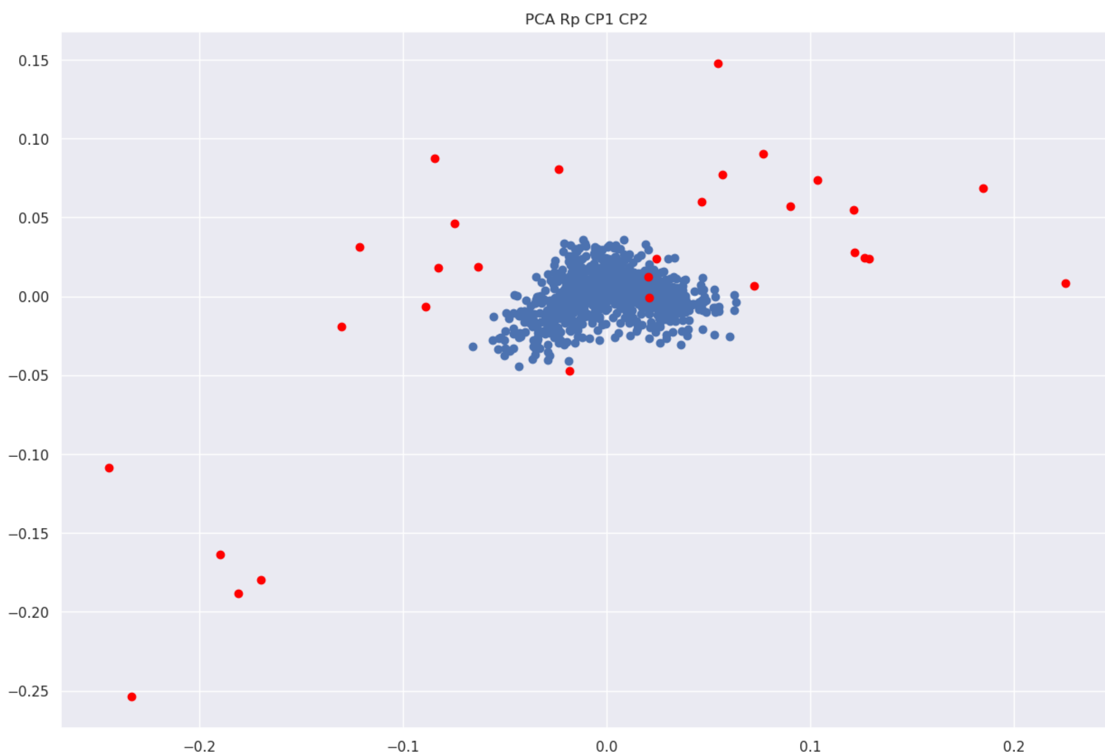
[214]:
```
fig = plt.figure(figsize= (15, 10))
ax1 = fig.add_subplot(221)
ax2 = fig.add_subplot(222)

sns.barplot(x=np.linspace(start=1, stop=3, num=3),
            y=V_p_eigen_values,
            color = 'green',
            ax=ax1).set_title('V_p_eigen_values', fontsize=15)

sns.barplot(x=np.linspace(start=1, stop=3, num=3),
            y=V_n_eigen_values[:3],
            color = 'green', ax=ax2).set_title('non-zero V_n_eigen_values ',␣
 ↪fontsize=15)
plt.show()

X_p_new_coord_non_isotrope = np.transpose(np.dot(V_p_eigen_vectors, np.
 ↪transpose(np.array(V_p))))
```



Comme nous le voyons dans le cas d'un nuage de points non isotrope, la première composante principale est très grande par rapport au cas isotrope, ceci parce que le premier (isotrope) vérifie l'uniformité dans toutes les orientations, tandis que dans le cas non isotrope il y a une direction qui détient une grande partie de la variance totale qui est le premier composant principal.

[291]:

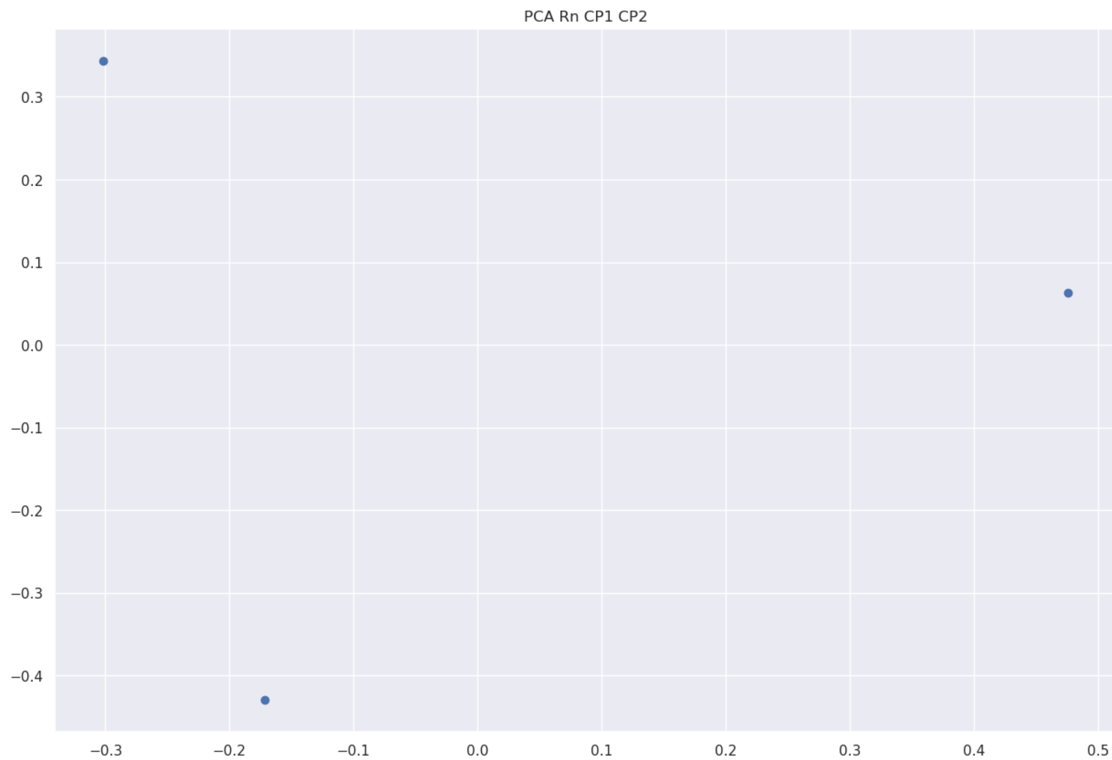
```
new_V = np.random.normal(0, 1, (30, 3))
new_V = pd.DataFrame(new_V)

new_V.columns = ['x', 'y', 'z']
new_V['x'] = np.sort(new_V['x'])
new_V['z'] = new_V['z'] + np.arctan2(new_V['x'], new_V['y'])
new_V = pd.DataFrame(new_V)/np.linalg.norm(new_V)
new_V_n = pd.DataFrame(np.transpose(new_V_p))

new_V = pd.DataFrame(new_V)/np.linalg.norm(new_V)

new_V_p = pd.DataFrame(new_V)
additional_point = np.dot(new_V_p, V_p_eigen_vectors)

fig = plt.figure(figsize= (15, 10))
ax1 = fig.add_subplot(111)
ax1.scatter(X_p_new_coord_non_isotrope[:, 0], X_p_new_coord_non_isotrope[:, 1])
ax1.scatter(additional_point[:, 0], additional_point[:, 1], c='red')
ax1.set_title('PCA Rp CP1 CP2')
plt.show()
```



[293]:

```
X_n_new_coord_non_isotrope = np.dot(V_n, V_n_eigen_vectors)
```

```
fig = plt.figure(figsize=(15, 10))
ax1 = fig.add_subplot(111)
ax1.scatter(X_n_new_coord_non_isotrope[:, 0], X_n_new_coord_non_isotrope[:, 1])
ax1.set_title('PCA Rn CP1 CP2')
plt.show()
```

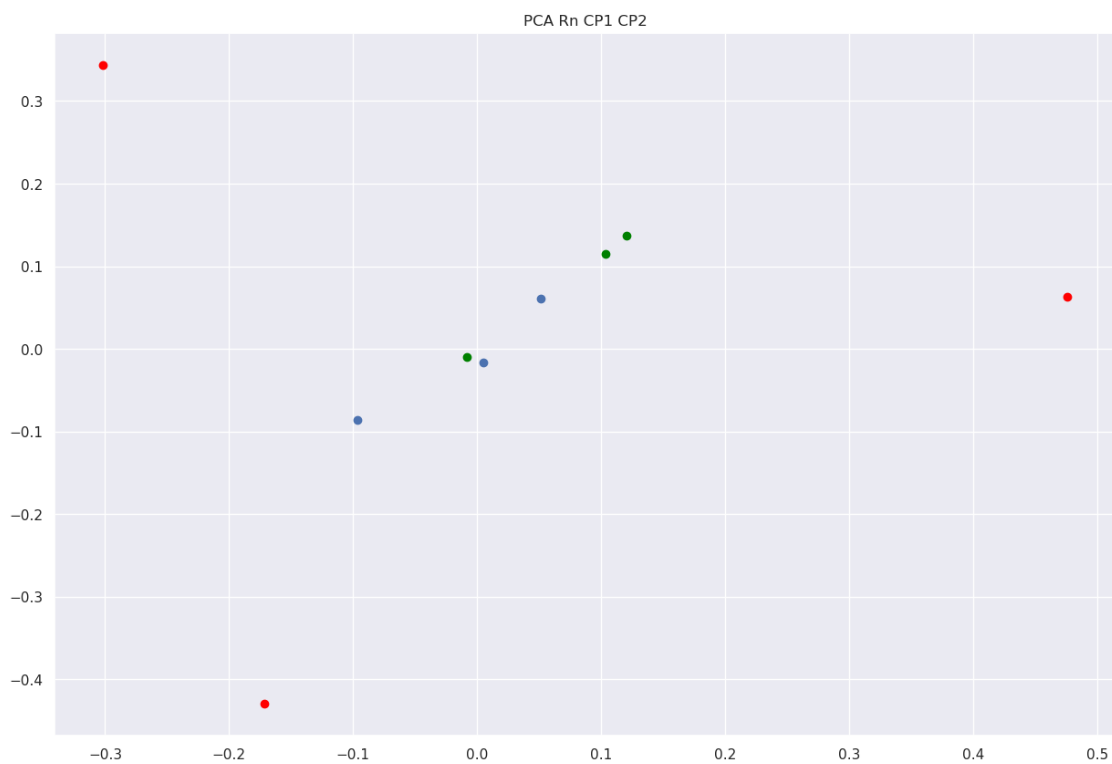


Formule de passage

[295]:
```
estimated_dual_vectors = np.zeros(V_n_eigen_vectors.shape)
for i in range(V_p_eigen_vectors.shape[0]):
    estimated_dual_vectors[i] = np.dot(V_p, np.transpose(V_p_eigen_vectors)[i])␣
 ↪/ np.sqrt(V_p_eigen_values[i])
print('The sum of absolute differences between the V_p_eigen_vectors and the␣
 ↪vectors calculated is:')
print(round(np.mean(abs(estimated_dual_vectors[:3]) - abs(V_n_eigen_vectors[:3].
 ↪astype(float))), 4))

estimated_projection = np.dot(V_n, estimated_dual_vectors)

new_V = np.random.normal(0, 1, (900, 3))
new_V = pd.DataFrame(new_V)

new_V.columns = ['x', 'y', 'z']
```

```
new_V['x'] = (6 * new_V['x'] + -15 * new_V['y'])
new_V['z'] = (3 * new_V['z'] + -12 * new_V['y'])
new_V = pd.DataFrame(new_V)/np.linalg.norm(new_V)
new_V = pd.DataFrame(new_V)
new_V_n = pd.DataFrame(np.transpose(new_V))

new_V_n = np.transpose(new_V)
additional_point = np.dot(new_V_n, estimated_dual_vectors)

fig = plt.figure(figsize= (15, 10))
ax1 = fig.add_subplot(111)
ax1.scatter(estimated_projection[:, 0], estimated_projection[:, 1])
ax1.scatter(X_n_new_coord_non_isotrope[:, 0], X_n_new_coord_non_isotrope[:, 1],
    c='red')
ax1.scatter(additional_point[:, 0], additional_point[:, 1], c='green')
ax1.set_title('PCA Rn CP1 CP2')
plt.show()
```

```
The sum of absolute differences between the V_p_eigen_vectors and the vectors
calculated is:
0.8215
```



À mesure que le nombre de dimensions augmente, la variance totale des données peut se disperser sur un plus grand nombre de composantes. Cela signifie que chaque composante individuelle explique une proportion plus faible de la variance totale, ce qui peut rendre l'interprétation des résultats plus difficile.

1.6 A - Partie 3

[296]:
```python
data = pd.read_excel('TP4_covC1234_DS19_20.xlsx', sheet_name='Feuil1')

# Remove the first column
data = data.iloc[:, 1:]
```

Traitement statistique des donnees

[297]:
```python
# Missing values represented by `?`
data.replace('?', np.nan, inplace=True)

# Remove the rows with missing values
data.dropna(inplace=True)

data.isnull().sum()
```

[297]:
```
B                  0
T                  0
E                  0
X                  0
9_ane              0
10_ane             0
13_ane             0
14_ane             0
1_M_2_PA           0
BTM                0
FormicAcid         0
aceticacid         0
NonaDecanoicAc     0
Tot_OcNoDecana     0
TYPE               0
SAISON             0
Campagne           0
Localisation       0
dtype: int64
```

[298]:
```python
data.describe()
```

[298]:
```
                B           T           E            X       9_ane  \
count  138.000000  138.000000  138.000000   138.000000  138.000000
mean    55.549380  208.588759  232.575160   883.284935  104.594599
std     33.461482  121.211625  430.588450  1235.511663   98.337371
min      0.000000   14.363178    0.000000    77.531698   11.659400
```

25%	22.995047	122.152279	115.743898	388.862905	52.562905
50%	51.822972	183.940552	152.687395	600.916311	75.211136
75%	76.072552	254.687341	227.745691	914.492120	121.364608
max	138.810642	675.650851	4844.955559	12987.880799	702.239764

	10_ane	13_ane	14_ane	1_M_2_PA	BTM \
count	138.000000	138.000000	138.000000	138.000000	138.000000
mean	266.418394	970.644372	1859.411419	311.633183	580.001283
std	476.821989	1498.088166	2383.823489	584.057749	1919.264999
min	0.000000	0.000000	0.000000	0.000000	36.620813
25%	73.441889	61.251710	70.950959	65.451691	209.225994
50%	177.613572	201.964257	1024.438774	128.358148	317.212636
75%	319.902277	593.251393	1917.443476	375.936027	487.307219
max	5316.464395	5176.410455	10996.742275	5191.044369	21891.220334

	FormicAcid	aceticacid	NonaDecanoicAc	Tot_OcNoDecana
count	138.000000	138.000000	138.000000	138.000000
mean	480.422784	342.809075	670.915135	630.614932
std	544.619533	668.040512	775.438631	806.915593
min	13.937401	0.000000	0.000000	0.000000
25%	57.525405	51.225189	55.616218	137.148926
50%	305.791366	172.396601	282.142846	336.084965
75%	742.841842	358.375749	1202.043049	708.645165
max	3618.024076	5624.216162	2981.690091	4466.795581

[299]:
```python
# Statistical indicators per `Campagne`, each `Campagne` in a separate table
for camp in data['Campagne'].unique():
    print('Campagne: ', camp)
    display(data[data['Campagne'] == camp].describe())
```

Campagne: BF2

	B	T	E	X	9_ane	10_ane \
count	18.000000	18.000000	18.000000	18.000000	18.000000	18.000000
mean	15.076719	102.754081	63.483194	210.014939	21.916648	36.558748
std	4.339949	38.150046	26.479410	83.844973	5.655037	13.135273
min	4.328710	65.709717	24.750344	77.531698	11.659400	17.842155
25%	13.141371	75.959049	45.107405	151.770654	17.236700	29.310866
50%	14.586954	87.624831	56.501705	194.284587	23.061192	35.891376
75%	17.464426	124.869620	75.953068	260.631303	25.697170	42.517963
max	24.171441	195.537372	121.441805	403.232080	30.461564	69.378070

	13_ane	14_ane	1_M_2_PA	BTM	FormicAcid	aceticacid \
count	18.000000	18.000000	18.000000	18.000000	18.000000	18.000000
mean	19.511359	43.447770	21.893003	114.283128	29.842710	12.765096
std	14.053689	34.987008	19.215836	60.702213	5.407451	7.036442
min	0.000000	11.190135	3.621062	36.620813	18.309706	3.354260
25%	12.813849	18.981295	9.054475	61.541217	25.257122	9.075636

```
50%     16.892346   29.926052  13.193060   92.425385   30.600086   12.189239
75%     23.214175   66.307222  25.273019  152.433715   34.509143   14.717507
max     56.732644  144.386207  72.403314  215.736621   36.768887   34.362957

       NonaDecanoicAc  Tot_OcNoDecana
count       18.000000       18.000000
mean        54.896148       67.671005
std         42.783932       53.233511
min          8.476058        0.000000
25%         19.295741       29.921632
50%         43.303068       53.932507
75%         77.024307       81.262525
max        142.691340      213.637752
```

```
Campagne:  BF3
```

```
               B           T           E           X       9_ane      10_ane  \
count  19.000000   19.000000   19.000000   19.000000   19.000000   19.000000
mean   19.354274  169.982896  157.683310  433.258081   52.480000  102.494935
std     3.217718   86.342073   56.201735  106.120372   33.067545   93.065739
min    13.576782  106.141376   94.339160  305.015268   28.367647   49.437428
25%    17.536413  132.821531  124.411171  368.219297   35.854005   62.035707
50%    18.960528  144.912568  135.888513  393.466339   47.063028   71.203366
75%    20.465743  166.154616  177.610712  469.974052   57.223689  102.634231
max    26.524218  496.957134  328.866328  726.778450  179.893186  468.416276

           13_ane     14_ane     1_M_2_PA         BTM  FormicAcid  aceticacid  \
count   19.000000  19.000000   19.000000   19.000000   19.000000   19.000000
mean    55.237776  30.761745   73.203228  307.478029   55.655680   58.402078
std     31.029644  18.343182   65.632581  169.638767    9.520422   78.961334
min      0.000000   7.395812   20.490173  167.527980   44.600394   23.675763
25%     40.274552  16.279505   37.993114  192.069673   48.555423   31.677059
50%     45.879663  28.339455   49.740404  264.949248   53.666971   39.220981
75%     66.206243  40.270221   87.873135  336.378769   58.492873   49.669188
max    148.925129  72.516856  316.020850  763.675034   84.086351  380.073994

       NonaDecanoicAc  Tot_OcNoDecana
count       19.000000       19.000000
mean        66.235082      141.991499
std         35.423214       79.840961
min         24.724491        0.000000
25%         46.025843      102.867248
50%         56.407743      144.972075
75%         84.805660      155.166261
max        165.015790      396.854143
```

```
Campagne:  CA1
```

```
               B           T            E            X        9_ane  \
count  20.000000   20.000000    20.000000    20.000000    20.000000
```

mean	39.859978	235.637253	230.200962	804.572250	88.285788
std	12.794591	110.574471	271.031858	588.737214	35.995389
min	0.000000	146.370818	103.607881	450.041130	45.937478
25%	34.771710	184.015900	137.745640	564.283839	67.284298
50%	38.841674	204.256026	162.815074	662.755807	78.001086
75%	45.414072	235.019822	194.974870	766.862490	111.391979
max	68.678793	613.833139	1345.466388	3161.133662	201.590658

	10_ane	13_ane	14_ane	1_M_2_PA	BTM \
count	20.000000	20.000000	20.000000	20.000000	20.000000
mean	127.807942	128.860629	379.664485	324.239304	642.791979
std	51.203304	75.589106	228.414015	709.355327	1375.567935
min	0.000000	0.000000	0.000000	56.470045	205.938279
25%	105.120962	79.281338	218.669881	102.332692	266.801473
50%	120.265739	134.951122	399.151119	135.429651	307.044114
75%	155.516112	157.733336	507.120123	206.106784	420.860016
max	221.527718	350.550726	908.691110	3301.128860	6472.325945

	FormicAcid	aceticacid	NonaDecanoicAc	Tot_OcNoDecana
count	20.000000	20.000000	20.000000	20.000000
mean	386.473397	814.325154	454.248342	348.759627
std	283.804434	1412.607623	286.486088	258.045233
min	180.806721	92.793744	82.206227	0.000000
25%	217.493759	142.085173	187.755757	173.727136
50%	297.308853	192.615457	450.375669	343.348190
75%	402.091761	339.061743	603.220232	488.997388
max	1360.139455	5624.216162	1071.785821	870.488320

Campagne: CA2

	B	T	E	X	9_ane \
count	29.000000	29.000000	29.000000	29.000000	29.000000
mean	105.556478	330.473288	523.390675	2083.814435	228.061505
std	14.954645	136.864151	849.761735	2240.554741	110.899129
min	74.521192	161.128847	0.000000	815.017945	118.855935
25%	97.093641	230.206031	244.065793	1091.335393	166.788891
50%	103.417565	298.358591	355.473739	1525.627953	208.448495
75%	112.834768	381.071831	470.177863	2131.892169	258.895869
max	138.810642	675.650851	4844.955559	12987.880799	702.239764

	10_ane	13_ane	14_ane	1_M_2_PA	BTM \
count	29.000000	29.000000	29.000000	29.000000	29.000000
mean	690.685507	3779.349060	5999.949335	834.440265	1450.934957
std	915.504764	598.265319	1743.607022	935.850115	3947.517071
min	56.201306	2643.765156	1460.345241	0.000000	228.187017
25%	397.558904	3293.666108	4966.982356	430.527952	479.319638
50%	506.283787	3779.749649	5459.467656	584.132221	585.935021
75%	676.959927	4153.668774	6823.087500	834.153456	914.717950
max	5316.464395	5176.410455	10996.742275	5191.044369	21891.220334

	FormicAcid	aceticacid	NonaDecanoicAc	Tot_OcNoDecana
count	29.000000	29.000000	29.000000	29.000000
mean	933.103144	445.092989	954.383625	1888.401752
std	175.847156	179.044424	674.366762	939.581127
min	652.669330	0.000000	0.000000	53.617055
25%	840.171341	356.894257	508.321422	1367.140532
50%	933.883790	384.981774	1046.247211	1506.475490
75%	1000.778018	525.886091	1422.247793	2489.960283
max	1383.805387	875.330690	2161.174659	4466.795581

Campagne: CA3

	B	T	E	X	9_ane	10_ane	\
count	24.000000	24.000000	24.000000	24.000000	24.000000	24.000000	
mean	52.001739	252.191829	171.947333	643.087978	68.959656	249.324598	
std	6.316959	63.338080	71.478691	228.876783	15.723494	58.790000	
min	40.621814	154.993492	93.927927	347.083206	50.432053	148.468540	
25%	46.337342	207.067805	124.390625	473.660207	55.461089	215.805111	
50%	51.009800	238.540065	165.420604	615.845365	65.561858	240.090290	
75%	58.563187	278.628749	205.647213	802.731156	76.300073	272.943270	
max	61.860864	397.597301	440.817277	1356.964075	113.530275	395.654408	

	13_ane	14_ane	1_M_2_PA	BTM	FormicAcid	\
count	24.000000	24.000000	24.000000	24.000000	24.000000	
mean	197.428142	1079.762165	167.674146	329.594021	213.366315	
std	96.809514	480.642518	138.023870	158.390298	93.354658	
min	0.000000	152.164592	55.562198	80.549567	13.937401	
25%	142.606128	752.844086	89.330428	213.706163	184.522538	
50%	201.964257	1102.711631	107.973863	318.461581	243.439232	
75%	271.305386	1395.543411	162.007730	416.362801	270.006161	
max	364.843310	2129.878719	535.458629	656.524816	370.314177	

	aceticacid	NonaDecanoicAc	Tot_OcNoDecana
count	24.000000	24.000000	24.000000
mean	214.477807	165.290178	276.281357
std	100.623042	154.313387	112.708157
min	0.000000	0.000000	44.886793
25%	154.998309	0.000000	206.574381
50%	188.655811	166.997980	303.797510
75%	236.963104	279.770288	342.453315
max	456.476730	547.493107	478.028818

Campagne: CA4

	B	T	E	X	9_ane	10_ane	\
count	28.000000	28.000000	28.000000	28.000000	28.000000	28.000000	
mean	68.582970	119.890215	144.557390	640.177626	107.425136	199.658865	
std	14.554742	48.509628	90.454348	359.342216	101.322501	84.803853	
min	8.383893	14.363178	13.574943	109.758387	56.744672	16.280538	

```
25%     63.885180   98.336874   90.207895   385.030380   74.775108  143.320741
50%     69.794745  112.767611  129.996277   580.607394   86.531583  198.000070
75%     75.631330  134.897352  174.777573   753.849816  104.280430  262.649502
max     90.284559  250.157975  470.285224  1838.077282  612.799425  367.643583

            13_ane       14_ane     1_M_2_PA         BTM   FormicAcid  \
count    28.000000    28.000000    28.000000   28.000000    28.000000
mean    558.271084  1704.504659  232.596805  332.063869   885.480959
std     324.033532   542.175875  186.131493  149.398661   828.418503
min      80.021979   492.909726    5.038233  117.075186    72.458616
25%     435.039852  1501.061188  114.909982  222.931870   505.013562
50%     512.203631  1687.130304  164.653069  320.616975   580.342657
75%     580.952004  1886.937734  272.437847  371.967345   756.453060
max    1771.421041  3727.510235  842.417054  695.746507  3618.024076

        aceticacid  NonaDecanoicAc  Tot_OcNoDecana
count    28.000000       28.000000       28.000000
mean    415.234784     1771.808397      526.405290
std     699.024820      619.638208      253.702961
min     121.743535      356.892675      128.158334
25%     134.288117     1423.833049      352.642707
50%     156.604735     1952.231829      461.056165
75%     265.623653     2150.739896      681.883429
max    3187.261794     2981.690091     1148.311924
```

[300]:

```
# Describe the data per `SAISON`
for saison in data['SAISON'].unique():
    print('SAISON: ', saison)
    display(data[data['SAISON'] == saison].describe())
```

```
SAISON:  hiver

               B           T            E            X       9_ane  \
count  81.000000   81.000000    81.000000    81.000000   81.000000
mean   33.140166  195.612314   158.881921   537.502826   59.411940
std    17.124605   97.472193   152.137386   386.388766   34.570732
min     0.000000   65.709717    24.750344    77.531698   11.659400
25%    17.626030  137.067950   108.154072   354.245700   30.461564
50%    34.622895  183.789855   135.888513   472.100396   55.581245
75%    49.372041  233.237497   176.064682   634.471771   73.973683
max    68.678793  613.833139  1345.466388  3161.133662  201.590658

           10_ane      13_ane      14_ane    1_M_2_PA         BTM  \
count   81.000000   81.000000   81.000000   81.000000   81.000000
mean   137.597660  107.607533  430.544626  151.776555  353.892283
std     99.801118   96.129659  527.171919  372.565150  705.930132
min      0.000000    0.000000    0.000000    3.621062   36.620813
25%     60.306966   31.328987   30.137847   38.289323  176.326494
```

```
50%     114.572193   68.764942   144.386207    89.332327   264.252071
75%     215.367264  167.563603   685.667608   131.192387   366.304894
max     468.416276  364.843310  2129.878719  3301.128860  6472.325945

        FormicAcid   aceticacid  NonaDecanoicAc  Tot_OcNoDecana
count    81.000000    81.000000       81.000000       81.000000
mean    178.331928   281.152860      188.870720      216.319280
std     203.459693   760.683524      228.896605      182.347527
min      13.937401     0.000000        0.000000        0.000000
25%      44.600394    24.072569       39.203236       80.664841
50%      84.086351   130.836201      101.411930      152.469300
75%     254.728787   196.111660      266.824679      320.011077
max    1360.139455  5624.216162     1071.785821      870.488320
SAISON:  été
                B           T            E             X       9_ane  \
count   57.000000   57.000000    57.000000     57.000000   57.000000
mean    87.394053  227.028971   337.297132   1374.659511  168.801534
std     23.700506  147.584800   633.640675   1761.380963  121.660265
min      8.383893   14.363178     0.000000    109.758387   56.744672
25%     70.318126  114.087361   128.589691    583.184939   86.902437
50%     86.778103  199.938413   228.352001    956.247946  128.504786
75%    103.417565  298.358591   361.542068   1552.851298  209.500043
max    138.810642  675.650851  4844.955559  12987.880799  702.239764

            10_ane       13_ane        14_ane       1_M_2_PA           BTM  \
count    57.000000    57.000000     57.000000      57.000000     57.000000
mean    449.479438  2197.065142   3889.906336     538.797864    901.314072
std     695.612096  1693.790520   2521.001165     739.428210   2849.678178
min      16.280538    80.021979    492.909726       0.000000    117.075186
25%     175.262365   512.250706   1672.883797     162.060717    319.754465
50%     322.577864  2643.765156   3727.510235     400.649801    454.471842
75%     506.283787  3779.749649   5459.467656     590.836464    614.097895
max    5316.464395  5176.410455  10996.742275    5191.044369  21891.220334

        FormicAcid   aceticacid  NonaDecanoicAc  Tot_OcNoDecana
count    57.000000    57.000000       57.000000       57.000000
mean    909.709790   430.425801     1355.925618     1219.350858
std     589.000581   501.844053      763.204550      971.768630
min      72.458616     0.000000        0.000000       53.617055
25%     581.139533   155.019208      807.891427      453.382842
50%     804.847510   351.765181     1422.247793      893.598432
75%     989.169836   450.521761     2018.240019     1506.475490
max    3618.024076  3187.261794     2981.690091     4466.795581
```

[301]:

```python
# Describe the data with `Campagne` BF2 and BF3 grouped together
print('Campagnes BF2 et BF3')
```

```python
display(data[data['Campagne'].str.startswith('BF')].describe())
```

```
Campagnes BF2 et BF3

               B           T           E           X        9_ane      10_ane  \
count  37.000000   37.000000   37.000000   37.000000   37.000000   37.000000
mean   17.273302  137.276986  111.856227  324.653309   37.611342   70.417871
std     4.332348   74.667451   64.720886  147.467265   28.313846   74.352953
min     4.328710   65.709717   24.750344   77.531698   11.659400   17.842155
25%    14.309193   91.828791   56.983950  198.176614   23.942037   36.037182
50%    17.521051  127.159599  118.650361  346.278511   30.185456   52.723442
75%    19.678814  158.588861  135.888513  403.232080   47.063028   71.203366
max    26.524218  496.957134  328.866328  726.778450  179.893186  468.416276

           13_ane      14_ane     1_M_2_PA         BTM  FormicAcid  aceticacid  \
count   37.000000   37.000000   37.000000   37.000000   37.000000   37.000000
mean    37.857357   36.933325   48.241497  213.491320   43.098019   36.200303
std     30.040050   28.064216   54.810206  160.349428   15.172564   60.626583
min      0.000000    7.395812    3.621062   36.620813   18.309706    3.354260
25%     16.638387   17.915708   15.008747   97.769647   31.421895   12.262799
50%     31.328987   29.714257   36.739595  188.823721   44.600394   23.734393
75%     53.312212   45.443490   57.104709  264.949248   53.666971   39.220981
max    148.925129  144.386207  316.020850  763.675034   84.086351  380.073994

       NonaDecanoicAc  Tot_OcNoDecana
count       37.000000       37.000000
mean        60.718844      105.835583
std         39.048685       77.095273
min          8.476058        0.000000
25%         28.578258       46.063908
50%         54.840564       94.457647
75%         83.026577      145.515455
max        165.015790      396.854143
```

[302]:
```python
# Describe the data with `Campagne` CA1, CA2, CA3, and CA4 grouped together
print('Campagnes CA1, CA2, CA3, et CA4')
display(data[data['Campagne'].str.startswith('CA')].describe())
```

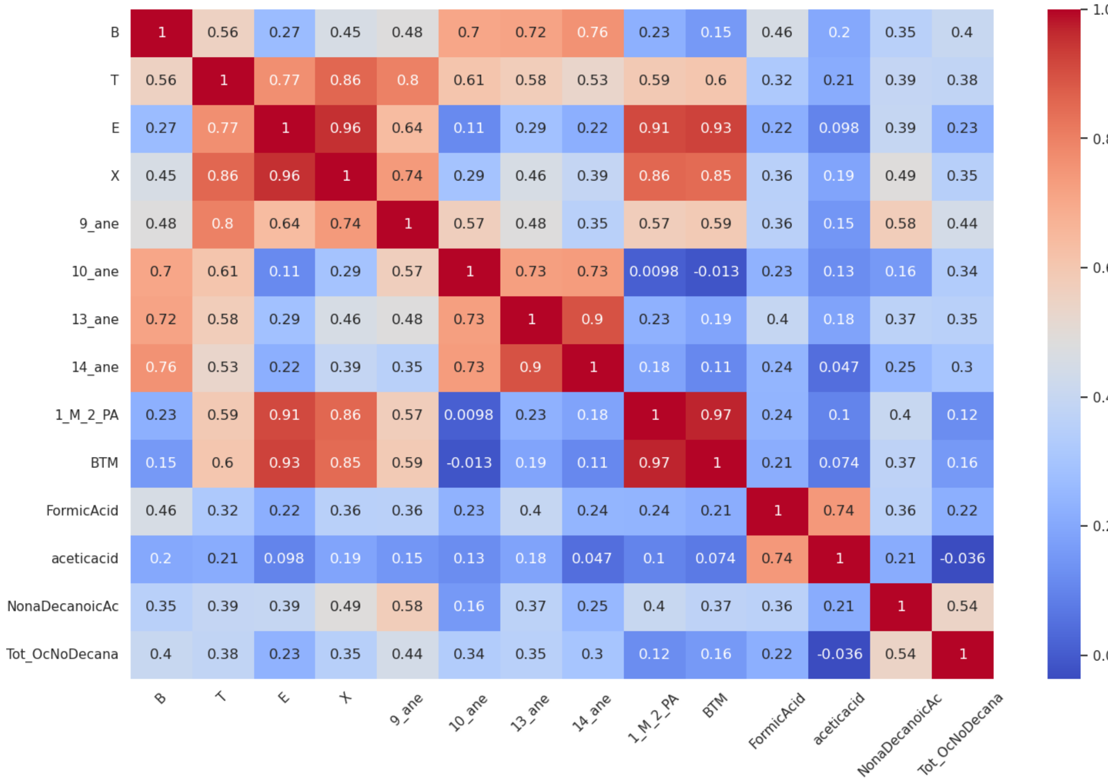
```
Campagnes CA1, CA2, CA3, et CA4

                B           T            E             X        9_ane  \
count  101.000000  101.000000   101.000000    101.000000  101.000000
mean    69.571310  234.712875   276.798928   1087.932164  129.133019
std     28.045318  124.701366   495.107553   1387.694606  103.399076
min      0.000000   14.363178     0.000000    109.758387   45.937478
25%     49.448437  150.686798   129.385560    531.802628   69.273768
50%     64.397748  211.732357   176.064682    733.147094   90.656027
75%     92.569623  280.688016   258.686004   1108.597735  158.798326
max    138.810642  675.650851  4844.955559  12987.880799  702.239764
```

```
          10_ane       13_ane        14_ane      1_M_2_PA           BTM  \
count  101.000000   101.000000    101.000000   101.000000    101.000000
mean   338.220566  1312.358427   2527.051909   408.123206    714.267309
std    538.582215  1623.099636   2470.985471   656.647082   2229.200793
min      0.000000     0.000000      0.000000     0.000000     80.549567
25%    148.678937   167.563603    747.382713   110.674575    250.784743
50%    232.039002   416.691750   1527.776925   205.602629    366.304894
75%    371.086279  3127.846498   4676.840299   467.676838    533.838792
max   5316.464395  5176.410455  10996.742275  5191.044369  21891.220334

        FormicAcid   aceticacid  NonaDecanoicAc  Tot_OcNoDecana
count   101.000000   101.000000      101.000000      101.000000
mean    640.630867   455.131100      894.452390      822.860832
std     556.405010   750.034743      796.871888      866.407041
min      13.937401     0.000000        0.000000        0.000000
25%     260.720126   152.371517      186.709785      292.026680
50%     548.570717   235.785849      716.442278      453.382842
75%     849.575270   386.610428     1470.401584     1148.311924
max    3618.024076  5624.216162     2981.690091     4466.795581
```

Correlation matrix

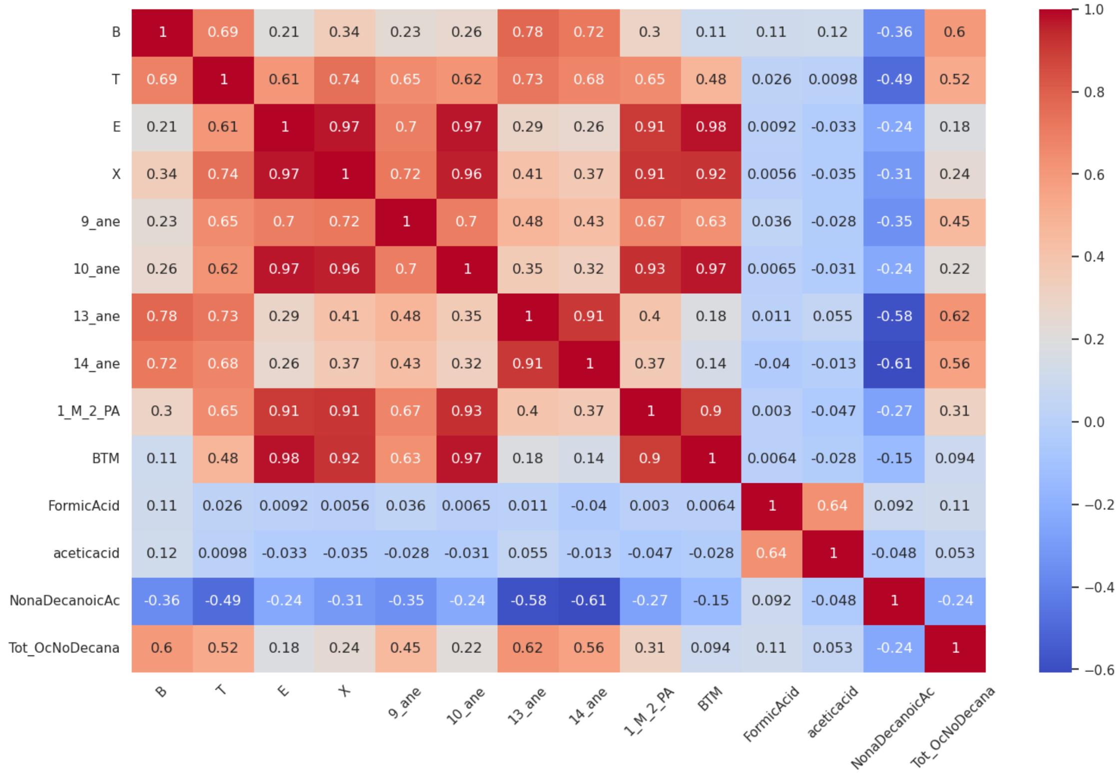
[303]:
```python
# For SAISON = hiver
data_hiver = data[data['SAISON'] == 'hiver']
numerical_data_hiver = data_hiver.select_dtypes(include=['float64', 'int64'])
corr_hiver = numerical_data_hiver.corr()
print("Saison = hiver")
plt.figure(figsize=(16, 10))
sns.heatmap(corr_hiver, annot=True, cmap='coolwarm')
plt.xticks(rotation=45)
plt.show()
```

```
Saison = hiver
```



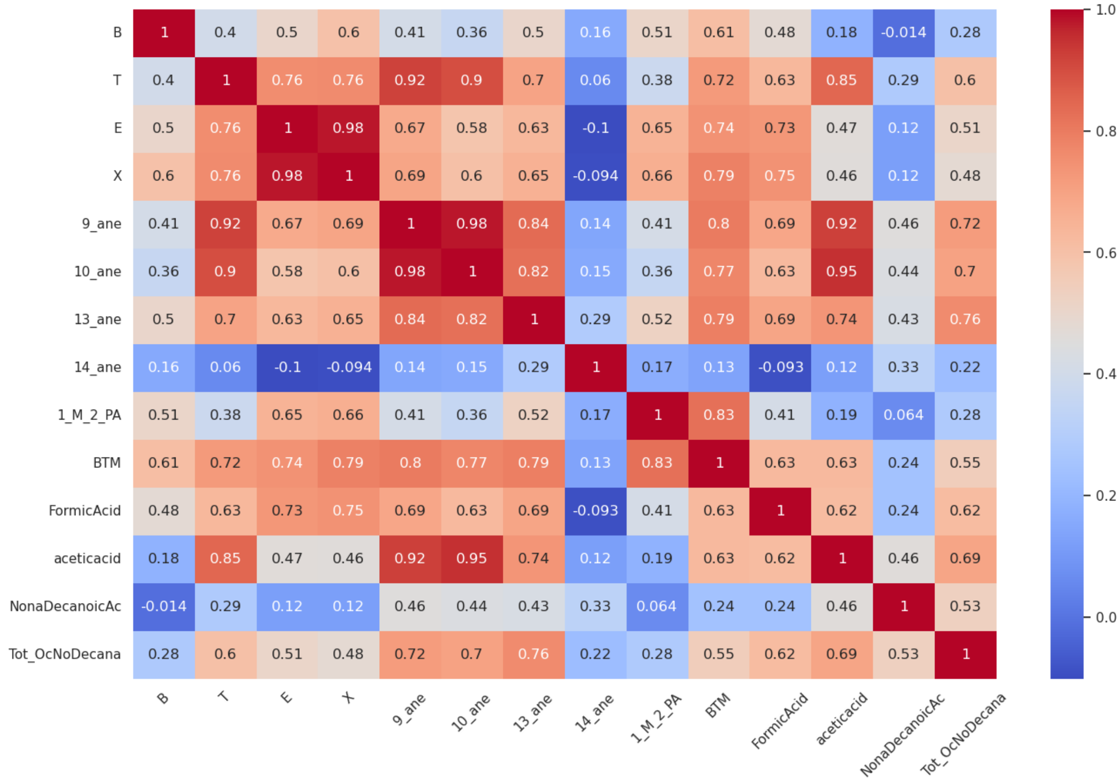
[304]:
```python
# For SAISON = été
data_ete = data[data['SAISON'] == 'été']
numerical_data_ete = data_ete.select_dtypes(include=['float64', 'int64'])
corr_ete = numerical_data_ete.corr()
print("Saison = été")
plt.figure(figsize=(16, 10))
sns.heatmap(corr_ete, annot=True, cmap='coolwarm')
plt.xticks(rotation=45)
plt.show()
```

```
Saison = été
```



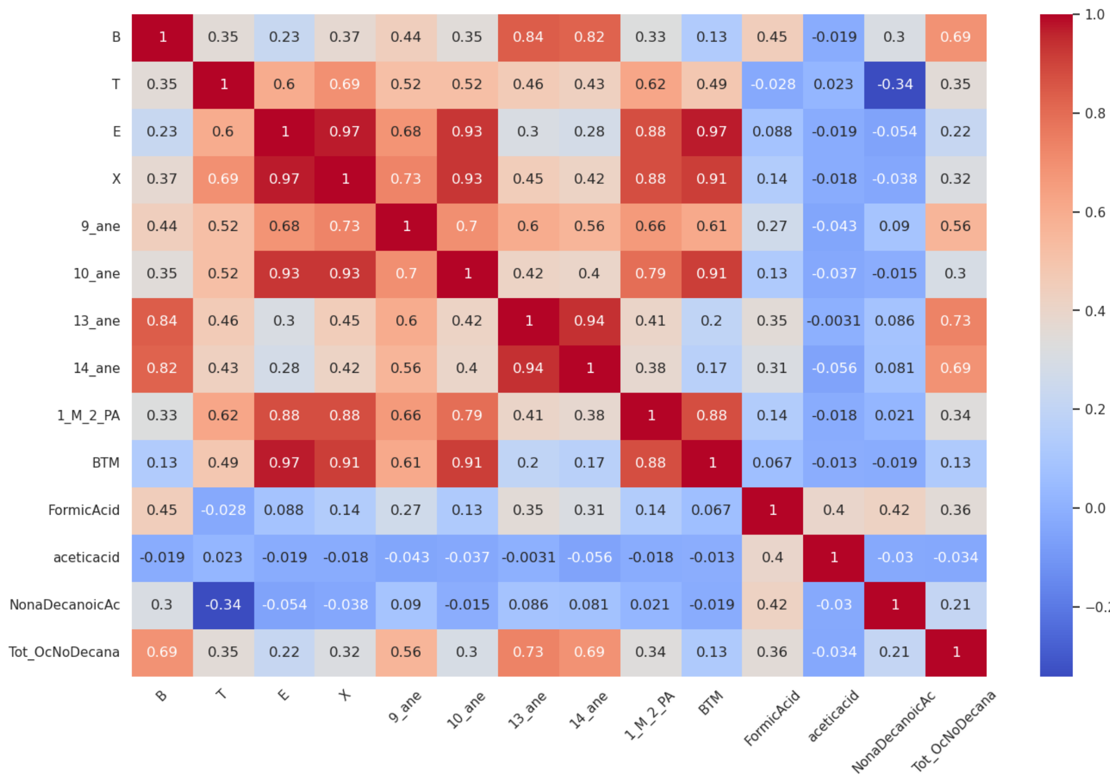
```
[305]: # For Campagne contains BF
data_BF = data[data['Campagne'].str.startswith("BF")]
numerical_data_BF = data_BF.select_dtypes(include=['float64', 'int64'])
corr_BF = numerical_data_BF.corr()
print("Campagne = BF")
plt.figure(figsize=(16, 10))
sns.heatmap(corr_BF, annot=True, cmap='coolwarm')
plt.xticks(rotation=45)
plt.show()
```

```
Campagne = BF
```



[306]:
```python
# For Campagne contains CA
data_CA = data[data['Campagne'].str.startswith("CA")]
numerical_data_CA = data_CA.select_dtypes(include=['float64', 'int64'])
corr_CA = numerical_data_CA.corr()
print("Campagne = CA")
plt.figure(figsize=(16, 10))
sns.heatmap(corr_CA, annot=True, cmap='coolwarm')
plt.xticks(rotation=45)
plt.show()
```

```
Campagne = CA
```



We notice a change in the correlations between variables from a period to the other, for instance, the correlation between 10-ane, and 1_M_2_PA and BTM, was almost 0 in the winter but became over 90% in the summer. Also the correlation between 14-ane and other chemical compounds was very small before the activity, and became quite considerable after the activity.

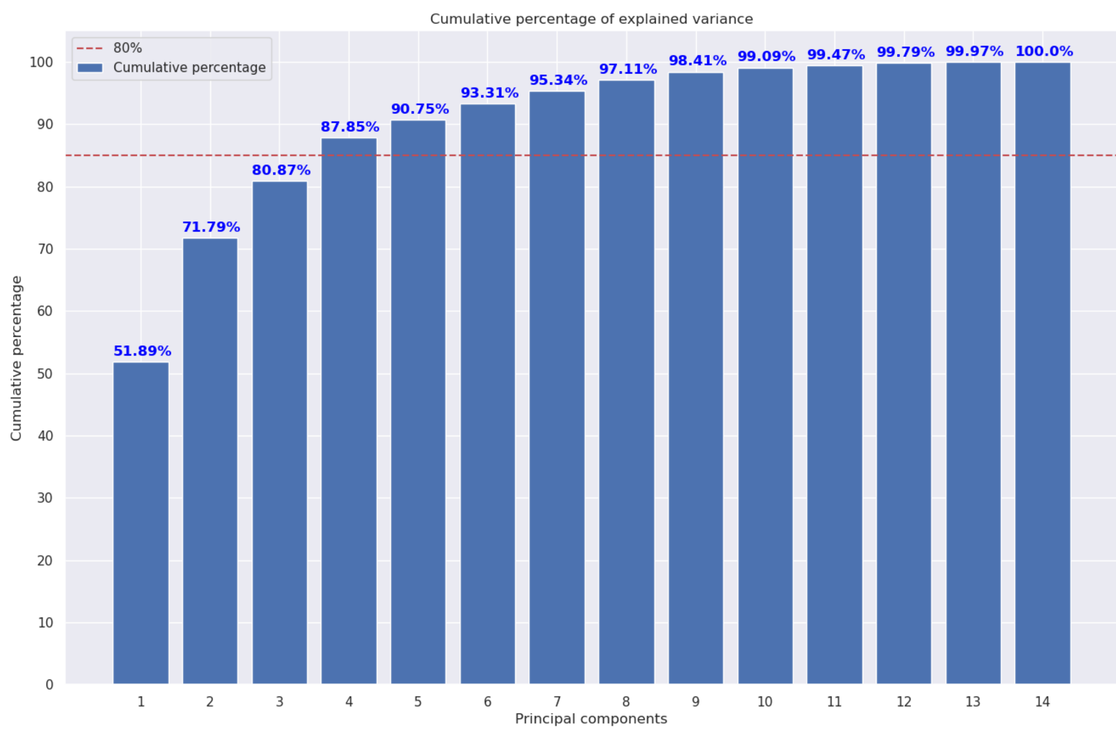
We also notice that the mean of the various features is higher in summer, and more variability (higher std) also appears during the summer which will affect PCA more.

Same thing can be said for when comparing before and after the activity.

[307]:
```
# Center and reduce data with the StandardScaler() function
from sklearn.preprocessing import StandardScaler

numerical_data = data.select_dtypes(include=['float64', 'int64'])

scaler = StandardScaler()
numerical_data = scaler.fit_transform(numerical_data)
```

[308]:
```
# PCA
pca = PCA()
pca.fit(numerical_data)

# Eigen values
```

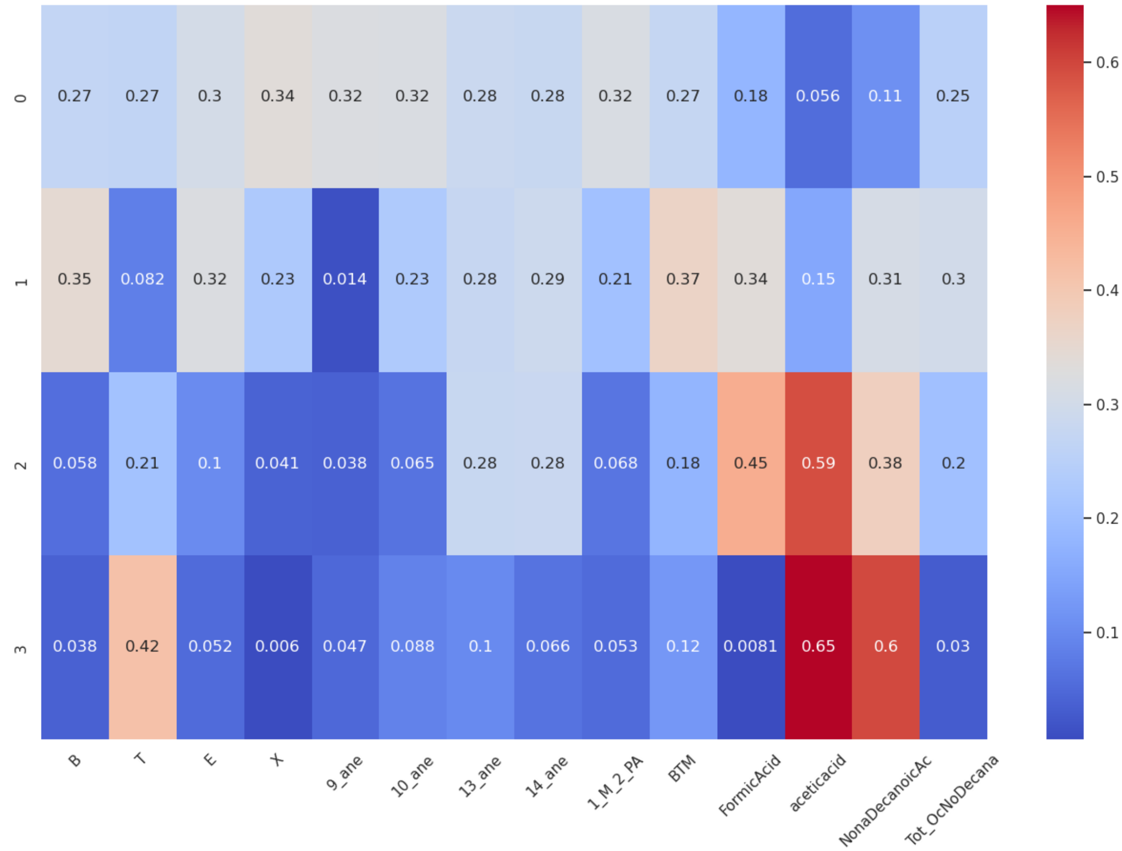
```
eigen_values = pca.explained_variance_

percentage_contributions = eigen_values / sum(eigen_values) * 100

cumulative_percentage = np.cumsum(percentage_contributions)

plt.figure(figsize=(16, 10))
plt.bar(range(1, len(cumulative_percentage) + 1), cumulative_percentage,␣
 ↪align='center', label='Cumulative percentage')
plt.axhline(y=85, color='r', linestyle='--', label='80%')
for i, v in enumerate(cumulative_percentage):
    plt.text(i+0.6, v + 1, str(round(v, 2)) + "%", color='blue',␣
 ↪fontweight='bold')
plt.xlabel('Principal components')
plt.ylabel('Cumulative percentage')
plt.title('Cumulative percentage of explained variance')
plt.xticks(range(1, len(cumulative_percentage) + 1))
plt.yticks(np.arange(0, 101, 10))
plt.legend()
plt.show()
```

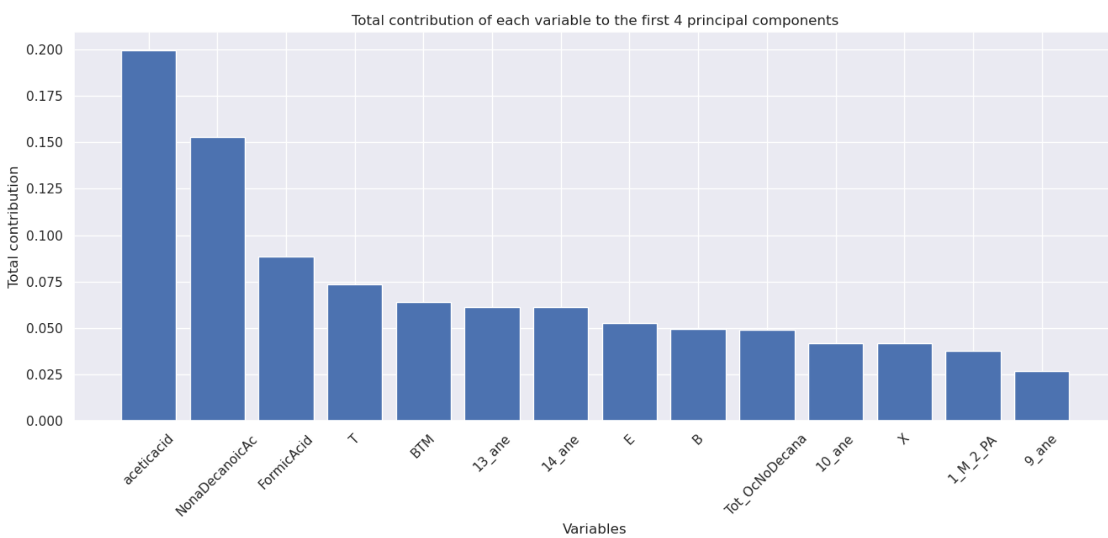


We can take up to 4 principal components, we will plot using 3 but do the analysis using 4.

[309]:

```
# How much of every variable is explained by the first 4 principal components?
eigen_vectors = pca.components_
eigen_vectors = pd.DataFrame(eigen_vectors, columns=data.
 ↪select_dtypes(include=['float64', 'int64']).columns)

# Heatmap of the first 4 principal components
plt.figure(figsize=(16, 10))
sns.heatmap(eigen_vectors.iloc[:4, :].abs(), annot=True, cmap='coolwarm')
plt.xticks(rotation=45)
plt.show()

# Calculate the total contribution of each variable to the first 4 principal␣
 ↪components
total_contribution = np.sum(np.square(eigen_vectors.iloc[:4, :]), axis=0)
total_contribution = pd.DataFrame(total_contribution, columns=['Total␣
 ↪contribution'])
total_contribution.sort_values(by='Total contribution', ascending=False,␣
 ↪inplace=True)
total_contribution['Total contribution'] = total_contribution['Total␣
 ↪contribution'] / sum(total_contribution['Total contribution'])

plt.figure(figsize=(16, 6))
plt.bar(total_contribution.index, total_contribution['Total contribution'],␣
 ↪align='center')
plt.xticks(rotation=45)
plt.xlabel('Variables')
plt.ylabel('Total contribution')
plt.title('Total contribution of each variable to the first 4 principal␣
 ↪components')
plt.show()
```

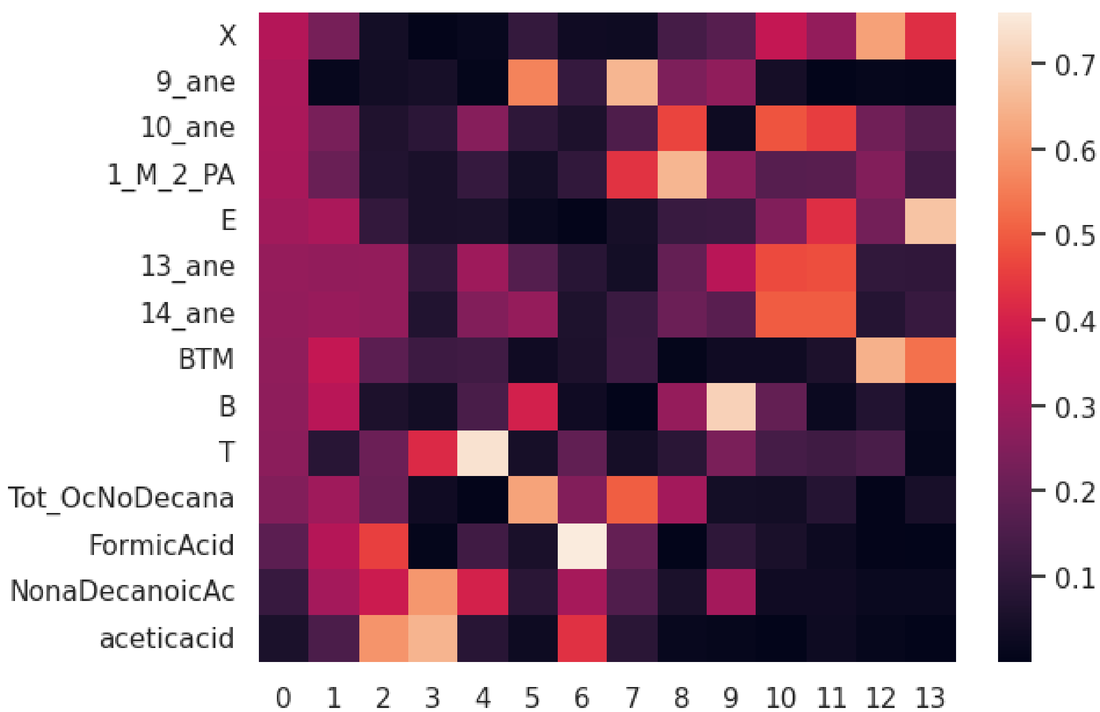




[310]:
```python
# Contribution of each variable to the principal components
variance_ratio = pca.explained_variance_ratio_
```

```
total_contributions = np.dot(np.abs(pca.components_), variance_ratio)

contributions = pd.DataFrame(pca.components_, columns=data.
 ↪select_dtypes(include=['float64', 'int64']).columns)
contributions = contributions.transpose()
contributions = contributions.abs()
contributions = contributions.sort_values(by=0, ascending=False)

print('Contribution of each variable to the principal components')
plt.figure()
sns.heatmap(contributions)
plt.show()
```

```
Contribution of each variable to the principal components
```




```
[311]: # Projection on 4 components
pca = PCA(n_components=4)
pca.fit(numerical_data)
pca.components_

# Plot the projection in 3D
pca_data = pca.transform(numerical_data)
pca_data = pd.DataFrame(pca_data, columns=['PC1', 'PC2', 'PC3', 'PC4'])
```

```python
# Quality of the projections
coord_squared = np.sum(pca_data ** 2, axis=1)
old_coord_squared = np.sum(numerical_data ** 2, axis=1)

quality = coord_squared / old_coord_squared
print("Quality of the projections (sorted):")
print(quality.sort_values(ascending=False))
```

```
Quality of the projections (sorted):
75     0.993252
3      0.988020
32     0.987438
2      0.985356
19     0.983339
         …
45     0.343512
123    0.329829
37     0.259235
127    0.131522
114    0.047059
Length: 138, dtype: float64
```

[312]:
```python
# Calculate the number of individuals with a quality of projection greater than␣
↪0.8
print("Precentage of individuals with a quality of projection greater than 0.8:
↪")
print(sum(quality >= 0.8) / len(quality) * 100)
```

```
Precentage of individuals with a quality of projection greater than 0.8:
71.01449275362319
```

[313]:
```python
# PCA with 3 components
pca = PCA(n_components=3)
pca.fit(numerical_data)
pca.components_

# Plot the projection in 3D
pca_data = pca.transform(numerical_data)
pca_data = pd.DataFrame(pca_data, columns=['PC1', 'PC2', 'PC3'])

fig = px.scatter_3d(pca_data, x='PC1', y='PC2', z='PC3', opacity=0.3)
fig.show()
```

From the results above, we can conclude: - It's hard to make sense of principal components. - The PCA is heavily affected by the difference between winter/summer and before/after: the higher variance in the summer / after, so the principal components are likely to be dominated by the patterns and variations in those periods. Hence, we're not able to find a *signature* for each period.

While normalization helps in putting variables on the same scale, it might not be sufficient here seeing there are substantial differences in variability between seasons and before and after the activity.

A possible solution would be to perform a seasonal separation, doing so could provide more interpretable results: we may apply a PCA on variables over the *same season*, before and after the activity, and figure out the axis with the most variance, this would be much more interpretable than taking the lot of the variables. This may be further applied to different variables, like the `TYPE`.