In [59]:
```
%time
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import sklearn as sk
from sklearn.decomposition import PCA
from sklearn.cluster import KMeans, DBSCAN
from scipy.stats import zscore
import scipy.cluster.hierarchy as ch
from sklearn.cluster import AgglomerativeClustering
from sklearn.preprocessing import LabelEncoder
pd.options.display.max_columns = None
```

```
CPU times: user 2 µs, sys: 0 ns, total: 2 µs
Wall time: 4.05 µs
```

In [60]:
```python
df = pd.read_csv("../data_cleaned/cleaned_dataset_no_zeros.csv")
df.head(20)
```

Out[60]:

	Species	Country.of.Origin	Variety	Processing.Method	Aroma	Flavor	Aftertaste
0	Arabica	Ethiopia	Caturra	Washed / Wet	8.67	8.83	8.67
1	Arabica	Ethiopia	Other	Washed / Wet	8.75	8.67	8.50
2	Arabica	Guatemala	Bourbon	Washed / Wet	8.42	8.50	8.42
3	Arabica	Ethiopia	Caturra	Natural / Dry	8.17	8.58	8.42
4	Arabica	Ethiopia	Other	Washed / Wet	8.25	8.50	8.25
5	Arabica	Ethiopia	Caturra	Washed / Wet	8.25	8.33	8.50
6	Arabica	Ethiopia	Caturra	Washed / Wet	8.67	8.67	8.58
7	Arabica	Ethiopia	Other	Natural / Dry	8.08	8.58	8.50
8	Arabica	Ethiopia	Caturra	Natural / Dry	8.17	8.67	8.25
9	Arabica	United States	Other	Washed / Wet	8.25	8.42	8.17
10	Arabica	United States	Other	Washed / Wet	8.08	8.67	8.33
11	Arabica	United States (Hawaii)	Caturra	Washed / Wet	8.33	8.42	8.08
12	Arabica	Ethiopia	Caturra	Washed / Wet	8.25	8.33	8.50
13	Arabica	United States	Other	Washed / Wet	8.00	8.50	8.58
14	Arabica	Indonesia	Caturra	Washed / Wet	8.33	8.25	7.83
15	Arabica	China	Catimor	Washed / Wet	8.42	8.25	8.08
16	Arabica	Ethiopia	Ethiopian Yirgacheffe	Natural / Dry	8.17	8.17	8.00
17	Arabica	United States	Other	Washed / Wet	8.00	8.25	8.08
18	Arabica	Costa Rica	Caturra	Washed / Wet	8.08	8.25	8.00
19	Arabica	Mexico	Other	Washed / Wet	8.17	8.25	8.17

In [61]:
```python
df.columns
```

Out[61]:
```
Index(['Species', 'Country.of.Origin', 'Variety', 'Processing.Method',
'Aroma',
       'Flavor', 'Aftertaste', 'Acidity', 'Body', 'Balance', 'Uniformit
y',
       'Clean.Cup', 'Sweetness', 'Cupper.Points', 'Total.Cup.Points',
       'Moisture', 'Category.One.Defects', 'Quakers', 'Color',
       'Category.Two.Defects', 'altitude_mean_meters'],
      dtype='object')
```

In [62]:
```python
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1103 entries, 0 to 1102
Data columns (total 21 columns):
 #   Column                Non-Null Count  Dtype  
---  ------                --------------  -----  
 0   Species               1103 non-null   object 
 1   Country.of.Origin     1103 non-null   object 
 2   Variety               1103 non-null   object 
 3   Processing.Method     1103 non-null   object 
 4   Aroma                 1103 non-null   float64
 5   Flavor                1103 non-null   float64
 6   Aftertaste            1103 non-null   float64
 7   Acidity               1103 non-null   float64
 8   Body                  1103 non-null   float64
 9   Balance               1103 non-null   float64
 10  Uniformity            1103 non-null   float64
 11  Clean.Cup             1103 non-null   float64
 12  Sweetness             1103 non-null   float64
 13  Cupper.Points         1103 non-null   float64
 14  Total.Cup.Points      1103 non-null   float64
 15  Moisture              1103 non-null   float64
 16  Category.One.Defects  1103 non-null   int64  
 17  Quakers               1103 non-null   float64
 18  Color                 1103 non-null   object 
 19  Category.Two.Defects  1103 non-null   int64  
 20  altitude_mean_meters  1103 non-null   float64
dtypes: float64(14), int64(2), object(5)
memory usage: 181.1+ KB
```

In [63]:
```
df.isna().sum()
```

Out[63]:
```
Species                 0
Country.of.Origin       0
Variety                 0
Processing.Method       0
Aroma                   0
Flavor                  0
Aftertaste              0
Acidity                 0
Body                    0
Balance                 0
Uniformity              0
Clean.Cup               0
Sweetness               0
Cupper.Points           0
Total.Cup.Points        0
Moisture                0
Category.One.Defects    0
Quakers                 0
Color                   0
Category.Two.Defects    0
altitude_mean_meters    0
dtype: int64
```

In [64]:
```
df.describe()
```

Out[64]:

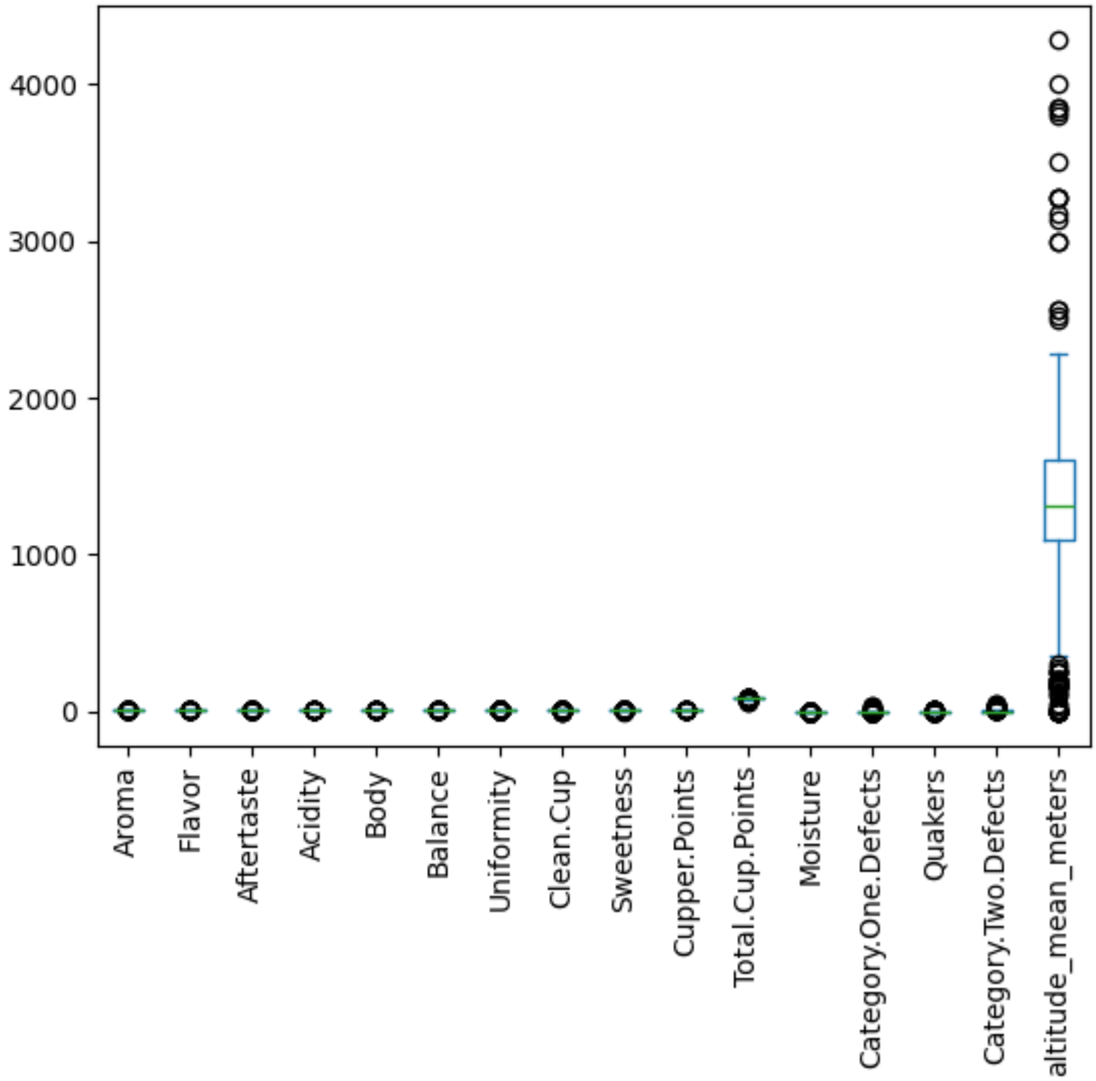
	Aroma	Flavor	Aftertaste	Acidity	Body	Balanc
count	1103.000000	1103.000000	1103.000000	1103.000000	1103.000000	1103.00000
mean	7.578368	7.527824	7.401496	7.535739	7.513654	7.51266
std	0.309181	0.331268	0.340065	0.313192	0.289467	0.35402
min	5.080000	6.170000	6.170000	5.250000	5.170000	5.25000
25%	7.420000	7.330000	7.250000	7.330000	7.330000	7.33000
50%	7.580000	7.580000	7.420000	7.500000	7.500000	7.50000
75%	7.750000	7.750000	7.580000	7.750000	7.670000	7.75000
max	8.750000	8.830000	8.670000	8.750000	8.580000	8.75000

In [65]:

```
fig = plt.figure()
df.plot.box(rot=90)
```

Out[65]: <Axes: >

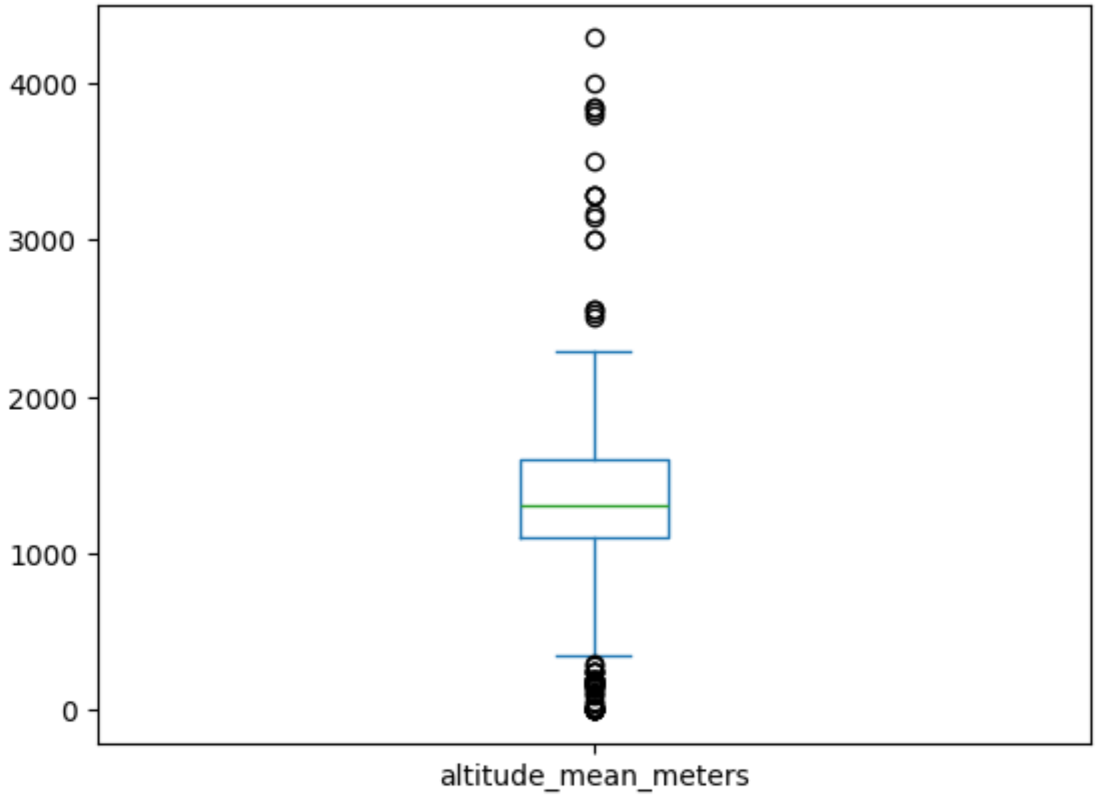
<Figure size 640x480 with 0 Axes>



In [66]:

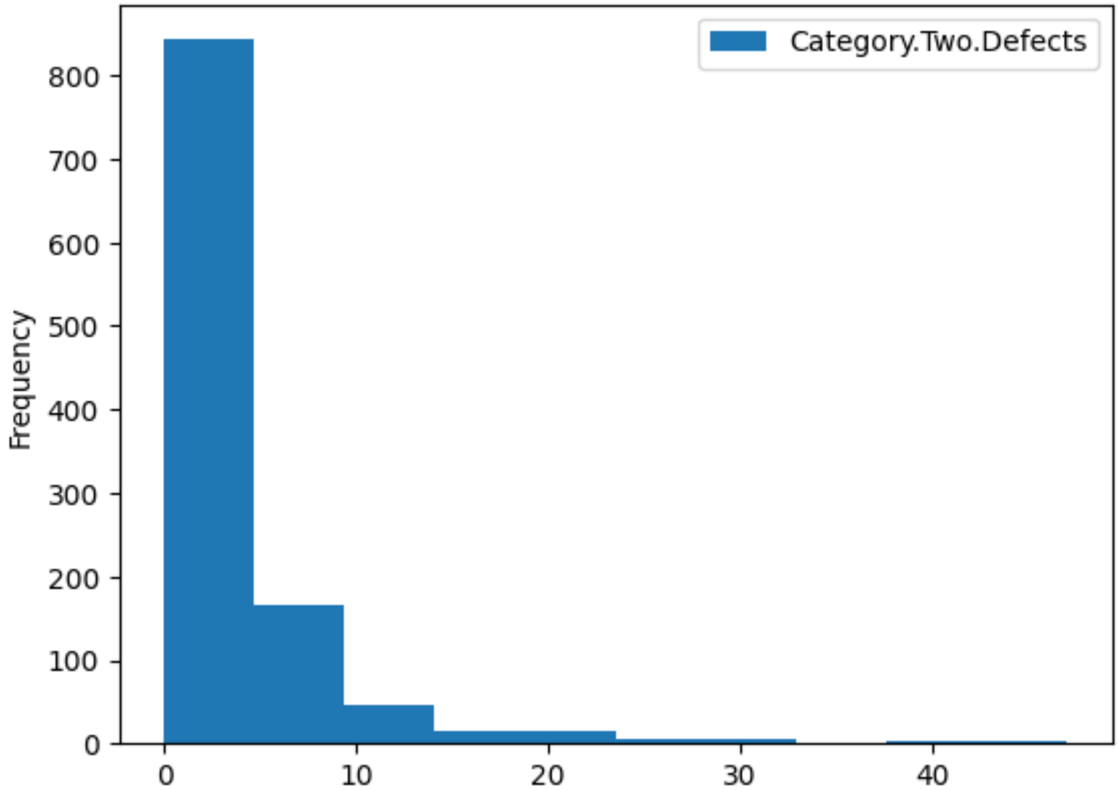
```
df['altitude_mean_meters'].plot.box()
```

Out[66]: <Axes: >



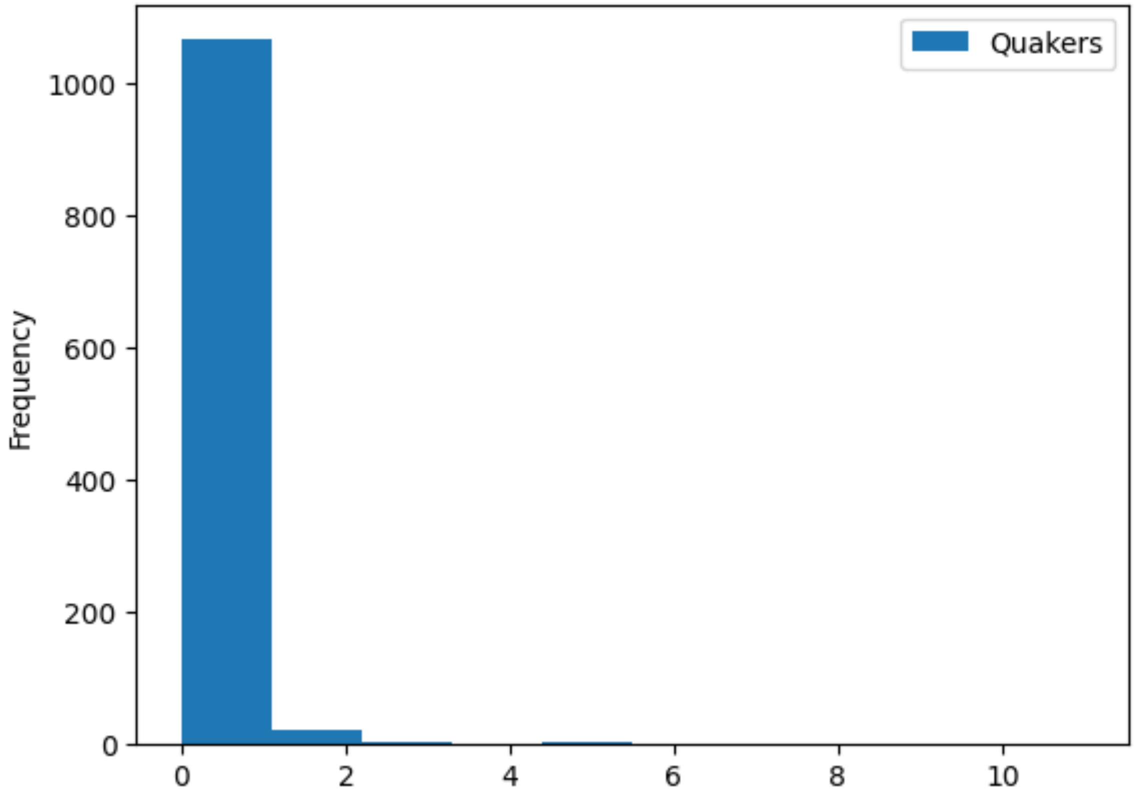
In [67]:
```
df[['Category.Two.Defects']].plot.hist()
```

Out[67]: <Axes: ylabel='Frequency'>



In [68]:
```
# we're gonna keep these outlying values, as they might have a high impac
df[['Quakers']].plot.hist()
```

Out[68]: <Axes: ylabel='Frequency'>



Data Exploration

In [69]:
```
# lets see which countries can boast the highest cup grades
df.groupby('Country.of.Origin')['Total.Cup.Points'].mean().reset_index().
```

Out[69]:

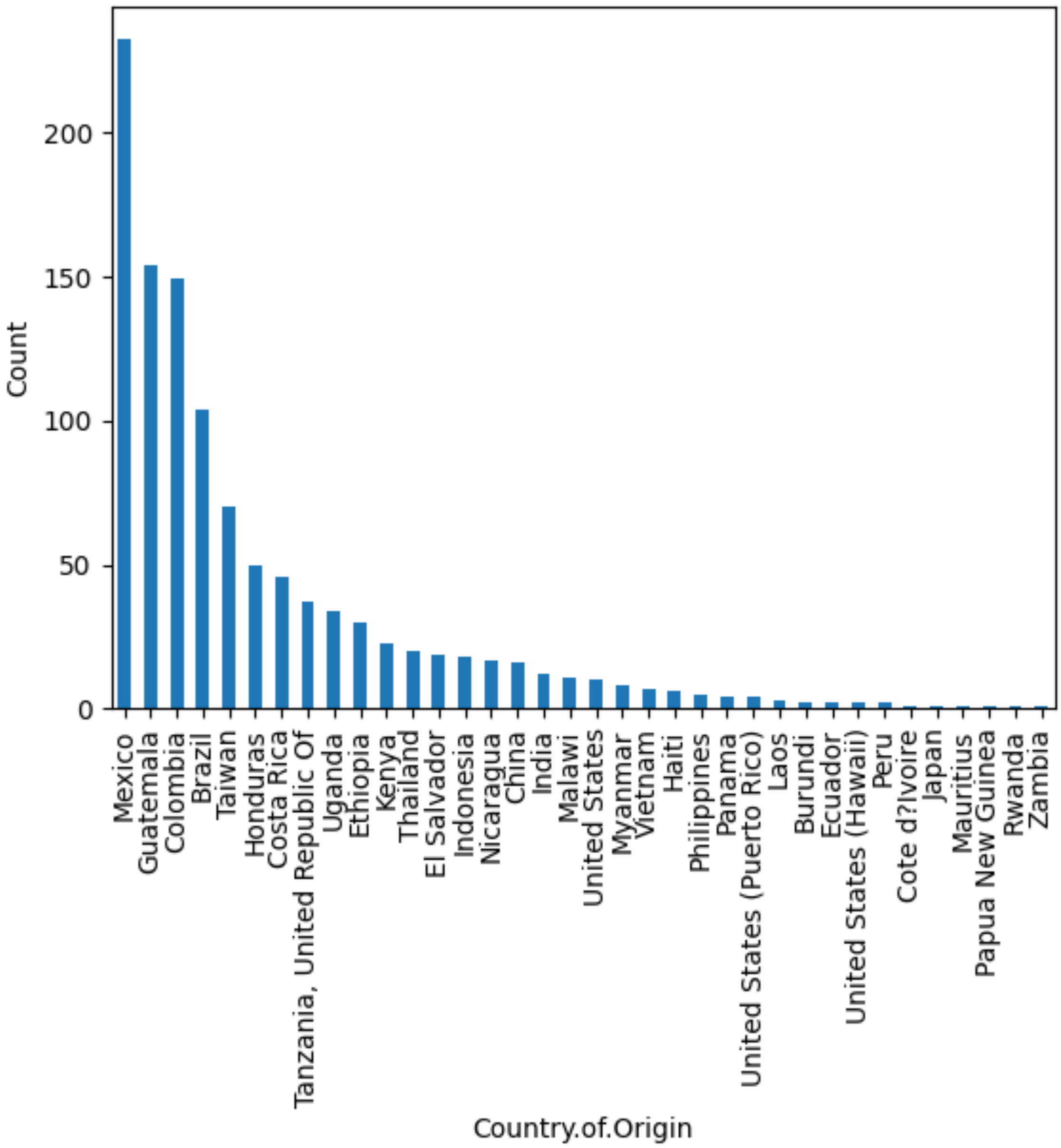
	Country.of.Origin	Total.Cup.Points
32	United States (Hawaii)	86.960000
8	Ethiopia	85.916333
23	Papua New Guinea	85.750000
14	Japan	84.670000
31	United States	84.433000
15	Kenya	84.271304
22	Panama	83.707500
30	Uganda	83.382941
3	Colombia	83.224832
7	El Salvador	83.115263
2	China	82.927500
26	Rwanda	82.830000
4	Costa Rica	82.800435
0	Brazil	82.711442
13	Indonesia	82.528333
29	Thailand	82.430000
28	Tanzania, United Republic Of	82.309459
34	Vietnam	82.274286
9	Guatemala	82.024221
27	Taiwan	81.947714
12	India	81.937500
35	Zambia	81.920000
16	Laos	81.833333
1	Burundi	81.830000
33	United States (Puerto Rico)	81.727500
17	Malawi	81.711818
6	Ecuador	80.955000
19	Mexico	80.863060
25	Philippines	80.834000
11	Honduras	80.832200
20	Myanmar	80.750000
18	Mauritius	80.500000
21	Nicaragua	80.010000

	Country.of.Origin	Total.Cup.Points
5	Cote d?Ivoire	79.330000
24	Peru	78.000000
10	Haiti	77.180000

Seems like a mixed bag from around the world. There seems to bare a small majority of african countries in the top half, an Hawaiian coffee seems to be a specialty!

In [70]:
```
df.groupby('Country.of.Origin').size().sort_values(ascending=False).plot.
```

Out[70]: <Axes: xlabel='Country.of.Origin', ylabel='Count'>



Though we see that there is a very skewed representation of countries in the dataset. Over a third of the coffee in the dataset is from Mexico!

In [71]:
```
df.groupby('Country.of.Origin')['Total.Cup.Points'].median().reset_index(
```

Out[71]:

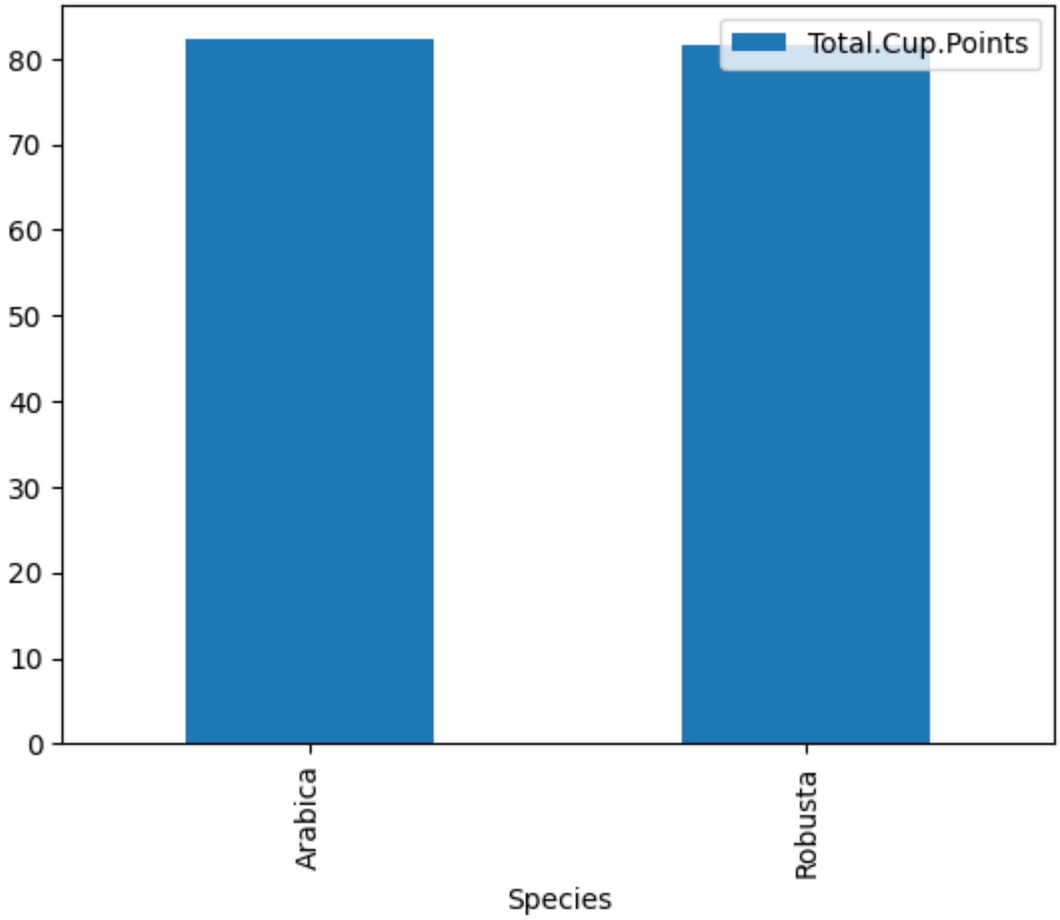
	Country.of.Origin	Total.Cup.Points
32	United States (Hawaii)	86.960
31	United States	86.625
23	Papua New Guinea	85.750
8	Ethiopia	85.250
14	Japan	84.670
15	Kenya	84.580
22	Panama	84.125
3	Colombia	83.250
2	China	83.170
4	Costa Rica	83.165
30	Uganda	83.085
7	El Salvador	82.920
34	Vietnam	82.830
26	Rwanda	82.830
13	Indonesia	82.665
29	Thailand	82.540
9	Guatemala	82.540
0	Brazil	82.500
28	Tanzania, United Republic Of	82.170
12	India	82.040
33	United States (Puerto Rico)	82.040
16	Laos	82.000
35	Zambia	81.920
27	Taiwan	81.875
1	Burundi	81.830
11	Honduras	81.625
17	Malawi	81.580
19	Mexico	81.580
25	Philippines	81.330
6	Ecuador	80.955
21	Nicaragua	80.920
20	Myanmar	80.625
18	Mauritius	80.500

	Country.of.Origin	Total.Cup.Points
5	Cote d?Ivoire	79.330
10	Haiti	79.000
24	Peru	78.000

Taking the median values, it seems aobut the same

In [72]:
```
df.groupby('Species')['Total.Cup.Points'].mean().reset_index().sort_value
```

Out[72]: `<Axes: xlabel='Species'>`



Surprinsingly, The Robusta species does not seem to have a much lower average score than Arabica, which we thought were far superior in taste

In [73]:
```
corr_mat = df.corr(numeric_only=True)
corr_mat
```

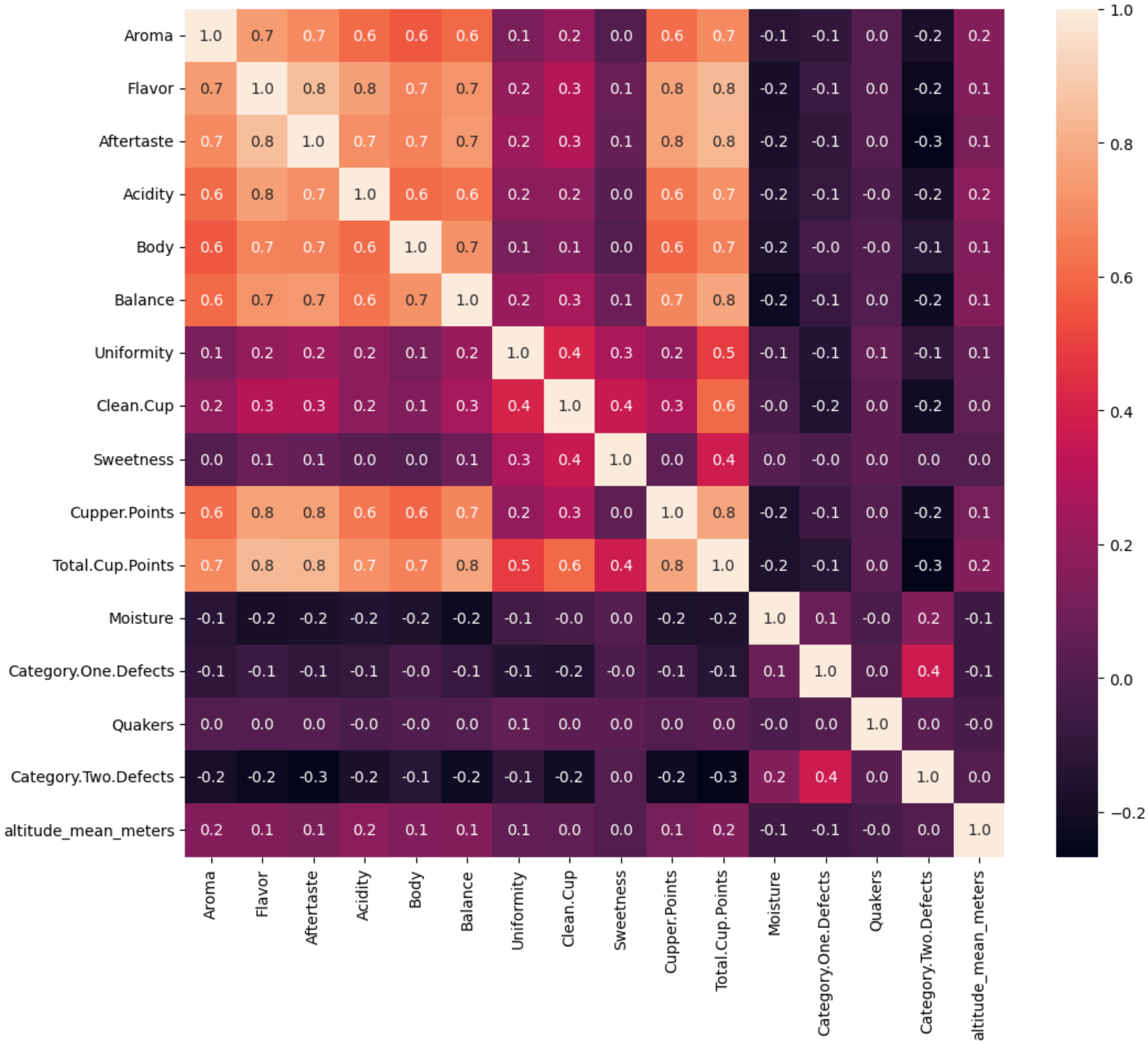
Out[73]:

	Aroma	Flavor	Aftertaste	Acidity	Body	Balan
Aroma	1.000000	0.743109	0.688130	0.606707	0.558217	0.6021
Flavor	0.743109	1.000000	0.849983	0.757027	0.668397	0.7221
Aftertaste	0.688130	0.849983	1.000000	0.705410	0.666111	0.7374
Acidity	0.606707	0.757027	0.705410	1.000000	0.604118	0.6247
Body	0.558217	0.668397	0.666111	0.604118	1.000000	0.7150
Balance	0.602133	0.722149	0.737439	0.624788	0.715045	1.0000
Uniformity	0.126962	0.207079	0.226183	0.178229	0.116480	0.2154
Clean.Cup	0.196811	0.297936	0.288698	0.176823	0.140021	0.2542
Sweetness	0.008310	0.077417	0.063372	0.022285	0.002498	0.0835
Cupper.Points	0.611088	0.764423	0.761057	0.642121	0.590999	0.6792
Total.Cup.Points	0.688725	0.836167	0.827814	0.708001	0.665436	0.7753
Moisture	-0.131316	-0.189600	-0.178685	-0.151101	-0.171327	-0.2270
Category.One.Defects	-0.104645	-0.069596	-0.103180	-0.090468	-0.035044	-0.0794
Quakers	0.007763	0.009010	0.007843	-0.017353	-0.002792	0.0010
Category.Two.Defects	-0.184304	-0.233813	-0.263210	-0.181162	-0.138092	-0.2188
altitude_mean_meters	0.155328	0.148021	0.133273	0.181499	0.142243	0.1444

In [74]:

```
plt.figure(figsize=(12, 10))
sns.heatmap(corr_mat, annot = True, fmt = ".1f")
```

Out[74]: <Axes: >



Unsurprisingly the different flavor parameters seems to correlate a lot with the Total Cup Points, and with each other. It seems that the main parameters that drags down the score is the amount of Category One and Two Defects, which we also suspected. Quakers doesn't seem to have a big impact on the overall Cup Point score. This might, of course, be biased by the low amount of values above zero

In [75]:
```
df.dtypes
```

Out[75]:
```
Species                   object
Country.of.Origin         object
Variety                   object
Processing.Method         object
Aroma                    float64
Flavor                   float64
Aftertaste               float64
Acidity                  float64
Body                     float64
Balance                  float64
Uniformity               float64
Clean.Cup                float64
Sweetness                float64
Cupper.Points            float64
Total.Cup.Points         float64
Moisture                 float64
Category.One.Defects       int64
Quakers                  float64
Color                     object
Category.Two.Defects       int64
altitude_mean_meters     float64
dtype: object
```

Lets label encode the categorical data, so we can see the nominal data affects the correlation score as well

In [76]:
```python
le = LabelEncoder()
cols_to_enc = df.select_dtypes(include='object').columns
enc_df = df.copy()

for col in cols_to_enc:
    enc_df[col] = le.fit_transform(df[col]).astype(int)

enc_df
```

Out[76]:

	Species	Country.of.Origin	Variety	Processing.Method	Aroma	Flavor	Aftertaste
0	0	8	5	4	8.67	8.83	8.67
1	0	8	13	4	8.75	8.67	8.50
2	0	9	2	4	8.42	8.50	8.42
3	0	8	5	0	8.17	8.58	8.42
4	0	8	13	4	8.25	8.50	8.25
...	...	...	...	...	...	...	...
1098	1	12	5	4	7.67	7.67	7.50
1099	1	12	5	0	7.58	7.42	7.42
1100	1	31	0	0	7.92	7.50	7.42
1101	1	6	5	4	7.50	7.67	7.75
1102	1	31	5	0	7.33	7.33	7.17

1103 rows × 21 columns

In [77]:
```python
enc_df.to_csv("../data_cleaned/encoded_df.csv", index=False)
```

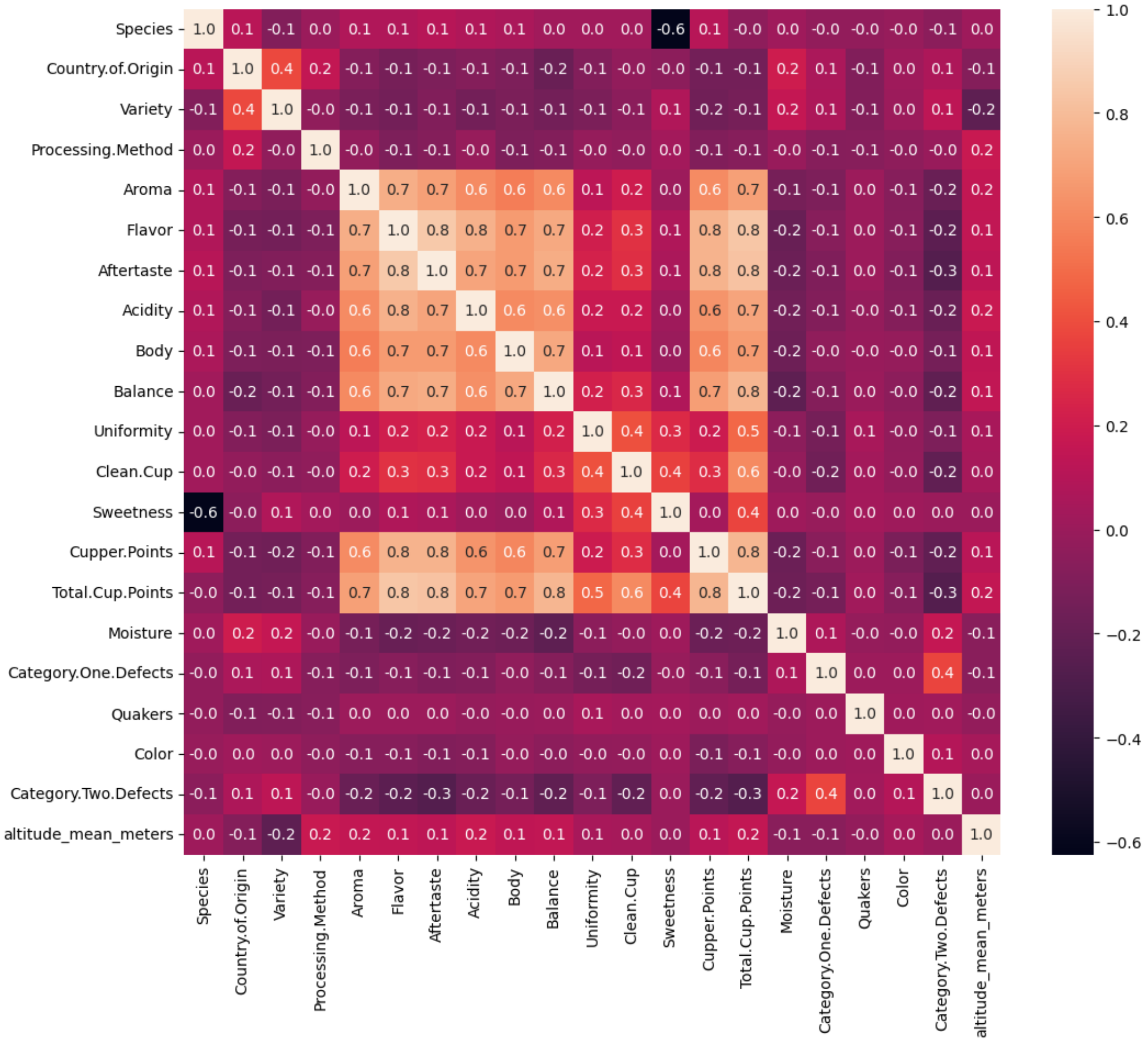
In [78]:
```python
# lets see how much variance it give us
df.describe()
```

Out[78]:

	Aroma	Flavor	Aftertaste	Acidity	Body	Balanc
count	1103.000000	1103.000000	1103.000000	1103.000000	1103.000000	1103.00000
mean	7.578368	7.527824	7.401496	7.535739	7.513654	7.51266
std	0.309181	0.331268	0.340065	0.313192	0.289467	0.35402
min	5.080000	6.170000	6.170000	5.250000	5.170000	5.25000
25%	7.420000	7.330000	7.250000	7.330000	7.330000	7.33000
50%	7.580000	7.580000	7.420000	7.500000	7.500000	7.50000
75%	7.750000	7.750000	7.580000	7.750000	7.670000	7.75000
max	8.750000	8.830000	8.670000	8.750000	8.580000	8.75000

In [79]:
```python
enc_corr_mat = enc_df.corr()
plt.figure(figsize=(12, 10))
sns.heatmap(enc_corr_mat, annot = True, fmt = ".1f")
```

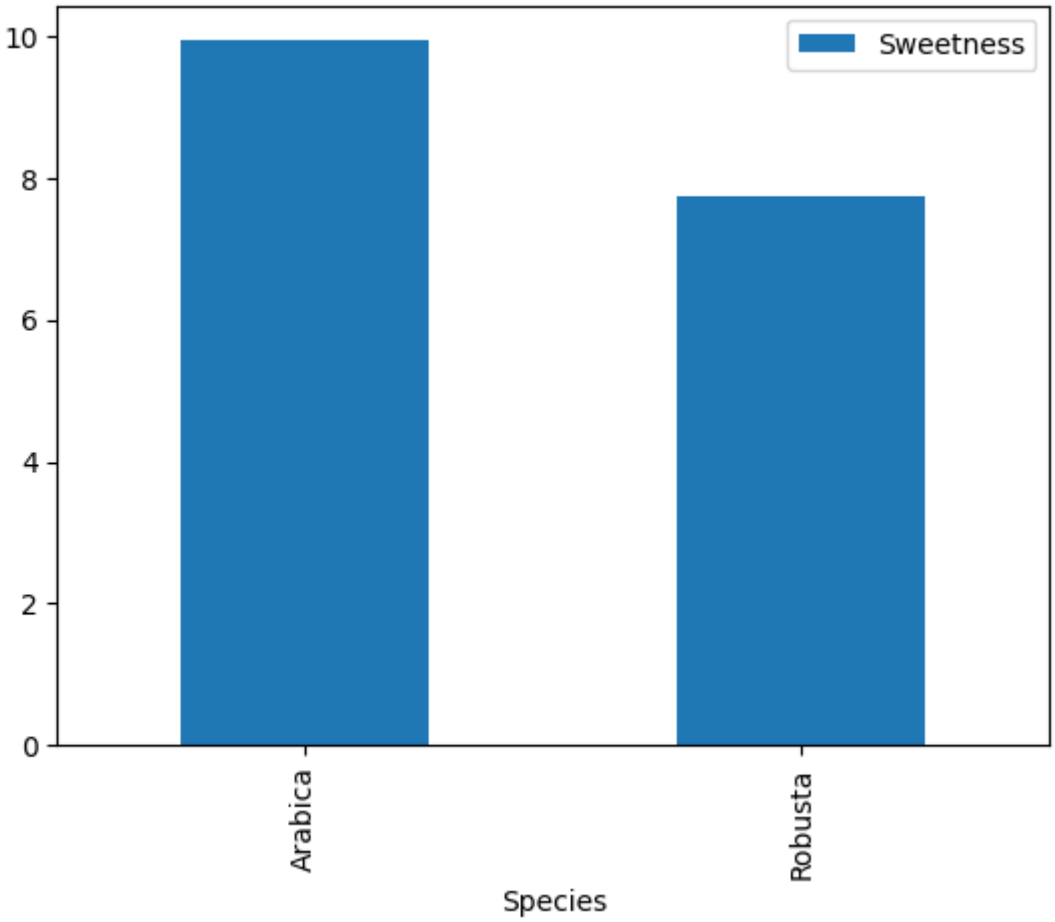
Out[79]: <Axes: >



The species of the coffee seems to have a significant impact on the sweetness

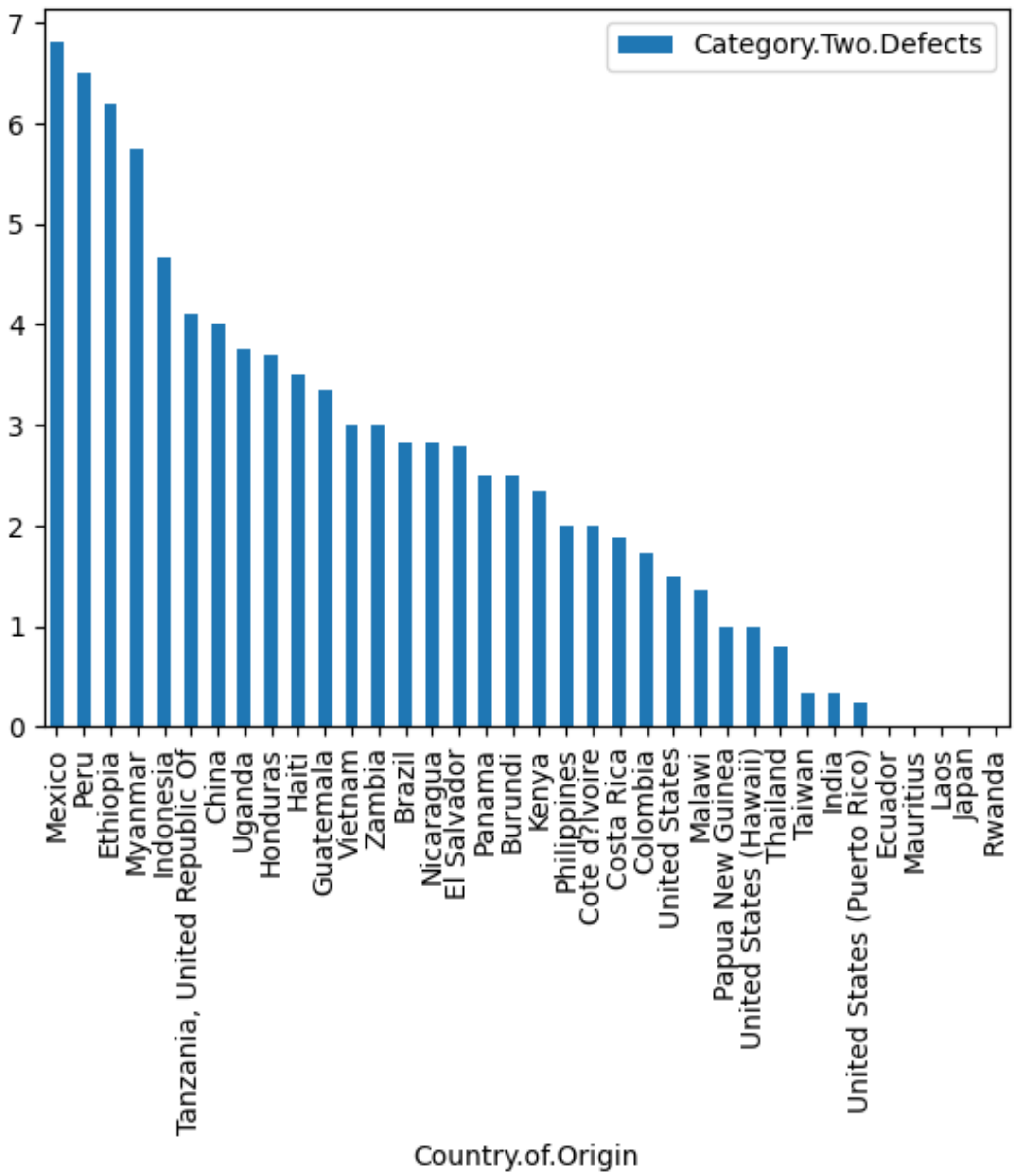
In [80]:
```
# Sweetnes grouped by species
df.groupby('Species')['Sweetness'].mean().reset_index().plot.bar(x='Speci
```

Out[80]: <Axes: xlabel='Species'>



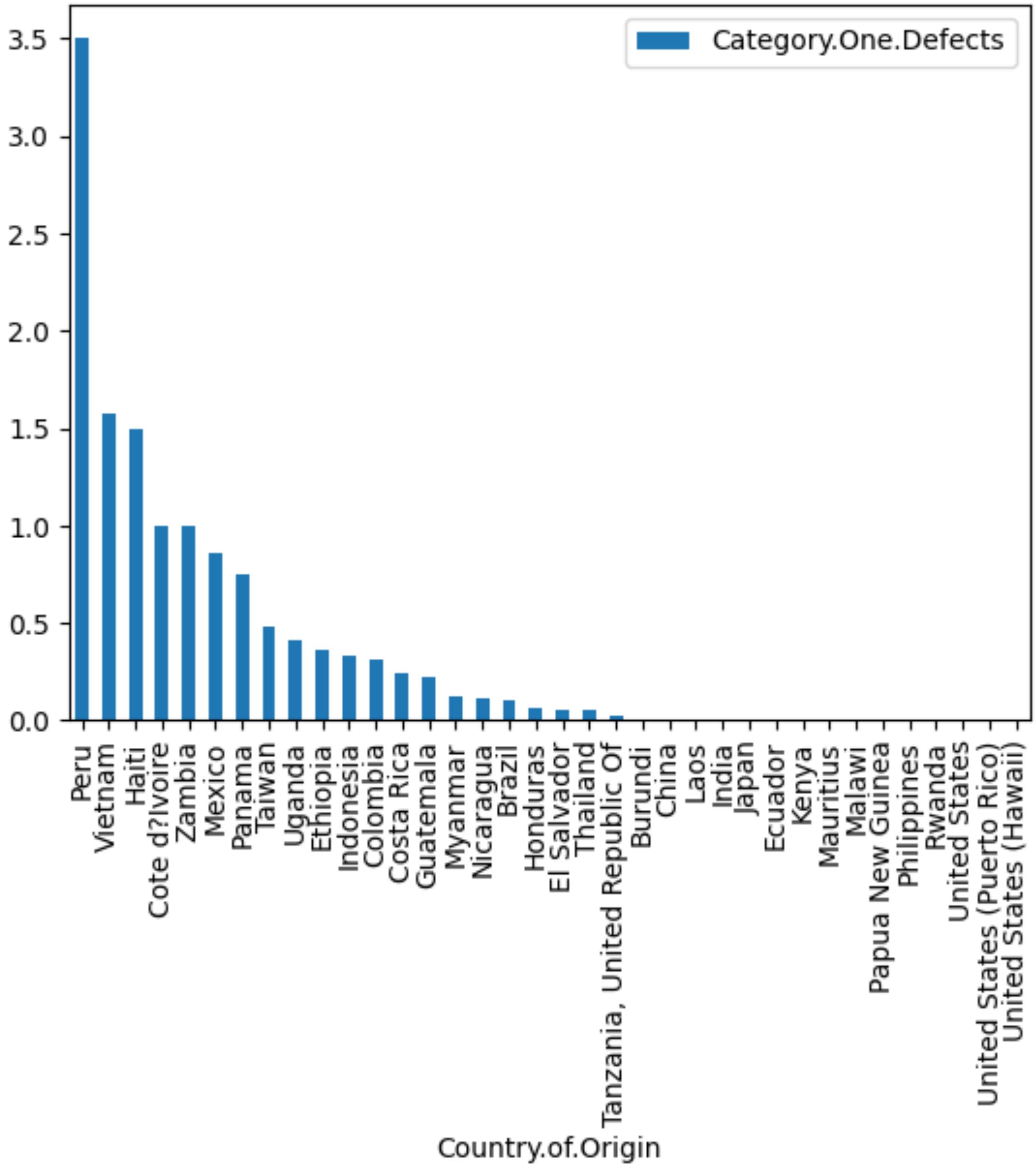
In [81]:
```
df.groupby('Country.of.Origin')['Category.Two.Defects'].mean().reset_inde
```

Out[81]: <Axes: xlabel='Country.of.Origin'>



In [82]:
```
df.groupby('Country.of.Origin')['Category.One.Defects'].mean().reset_inde
```

Out[82]:
```
<Axes: xlabel='Country.of.Origin'>
```



Interestingly though, we also find Ethiopia among the countries with the highest mean in Category 2 defect parameters, even though it is the country with the averagely highest scoring coffee. This indicates that it takes rather large amounts of defects in the coffee to really make an impact on the overall score.

Clustering model training

We'll try to extract more information with clustering models. For this purpose we drop our previous target feature "Total Cup Points" and scale the feature values in the dataset, so we can do a principal component analysis

In [83]:
```
# df_cls = enc_df.drop('Total Cup Points', axis=1)
df_cls = enc_df.copy()
```

In [84]:
```
df_cls[df_cls.columns] = sk.preprocessing.StandardScaler().fit_transform(
```

In [85]:
```
df_cls.sample(5)
```

Out[85]:

	Species	Country.of.Origin	Variety	Processing.Method	Aroma	Flavor
962	-0.152286	-0.441966	-0.958392	0.526081	-0.253585	-1.594069
307	-0.152286	-1.070443	-0.620082	0.526081	-0.253585	0.157575
849	-0.152286	0.710241	0.282078	-1.445381	-1.321406	-0.325637
1002	-0.152286	0.605495	1.635319	0.526081	-0.803674	-1.594069
292	-0.152286	1.548210	0.845929	0.526081	0.555370	0.429382

In [86]:

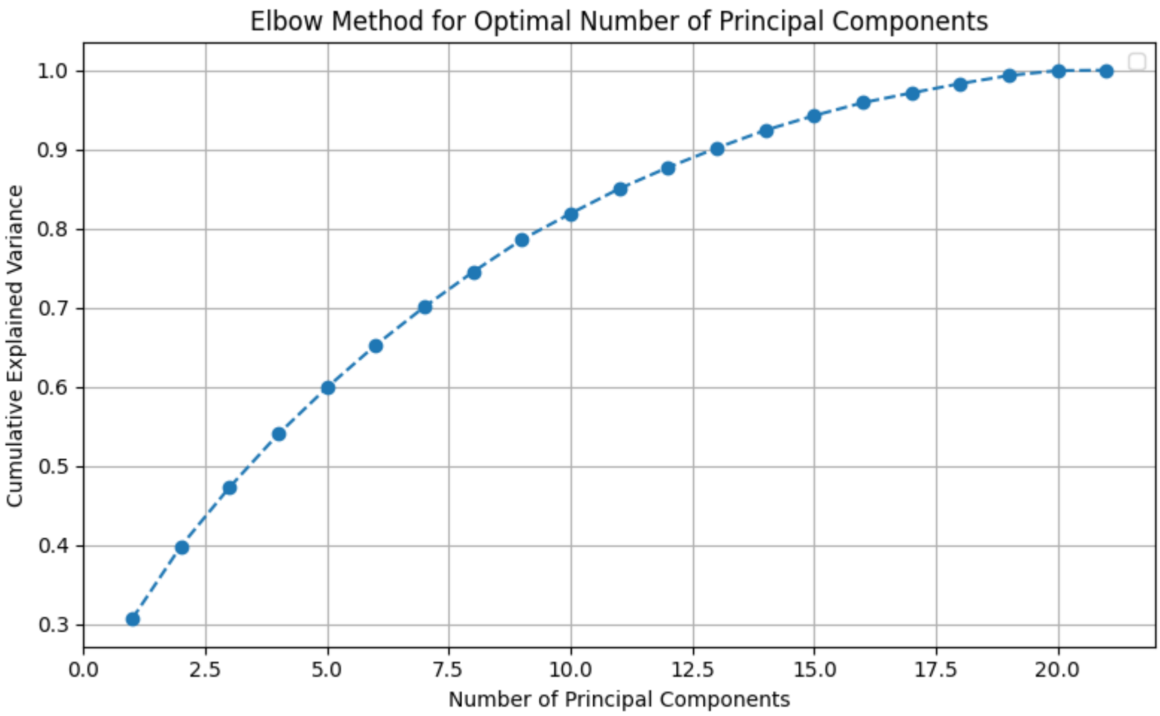
```
pca = PCA()
pca.fit(df_cls)
explained_variance = pca.explained_variance_ratio_
cumulative_variance = np.cumsum(explained_variance)
# 3 principal components
cumulative_variance[2]
```

Out[86]: np.float64(0.4725891234734746)

In [87]:

```
plt.figure(figsize=(8, 5))
plt.plot(range(1, len(cumulative_variance) + 1), cumulative_variance, mar
plt.xlabel('Number of Principal Components')
plt.ylabel('Cumulative Explained Variance')
plt.title('Elbow Method for Optimal Number of Principal Components')
plt.grid(True)
plt.legend()
plt.tight_layout()
plt.show()
```

```
/tmp/ipykernel_12403/3103998374.py:7: UserWarning: No artists with labels
found to put in legend.  Note that artists whose label start with an under
score are ignored when legend() is called with no argument.
  plt.legend()
```



Not as much as we hoped for. For 3 principal components, we get just above 50% explained variance, which is not a lot. Lets try and extract high correlating features and do the PCA again

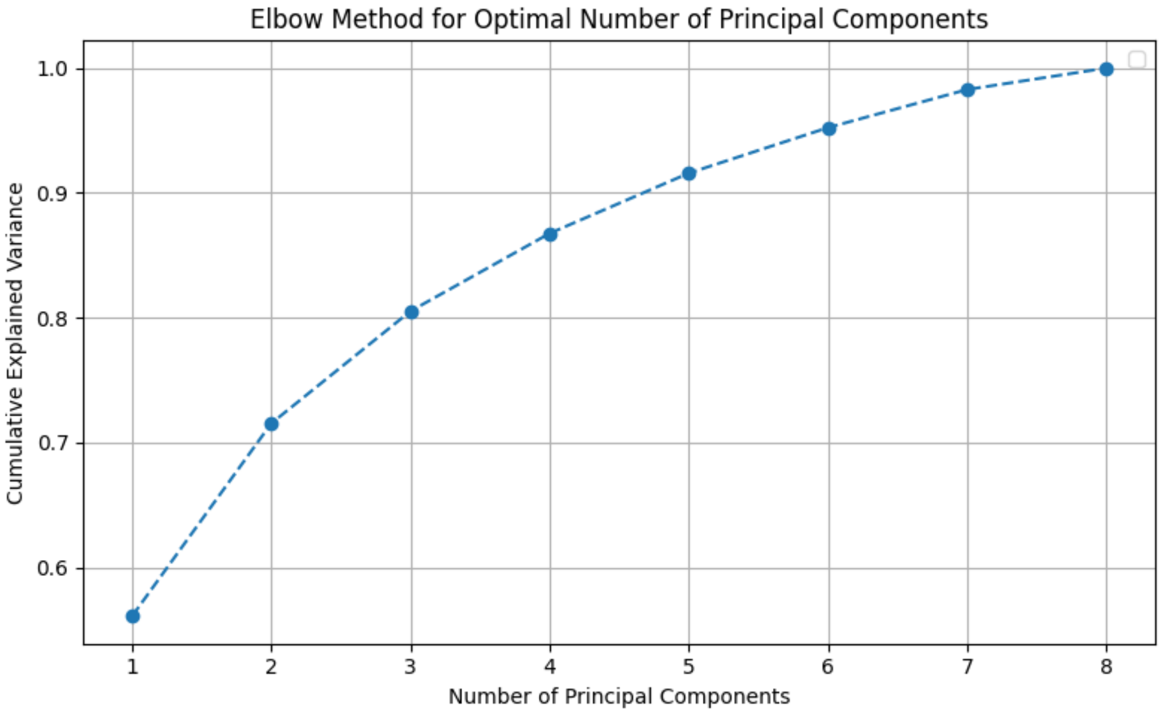
In [88]:
```
df_cls_ext = enc_df[["Aroma","Flavor","Acidity","Body","Balance","Afterta
df_cls_ext[df_cls_ext.columns] = sk.preprocessing.StandardScaler().fit_tr
```

In [89]:
```
pca = PCA()
pca.fit(df_cls_ext)
explained_variance = pca.explained_variance_ratio_
cumulative_variance = np.cumsum(explained_variance)
# 3 principal components
cumulative_variance[2]
```

Out[89]:
```
np.float64(0.8053004618615184)
```

In [90]:
```
plt.figure(figsize=(8, 5))
plt.plot(range(1, len(cumulative_variance) + 1), cumulative_variance, mar
plt.xlabel('Number of Principal Components')
plt.ylabel('Cumulative Explained Variance')
plt.title('Elbow Method for Optimal Number of Principal Components')
plt.grid(True)
plt.legend()
plt.tight_layout()
plt.show()
```

```
/tmp/ipykernel_12403/3103998374.py:7: UserWarning: No artists with labels
found to put in legend.  Note that artists whose label start with an under
score are ignored when legend() is called with no argument.
  plt.legend()
```



Now we have an explained variance of above 70% with 2 principal components. Much better!

In [91]:
```
pca_2 = PCA(n_components=2)
pca_2_result = pca_2.fit_transform(df_cls_ext)
dataset_pca = pd.DataFrame(abs(pca_2.components_), columns=df_cls_ext.col
dataset_pca
```

Out[91]:

	Aroma	Flavor	Acidity	Body	Balance	Aftertaste	Uniformity	Swee
PC_1	0.381225	0.436044	0.392771	0.381476	0.404040	0.428197	0.128396	0.0
PC_2	0.103547	0.019839	0.057700	0.113975	0.009413	0.009358	0.659328	0.7

Here is our principal components. We see that PC1 is weighted across all the features, with a dive in Uniformity and Sweetness, while PC2 is mostly weighted be these.

In [92]:

```
df_pca = pd.DataFrame(pca_2_result, columns=['PC_1', 'PC_2'])
df_pca.head()
```

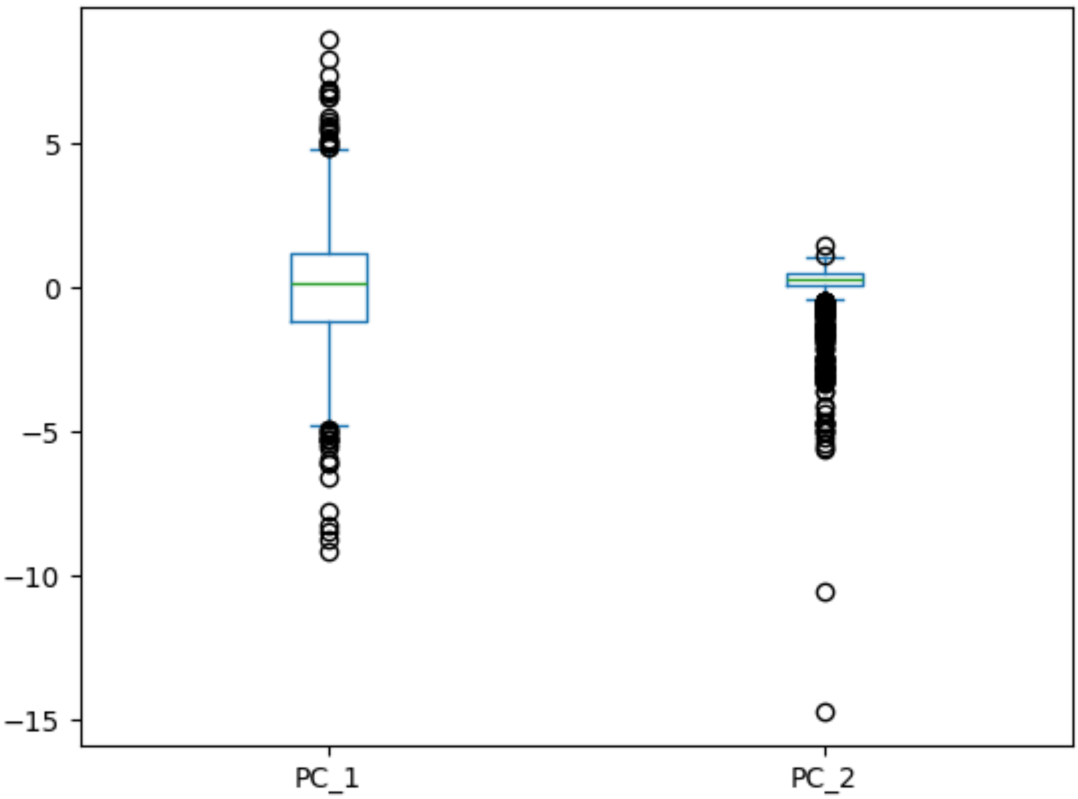
Out[92]:

	PC_1	PC_2
0	8.565309	-0.713374
1	7.920370	-0.663066
2	6.869235	-0.475166
3	6.696222	-0.467683
4	6.561643	-0.466118

In [93]:

```
df_pca.plot.box()
```

Out[93]: <Axes: >



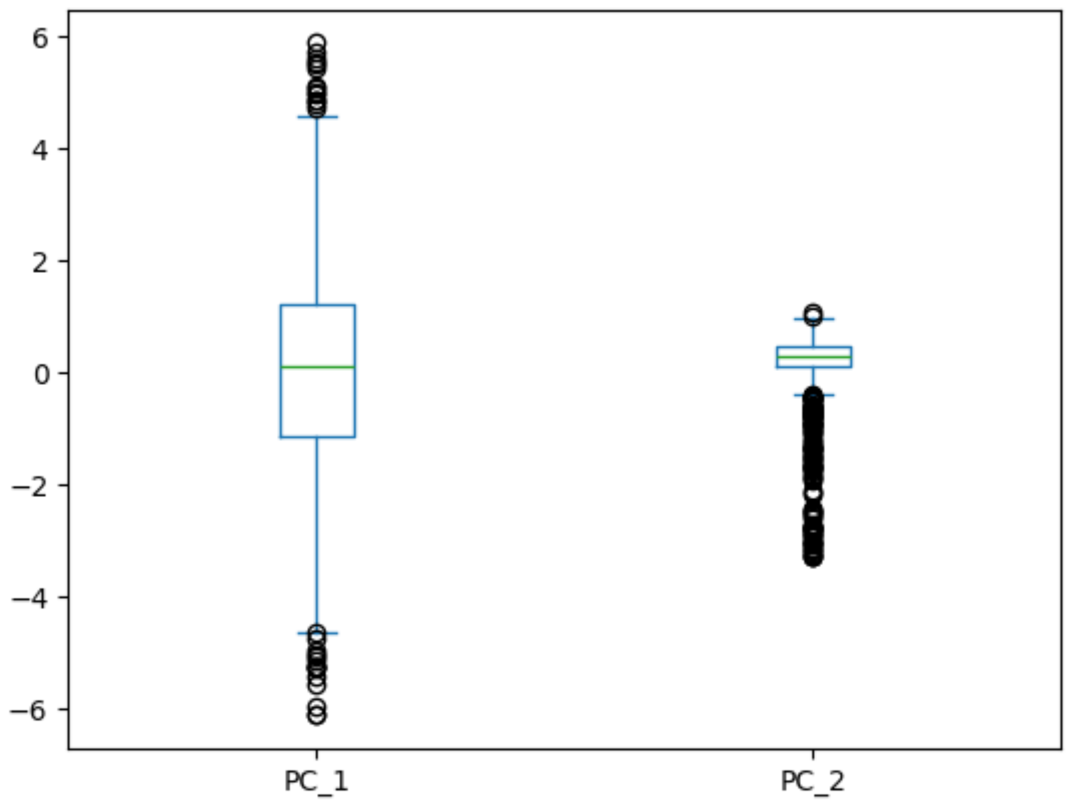
We have also introduced some serious outliers. Lets remove them

In [94]:

```
z_scores = np.abs(zscore(df_pca))
df_pca = df_pca[(z_scores < 3).all(axis=1)]
```

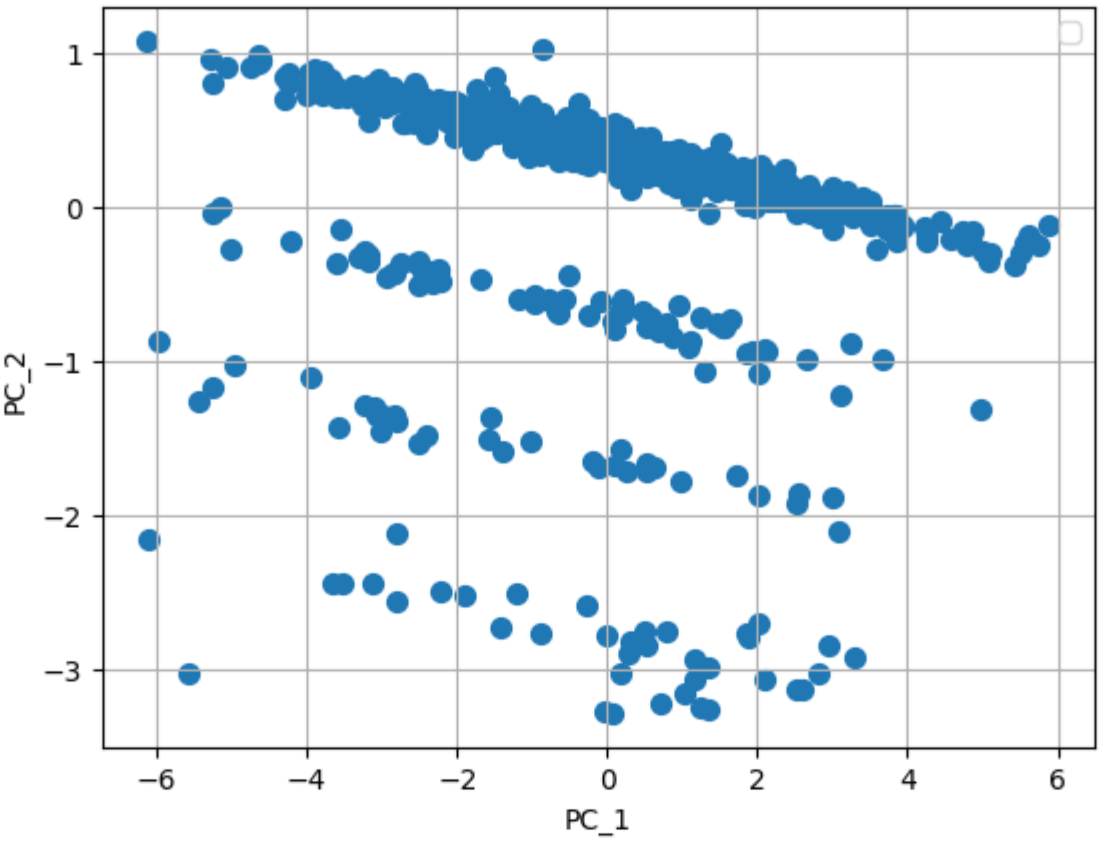
In [95]:
```
df_pca.plot.box()
```

Out[95]: <Axes: >



In [96]:
```
fig = plt.figure()
plt.scatter(df_pca['PC_1'], df_pca['PC_2'], s=50, cmap='viridis')
plt.xlabel('PC_1')
plt.ylabel('PC_2')
plt.grid(True)
plt.legend()
plt.show()
```

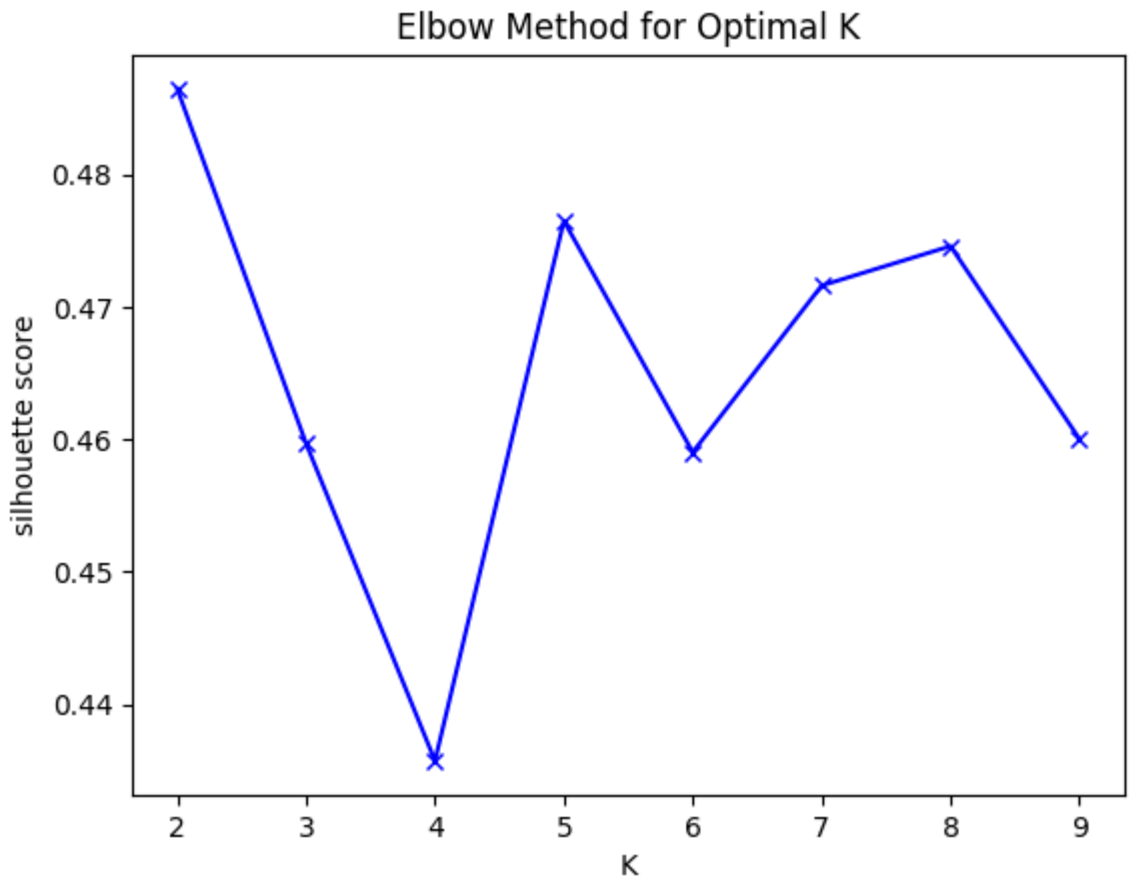
```
/tmp/ipykernel_12403/519479020.py:2: UserWarning: No data for colormapping
provided via 'c'. Parameters 'cmap' will be ignored
  plt.scatter(df_pca['PC_1'], df_pca['PC_2'], s=50, cmap='viridis')
/tmp/ipykernel_12403/519479020.py:6: UserWarning: No artists with labels f
ound to put in legend.  Note that artists whose label start with an unders
core are ignored when legend() is called with no argument.
  plt.legend()
```


PC_2
PC_1
1
0
−1
−2
−3
−6
−4
−2
0
2
4
6

In [97]:
```
# Calculating optimal number of clusters in a K-means algorithm using sil
scores = []
K = range(2,10)
for k in K:
    model = KMeans(n_clusters=k, n_init=10)
    model.fit(df_pca)
    score = sk.metrics.silhouette_score(df_pca, model.labels_, metric='eu
    print("\nNumber of clusters =", k)
    print("Silhouette score =", score)
    scores.append([k, score])
```

```
Number of clusters = 2
Silhouette score = 0.4864683885974626

Number of clusters = 3
Silhouette score = 0.45968642227744294

Number of clusters = 4
Silhouette score = 0.4357283895887136

Number of clusters = 5
Silhouette score = 0.4764977680674508

Number of clusters = 6
Silhouette score = 0.4590307090562025

Number of clusters = 7
Silhouette score = 0.4716143428820624

Number of clusters = 8
Silhouette score = 0.4745932627502572

Number of clusters = 9
Silhouette score = 0.4600339588086069
```

In [98]:
```
score_df = pd.DataFrame(scores, columns=['k', 'scores'])
fig = plt.figure()
plt.title('Elbow Method for Optimal K')
plt.plot(score_df.k, score_df.scores, 'bx-')
plt.xlabel('K')
plt.ylabel('silhouette score')
plt.show()
```

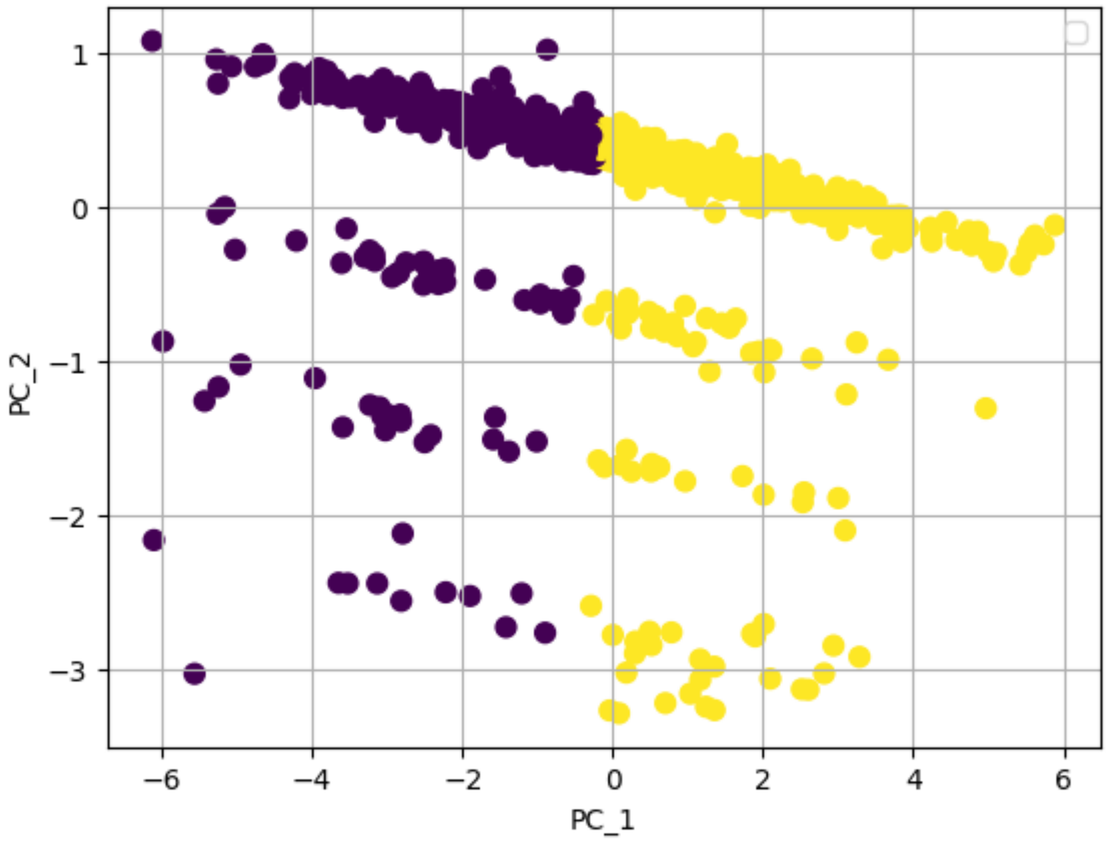


Using silhouette score for each amount of clusters, we se that we achieve a maximum score of 0,473 on 2 clusters. Let's try and visualize them

In [99]:
```
kmeans = KMeans(init='k-means++', n_clusters=2, n_init=10)
prediction = kmeans.fit_predict(df_pca)
```

In [100…
```
fig = plt.figure()
plt.scatter(df_pca['PC_1'], df_pca['PC_2'], c=prediction, s=50, cmap='vir
plt.xlabel('PC_1')
plt.ylabel('PC_2')
plt.grid(True)
plt.legend()
plt.show()
```

```
/tmp/ipykernel_12403/3703295130.py:6: UserWarning: No artists with labels
found to put in legend.  Note that artists whose label start with an under
score are ignored when legend() is called with no argument.
  plt.legend()
```



Well, its doesn't seem like the K-means algorithm finds any clusters that makes visual sense. Lets try to the PCA again with an additional PC. The extra dimension and 10% added explained variance, might give additional insights

In [101…
```
pca_3 = PCA(n_components=3)
pca_3_result = pca_3.fit_transform(df_cls_ext)
dataset_pca = pd.DataFrame(abs(pca_3.components_), columns=df_cls_ext.col
dataset_pca
```

Out[101…

	Aroma	Flavor	Acidity	Body	Balance	Aftertaste	Uniformity	Swe
PC_1	0.381225	0.436044	0.392771	0.381476	0.404040	0.428197	0.128396	0.0
PC_2	0.103547	0.019839	0.057700	0.113975	0.009413	0.009358	0.659328	0.7
PC_3	0.049970	0.040739	0.022757	0.067166	0.034935	0.002558	0.731547	0.6

Here are our components. With PC1 weighted across most parameters, PC2 mostly weighted by Sweetness and Uniformity and PC3 weighted mainly by Uniformity

In [102…
```
df_pca = pd.DataFrame(pca_3_result, columns=['PC_1', 'PC_2', 'PC_3'])
df_pca.head()
```

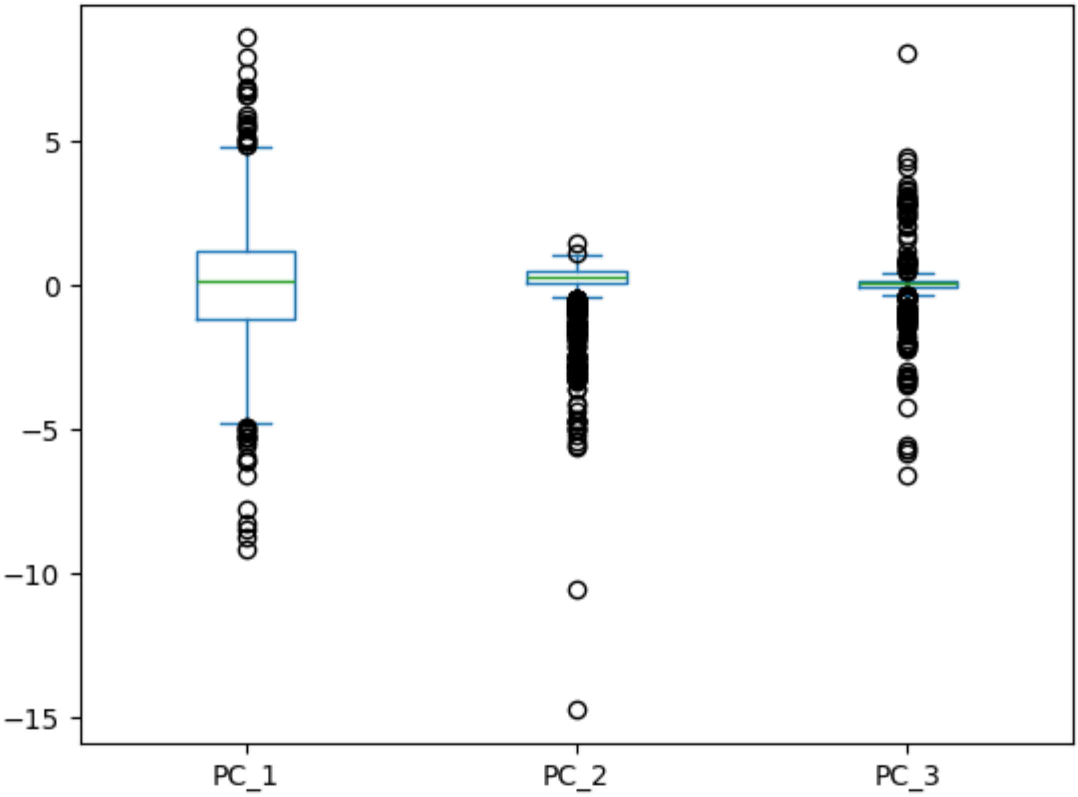
Out[102…

	PC_1	PC_2	PC_3
0	8.565309	-0.713374	-0.498447
1	7.920370	-0.663066	-0.486764
2	6.869235	-0.475166	-0.403830
3	6.696222	-0.467683	-0.395929
4	6.561643	-0.466118	-0.383813

In [103…

```
df_pca.plot.box()
```

Out[103… <Axes: >



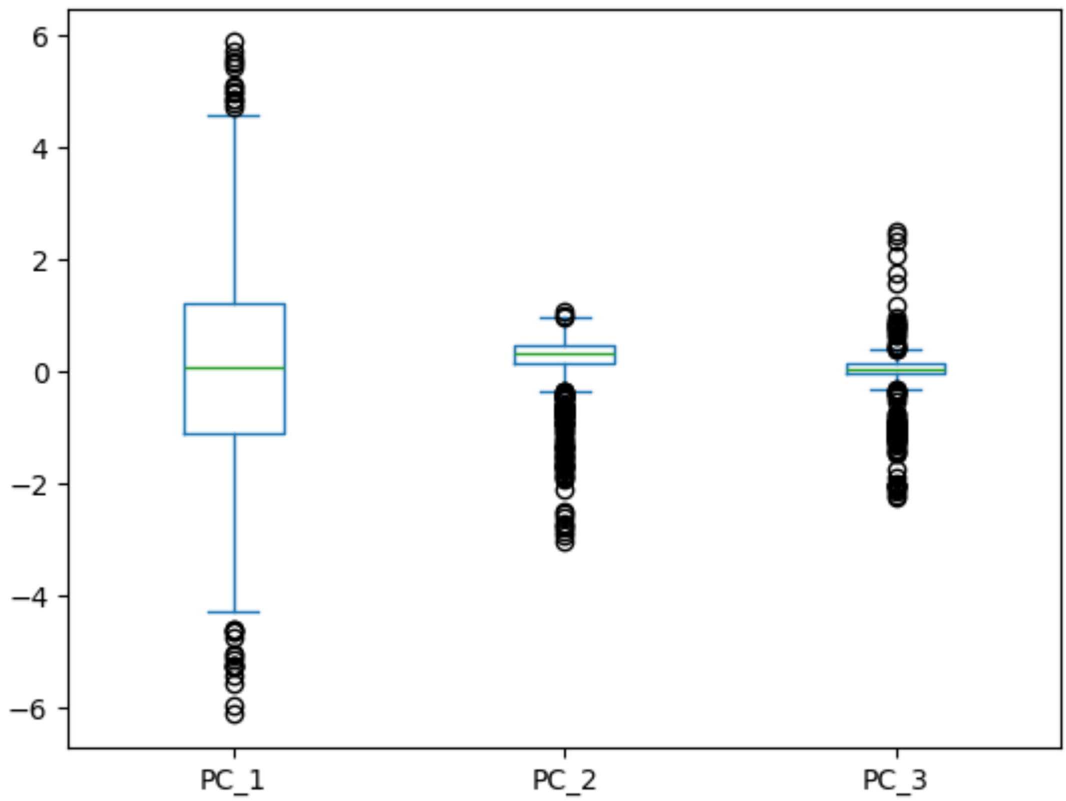
In [104…

```
z_scores = np.abs(zscore(df_pca))
df_pca = df_pca[(z_scores < 3).all(axis=1)]
```

In [105…

```
df_pca.plot.box()
```

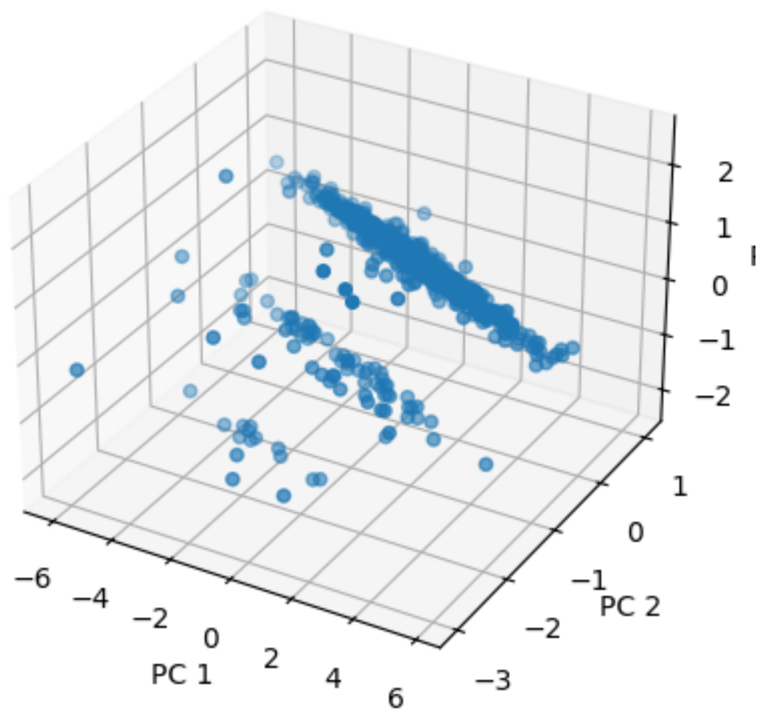
Out[105… <Axes: >



In [106…

```
fig = plt.figure()
ax = fig.add_subplot(projection='3d')
ax.scatter(df_pca['PC_1'], df_pca['PC_2'], df_pca['PC_3'])

ax.set_xlabel('PC 1')
ax.set_ylabel('PC 2')
ax.set_zlabel('PC 3')
```

Out[106… Text(0.5, 0, 'PC 3')

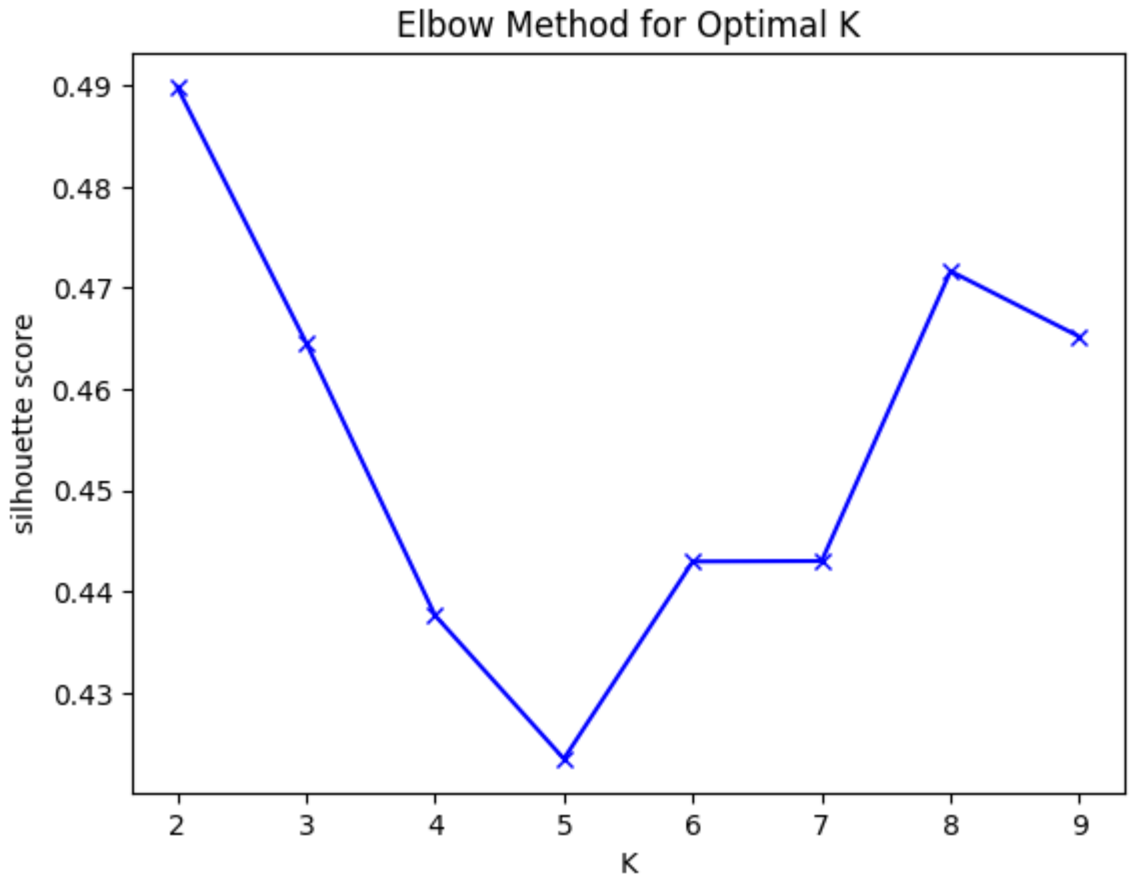


Here is our 3D points. Let's start with doing doing a K-means clustering algorithm. First we need to find the optimal K (Number of clusters)

In [107…
```
# Calculating optimal number of clusters in a K-means algorithm using sil
scores = []
K = range(2,10)
for k in K:
    model = KMeans(n_clusters=k, n_init=10)
    model.fit(df_pca)
    score = sk.metrics.silhouette_score(df_pca, model.labels_, metric='eu
    print("\nNumber of clusters =", k)
    print("Silhouette score =", score)
    scores.append([k, score])
```

```
Number of clusters = 2
Silhouette score = 0.4898576695192007

Number of clusters = 3
Silhouette score = 0.4645804564710879

Number of clusters = 4
Silhouette score = 0.4376410764623363

Number of clusters = 5
Silhouette score = 0.4234582724839815

Number of clusters = 6
Silhouette score = 0.442960181970954

Number of clusters = 7
Silhouette score = 0.443005556219866

Number of clusters = 8
Silhouette score = 0.47164334262945723

Number of clusters = 9
Silhouette score = 0.4651752303653036
```

In [108…
```
score_df = pd.DataFrame(scores, columns=['k', 'scores'])
fig = plt.figure()
plt.title('Elbow Method for Optimal K')
plt.plot(score_df.k, score_df.scores, 'bx-')
plt.xlabel('K')
plt.ylabel('silhouette score')
plt.show()
```



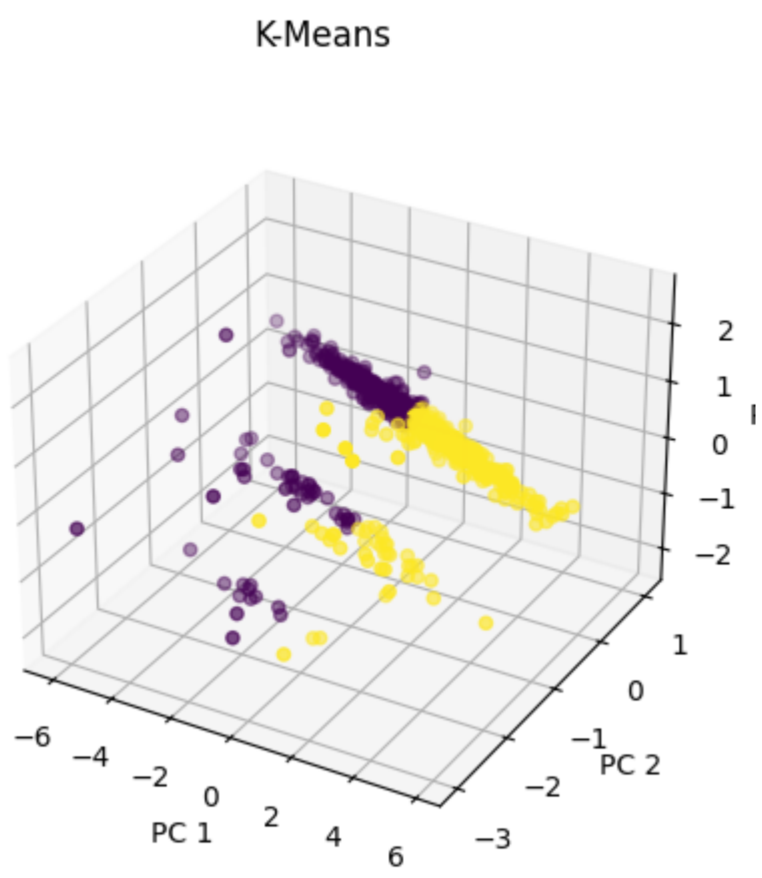
In [109…
```
kmeans = KMeans(init='k-means++', n_clusters=2, n_init=10)
prediction = kmeans.fit_predict(df_pca)
```

In [110…
```
prediction
```

Out[110…
```
array([1, 1, 1, ..., 1, 1, 1], shape=(1042,), dtype=int32)
```

In [111…
```
fig = plt.figure()
fig.suptitle("K-Means")
ax = fig.add_subplot(projection='3d')
ax.scatter(df_pca['PC_1'], df_pca['PC_2'], df_pca['PC_3'], c=prediction)

ax.set_xlabel('PC 1')
ax.set_ylabel('PC 2')
ax.set_zlabel('PC 3')
```

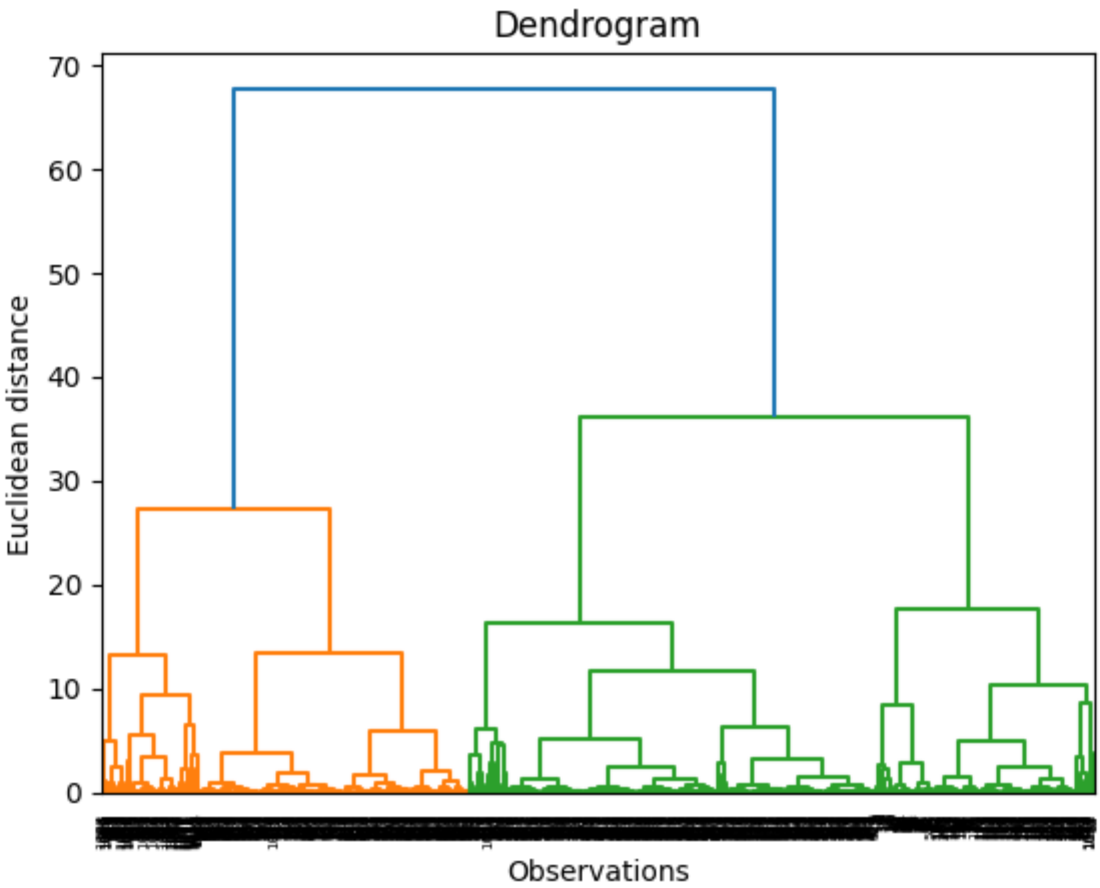
Out[111…
```
Text(0.5, 0, 'PC 3')
```



Well, the K-means method doesn't seem to agree with us. Lets try doing agglomerative clustering instead

In [112…

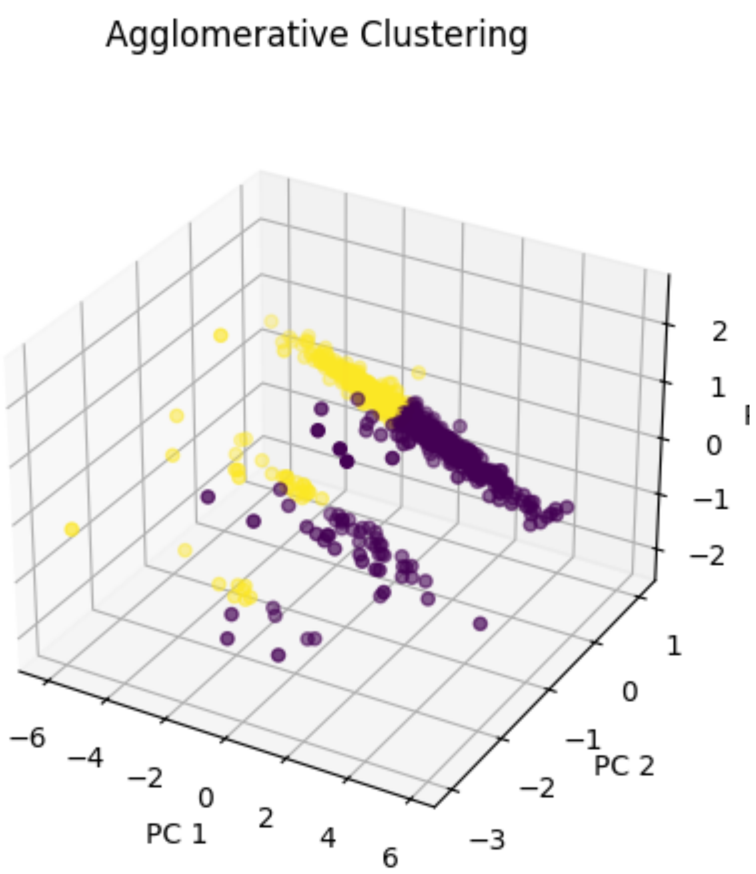
```
# Dendogram for agglomerative clustering
plt.figure()
dendogram = ch.dendrogram(ch.linkage(df_pca, method = 'ward'))
plt.title('Dendrogram')
plt.xlabel('Observations')
plt.ylabel('Euclidean distance')
plt.show()
```



In [113…
```
model = AgglomerativeClustering(2, linkage = 'ward')
aggmodel_pred = model.fit_predict(df_pca)
```

In [114…
```
fig = plt.figure()
fig.suptitle("Agglomerative Clustering")
ax = fig.add_subplot(projection='3d')
ax.scatter(df_pca['PC_1'], df_pca['PC_2'], df_pca['PC_3'], c=aggmodel_pre

ax.set_xlabel('PC 1')
ax.set_ylabel('PC 2')
ax.set_zlabel('PC 3')
```

Out[114… Text(0.5, 0, 'PC 3')



Well that doesn't seem to agree either. Lets try running a DBSCAN

In [115…

```
#DBSCAN for automatically determining amount of clusters
# Tried to play a little around with eps here
dbscan = DBSCAN(eps=0.7, min_samples=10)
dbscan_pred = dbscan.fit_predict(df_pca)
dbscan_pred
```

Out[115…

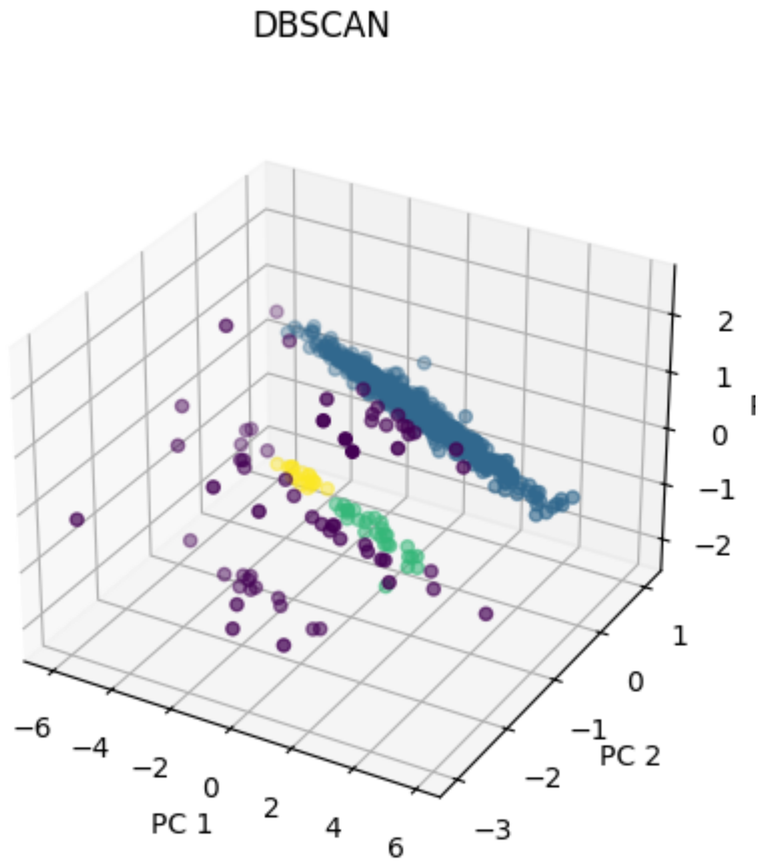
```
array([ 0,  0,  0, ..., -1, -1, -1], shape=(1042,))
```

In [116…

```
fig = plt.figure()
fig.suptitle("DBSCAN")
ax = fig.add_subplot(projection='3d')
ax.scatter(df_pca['PC_1'], df_pca['PC_2'], df_pca['PC_3'], c=dbscan_pred)

ax.set_xlabel('PC 1')
ax.set_ylabel('PC 2')
ax.set_zlabel('PC 3')
```

Out[116…

```
Text(0.5, 0, 'PC 3')
```



The DBSCAN clustering seems to yield the best results so far. There's a clear large cluster, showing the correlation between PC1 and PC2. Two smaller clusters showing a concentration of data points in the same correlation between PC1 and PC2, but is offset on PC2 and PC3. Showing 2 potential subcategories of data along both axises of PC2 and PC3.

In this case we suspect the clusters mostly represent the bean species, since both PC2 and PC3 are mainly weighted by Unifomity and Sweetness. We found in earlier analysis, that the main difference between Arabica and Robusta beans seem to be in sweetness. This fits with a cluster split along PC2 and PC3 axises, along with the much smaller cluster size in terms of data points, since Robusta beans are less represented in the dataset.