```
In [2]: %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
```

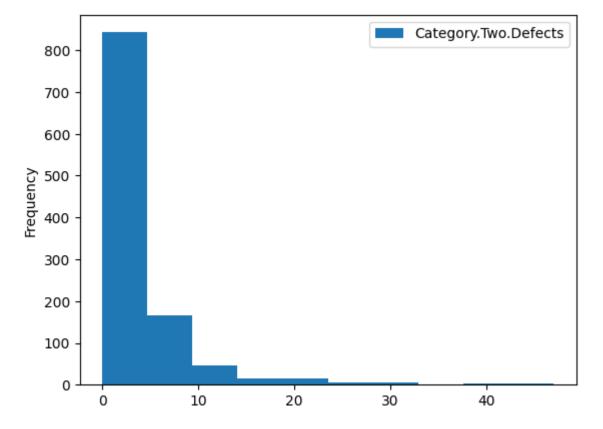
CPU times: user 4 $\mu s,$ sys: 0 ns, total: 4 μs Wall time: 9.06 μs

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

2 of 32

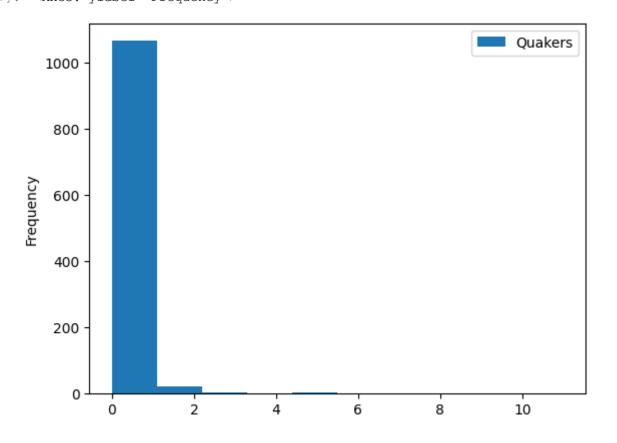
```
In [4]: df.columns
Out[4]: Index(['Species', 'Country.of.Origin', 'Variety', 'Processing.Method', 'A
        roma',
                'Flavor', 'Aftertaste', 'Acidity', 'Body', 'Balance', 'Uniformit
        у',
                'Clean.Cup', 'Sweetness', 'Cupper.Points', 'Total.Cup.Points',
                'Moisture', 'Category.One.Defects', 'Quakers', 'Color',
                'Category.Two.Defects', 'altitude_mean_meters'],
               dtype='object')
In [5]: df.info()
       <class 'pandas.core.frame.DataFrame'>
       RangeIndex: 1103 entries, 0 to 1102
       Data columns (total 21 columns):
        # Column
                                  Non-Null Count Dtype
       ---
                                  _____
          Species
                                  1103 non-null object
        0
          Country.of.Origin 1103 non-null object
        1
                                 1103 non-null object
        2 Variety
        3 Processing.Method 1103 non-null object
                                 1103 non-null float64
          Aroma
        4
          Flavor
                                 1103 non-null float64
        5
        6 Aftertaste
                                 1103 non-null float64
        7
          Acidity
                                 1103 non-null float64
                                 1103 non-null float64
          Body
        8
                              1103 non-null float64
1103 non-null float64
1103 non-null float64
        9 Balance
        10 Uniformity
        11 Clean.Cup
        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 [6]: df[['Category.Two.Defects']].plot.hist()
Out[6]: <Axes: ylabel='Frequency'>
```

11/05/2025, 10.14



We're gonna keep these outlying values, as they might have a high impact on the quality score

```
In [7]: df[['Quakers']].plot.hist()
Out[7]: <Axes: ylabel='Frequency'>
```



Data Exploration

Lets see which countries can boast the highest cup grades

```
In [8]: df.groupby('Country.of.Origin')['Total.Cup.Points'].mean().reset_index().
```

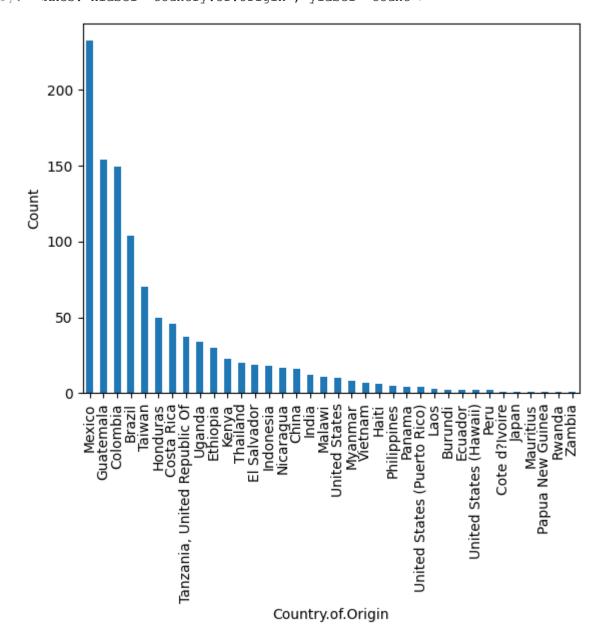
Out[8]:		Country.of.Origin	Total.Cup.Points
	32	United States (Hawaii)	86.960000
	8	Ethiopia	85.916333
	23	Papua New Guinea	85.750000
	14	Japan	84.670000
	31	United States	84.433000
	15	Kenya	84.271304
	22	Panama	83.707500
	30	Uganda	83.382941
	3	Colombia	83.224832
	7	El Salvador	83.115263
	2	China	82.927500
	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
	5	Cote d?Ivoire	79.330000
	24	Peru	78.000000

Country.of.Origin Total.Cup.Points

10 Haiti 77.180000

Seems like a mixed bag from around the world. Quality doens't seem to be linked rigonally, but there is a small majority of african countries in the top half, and Hawaiian coffee seems to be a specialty!

```
In [9]: df.groupby('Country.of.Origin').size().sort_values(ascending=False).plot.}
Out[9]: <Axes: xlabel='Country.of.Origin', ylabel='Count'>
```



Though we see that there is a very skewed representation of countries in the dataset. About 1/4 of the coffee in the dataset is from Mexico!

```
In [10]: df.groupby('Country.of.Origin')['Total.Cup.Points'].median().reset_index()
```

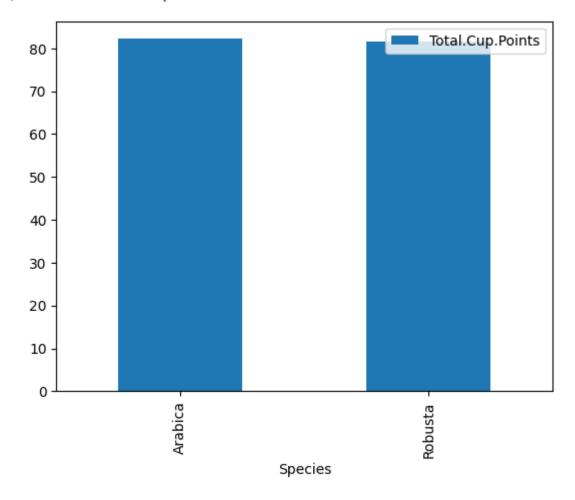
Out[10]:	Country.of.Origin	Total.Cup.Points
32	United States (Hawaii)	86.960
31	United States	86.625
23	Papua New Guinea	85.750
8	Ethiopia	85.250
14	Japan	84.670
15	Kenya	84.580
22	Panama	84.125
3	Colombia	83.250
2	China	83.170
4	Costa Rica	83.165
30	Uganda	83.085
7	El Salvador	82.920
34	Vietnam	82.830
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
5	Cote d?Ivoire	79.330
10	Haiti	79.000

Country.of.Origin Total.Cup.Points

24 Peru 78.000

Taking the median values, it seems about the same

```
In [11]: df.groupby('Species')['Total.Cup.Points'].mean().reset_index().sort_values
Out[11]: <Axes: xlabel='Species'>
```

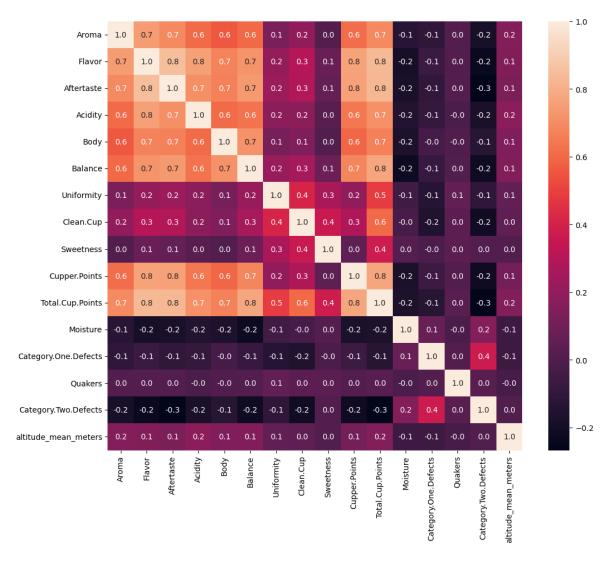


Surprinsingly, The Robusta species does not seem to have a much lower average score than Arabica, which we thought were far superior in taste

Out[12]:		Aroma	Flavor	Aftertaste	Acidity	Body	Balance				
	Aroma	1.000000	0.743109	0.688130	0.606707	0.558217	0.602133				
	Flavor	0.743109	1.000000	0.849983	0.757027	0.668397	0.722149				
	Aftertaste	0.688130	0.849983	1.000000	0.705410	0.666111	0.737439				
	Acidity	0.606707	0.757027	0.705410	1.000000	0.604118	0.624788				
	Body	0.558217	0.668397	0.666111	0.604118	1.000000	0.715045				
	Balance	0.602133	0.722149	0.737439	0.624788	0.715045	1.000000				
	Uniformity	0.126962	0.207079	0.226183	0.178229	0.116480	0.215432				
	Clean.Cup	0.196811	0.297936	0.288698	0.176823	0.140021	0.254276				
	Sweetness	0.008310	0.077417	0.063372	0.022285	0.002498	0.083593				
	Cupper.Points	0.611088	0.764423	0.761057	0.642121	0.590999	0.679213				
	Total.Cup.Points	0.688725	0.836167	0.827814	0.708001	0.665436	0.775314				
	Moisture	-0.131316	-0.189600	-0.178685	-0.151101	-0.171327	-0.227089				
	Category.One.Defects	-0.104645	-0.069596	-0.103180	-0.090468	-0.035044	-0.079425				
	Quakers	0.007763	0.009010	0.007843	-0.017353	-0.002792	0.001002				
	Category.Two.Defects	-0.184304	-0.233813	-0.263210	-0.181162	-0.138092	-0.218804				
	altitude_mean_meters	0.155328	0.148021	0.133273	0.181499	0.142243	0.144477				
In [13]:	[13]: plt.figure(figsize=(12, 10))										

```
In [13]: plt.figure(figsize=(12, 10))
sns.heatmap(corr_mat, annot = True, fmt = ".1f")
```

Out[13]: <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 [14]: df.dtypes

```
Out[14]: Species
                                      object
          Country.of.Origin
                                    object
                                      object
          Variety
          Processing.Method object
                                    float64
          Aroma
          Flavor
                                    float64
          Aftertaste
                                    float64
          Acidity
                                    float64
                                   float64
          Body
          Balance
                                   float64
          Uniformity
                                    float64
          Clean.Cup
                                   float64
          Clean.cur
Sweetness Inca:
Cupper.Points float64
Total.Cup.Points float64
int64
          Category.One.Defects int64
Quakers float64
Color object
          color object
Category.Two.Defects int64
          altitude_mean_meters float64
          dtype: object
```

Lets label encode the categorical data into discrete values, so we can see how the nominal data affects the correlation score as well.

```
In [15]: 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[15]:		Species	Country.of.Origin	Variety	Processing.Method	Aroma	Flavor	Aftertast
	0	0	8	5	4	8.67	8.83	8.6
	1	0	8	13	4	8.75	8.67	8.5
	2	0	9	2	4	8.42	8.50	8.4
	3	0	8	5	0	8.17	8.58	8.4
	4	0	8	13	4	8.25	8.50	8.2
	1098	1	12	5	4	7.67	7.67	7.5
	1099	1	12	5	0	7.58	7.42	7.4
	1100	1	31	0	0	7.92	7.50	7.4
	1101	1	6	5	4	7.50	7.67	7.7
	1102	1	31	5	0	7.33	7.33	7.1

1103 rows × 21 columns

In [16]: enc_df.to_csv("../data_cleaned/encoded_df.csv", index=False)

Lets see how much variance it give us

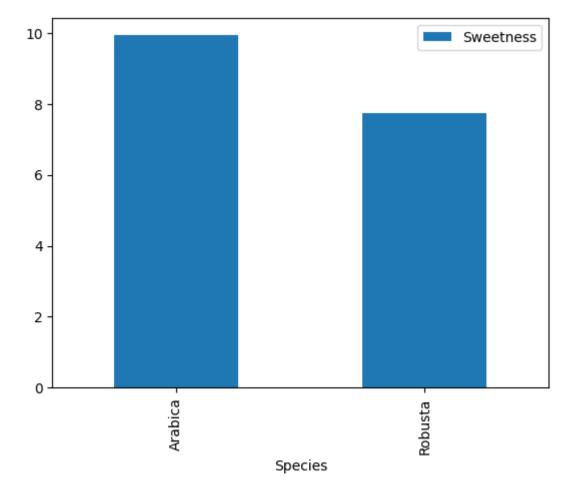
In [17]: df.describe()

Out[17]:		Aroma	Flavor	Aftertaste	Acidity	Body	Balance
	count	1103.000000	1103.000000	1103.000000	1103.000000	1103.000000	1103.000000
	mean	7.578368	7.527824	7.401496	7.535739	7.513654	7.512665
	std	0.309181	0.331268	0.340065	0.313192	0.289467	0.354021
	min	5.080000	6.170000	6.170000	5.250000	5.170000	5.250000
	25%	7.420000	7.330000	7.250000	7.330000	7.330000	7.330000
	50%	7.580000	7.580000	7.420000	7.500000	7.500000	7.500000
	75%	7.750000	7.750000	7.580000	7.750000	7.670000	7.750000
	max	8.750000	8.830000	8.670000	8.750000	8.580000	8.750000

```
In [18]: enc_corr_mat = enc_df.corr()
            plt.figure(figsize=(12, 10))
            sns.heatmap(enc_corr_mat, annot = True, fmt = ".1f")
Out[18]: <Axes: >
                                                                                                      - 1.0
                   Country.of.Origin - 0.1 1.0 0.4 0.2 -0.1 -0.1 -0.1 -0.1 -0.1 -0.2 -0.1 -0.0 -0.0 -0.1 -0.1 0.2 0.1 -0.1 0.0 0.1 -0.1
                    - 0.8
            Aroma - 0.1 -0.1 -0.1 -0.0 1.0 0.7 0.7 0.6 0.6 0.6 0.1 0.2 0.0 0.6 0.7 -0.1 -0.1 0.0 -0.1 -0.2 0.2
                                                                                                      - 0.6
                    Flavor - 0.1 -0.1 -0.1 -0.1 0.7 1.0 0.8 0.8 0.7 0.7 0.2 0.3 0.1 0.8 0.8 -0.2 -0.1 0.0 -0.1 -0.2 0.1
                  Aftertaste - 0.1 -0.1 -0.1 -0.1 0.7 0.8 1.0 0.7 0.7 0.7 0.2 0.3 0.1 0.8 0.8 -0.2 -0.1 0.0 -0.1 -0.3 0.1
                    Acidity - 0.1 -0.1 -0.1 -0.0 0.6 0.8 0.7 1.0 0.6 0.6 0.2 0.2 0.0 0.6 0.7 -0.2 -0.1 -0.0 -0.1 -0.2 0.2
                                                                                                       - 0.4
                     Body - 0.1 -0.1 -0.1 -0.1 0.6 0.7 0.7 0.6 1.0 0.7 0.1 0.1 0.0 0.6 0.7 -0.2 -0.0 -0.0 -0.0 0.1 0.1
                   Balance - 0.0 -0.2 -0.1 -0.1 0.6 0.7 0.7 0.6 0.7 1.0 0.2 0.3 0.1 0.7 0.8 -0.2 -0.1 0.0 -0.0 -0.2 0.1
                 Uniformity - 0.0 -0.1 -0.1 -0.0 0.1 0.2 0.2 0.2 0.1 0.2 1.0 0.4 0.3 0.2 0.5 -0.1 -0.1 0.1 -0.0 -0.1 0.1
                                                                                                      - 0.2
                  Clean.Cup - 0.0 -0.0 -0.1 -0.0 0.2 0.3 0.3 0.2 0.1 0.3 0.4 1.0 0.4 0.3 0.6 -0.0 -0.2 0.0 -0.0 -0.2 0.0
                 Sweetness - -0.6 -0.0 0.1 0.0 0.0 0.1 0.1 0.0 0.0 0.1 0.3 0.4 1.0 0.0 0.4 0.0 -0.0 0.0 0.0 0.0 0.0
                                                                                                       - 0.0
               Cupper.Points - 0.1 -0.1 -0.2 -0.1 0.6 0.8 0.8 0.8 0.6 0.6 0.7 0.2 0.3 0.0 1.0 0.8 -0.2 -0.1 0.0 -0.1 -0.2 0.1
              Total.Cup.Points - 0.0 -0.1 -0.1 -0.1 -0.1 0.7 0.8 0.8 0.7 0.7 0.8 0.5 0.6 0.4 0.8 1.0 -0.2 -0.1 0.0 -0.1 -0.3 0.2
                   Moisture - 0.0 0.2 0.2 -0.0 -0.1 -0.2 -0.2 -0.2 -0.2 -0.2 -0.1 -0.0 0.0 -0.2 -0.2 1.0 0.1 -0.0 -0.0 0.2 -0.1
                                                                                                      - -0.2
          Category.Two.Defects - -0.1 0.1 0.1 -0.0 -0.2 -0.2 -0.3 -0.2 -0.1 -0.2 -0.1 -0.2 -0.1 -0.2 0.0 -0.2 -0.3 0.2 0.4 0.0 0.1 1.0 0.0
          altitude_mean_meters - 0.0 -0.1 -0.2 0.2 0.2 0.1 0.1 0.2 0.1 0.1 0.1 0.0 0.0 0.1 0.2 -0.1 -0.1 -0.0 0.0 0.0 1.0
                                                                        Total.Cup.Points
                                                                                            altitude mean meters
```

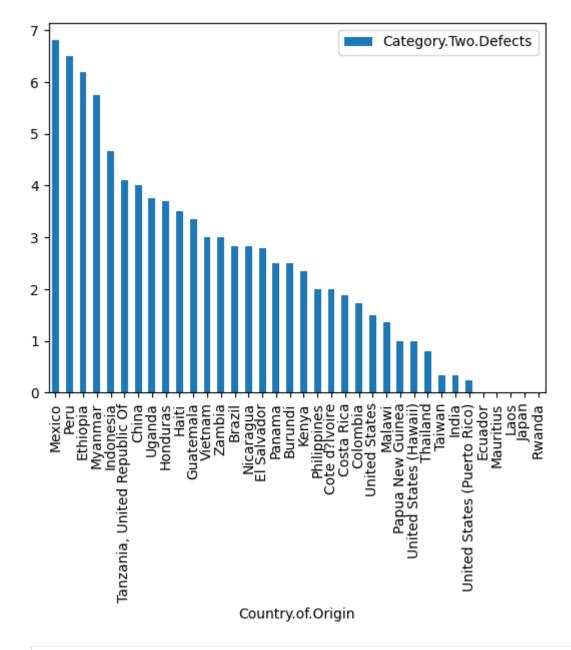
The species of the coffee seems to have a significant impact on the sweetness

```
In [19]: # Sweetnes grouped by species
df.groupby('Species')['Sweetness'].mean().reset_index().plot.bar(x='Specie)
Out[19]: <Axes: xlabel='Species'>
```



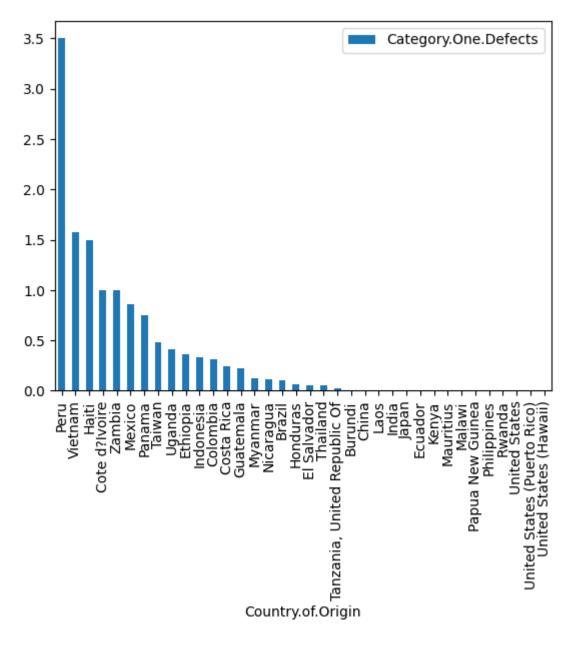
So this is where the Arabica beans stand out! It's on average around 20% sweeter than Robousta beans

```
In [20]: df.groupby('Country.of.Origin')['Category.Two.Defects'].mean().reset_inde:
Out[20]: <Axes: xlabel='Country.of.Origin'>
```



In [21]: df.groupby('Country.of.Origin')['Category.One.Defects'].mean().reset_index

Out[21]: <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 4th 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 [23]: df_cls = enc_df.drop('Total.Cup.Points', axis=1)
# df_cls = enc_df.copy()

In [24]: df_cls[df_cls.columns] = sk.preprocessing.StandardScaler().fit_transform(d:
In [25]: df_cls.sample(5)
```

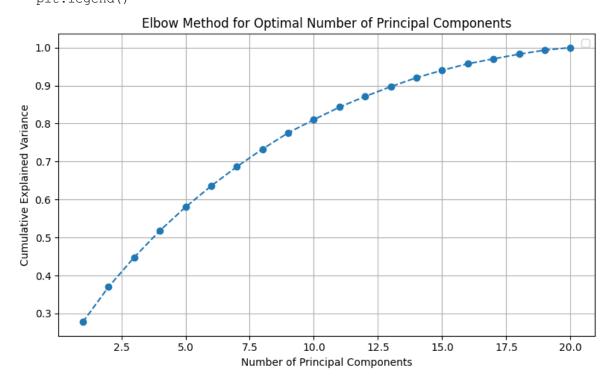
Out[25]:	Species		Country.of.Origin	Variety	Processing.Method	Aroma	Flavor
	113	-0.152286	-1.070443	0.282078	0.526081	0.814236	0.429382
	150	-0.152286	1.652957	-0.845622	-2.102535	0.814236	0.670988
	49	-0.152286	-0.651458	-0.958392	-0.131073	0.814236	1.426007
	828	-0.152286	2.071941	0.282078	0.526081	0.296504	0.670988
	958	-0.152286	0.605495	1.635319	0.526081	-1.062540	-2.107482

```
In [26]: 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[26]: np.float64(0.4478511071920876)

```
In [27]: plt.figure(figsize=(8, 5))
    plt.plot(range(1, len(cumulative_variance) + 1), cumulative_variance, marl
    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_11022/3103998374.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()

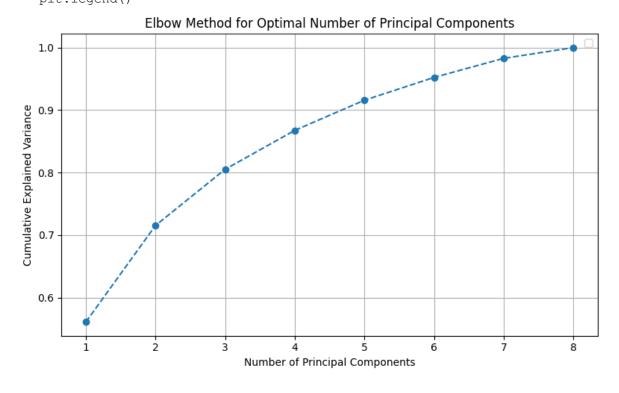


Not as much as we hoped for. For 3 principal components, we get just above 50% explained variance, which is not a lot. Lets try and extract high correlating features and

do the PCA again

```
In [28]: df_cls_ext = enc_df[["Aroma", "Flavor", "Acidity", "Body", "Balance", "Aftertage of the control of the
                                   df_cls_ext[df_cls_ext.columns] = sk.preprocessing.StandardScaler().fit_tran
In [29]: 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 [29]: np.float64(0.8053004618615184)
In [30]: plt.figure(figsize=(8, 5))
                                   plt.plot(range(1, len(cumulative_variance) + 1), cumulative_variance, marl
                                   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_11022/3103998374.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 [31]: 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.columnset_pca
```

Out[31]:		Aroma	Flavor	Acidity	Body	Balance	Aftertaste	Uniformity	Sweet
	PC_1	0.381225	0.436044	0.392771	0.381476	0.404040	0.428197	0.128396	0.04
	PC_2	0.103547	0.019839	0.057700	0.113975	0.009413	0.009358	0.659328	0.73

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.

```
Out [32]: PC_1 PC_2

0 8.565309 -0.713374

1 7.920370 -0.663066

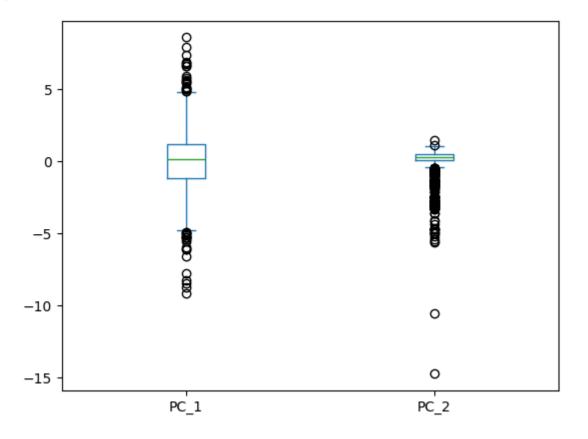
2 6.869235 -0.475166

3 6.696222 -0.467683

4 6.561643 -0.466118
```

```
In [33]: df_pca.plot.box()
```

Out[33]: <Axes: >

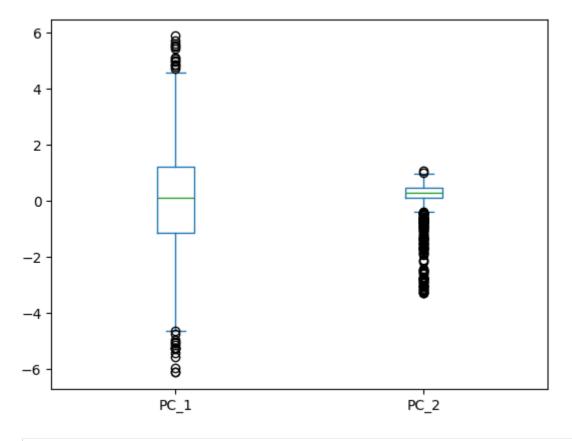


We have also introduced some serious outliers. Lets remove them

```
In [34]: z_scores = np.abs(zscore(df_pca))
df_pca = df_pca[(z_scores < 3).all(axis=1)]</pre>
```

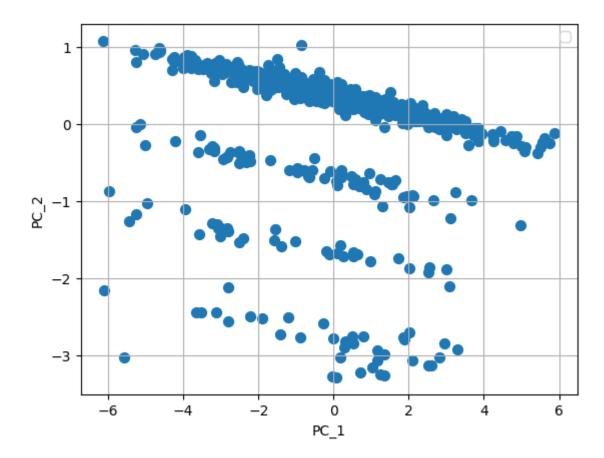
```
In [35]: df_pca.plot.box()
```

Out[35]: <Axes: >



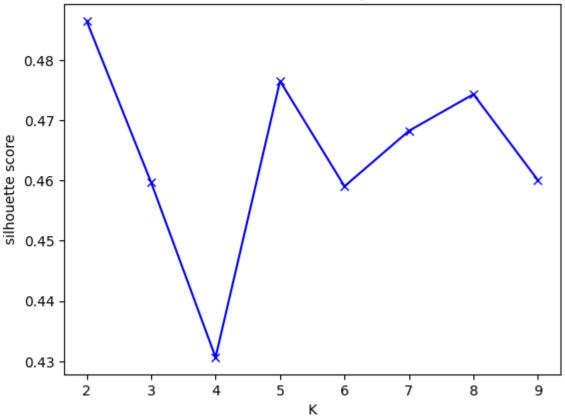
```
In [36]: fig = plt.figure()
    plt.scatter(df_pca['PC_1'], df_pca['PC_2'], s=50)
    plt.xlabel('PC_1')
    plt.ylabel('PC_2')
    plt.grid(True)
    plt.legend()
    plt.show()
```

/tmp/ipykernel_11022/573061907.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()



```
In [37]: # Calculating optimal number of clusters in a K-means algorithm using sill
         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='euc
             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 = 0.4596864222774429
        Number of clusters = 4
        Silhouette score = 0.4306487916313575
        Number of clusters = 5
        Silhouette score = 0.4764977680674508
        Number of clusters = 6
        Silhouette score = 0.4590307090562025
        Number of clusters = 7
        Silhouette score = 0.468243031713899
        Number of clusters = 8
        Silhouette score = 0.4743114637983735
        Number of clusters = 9
        Silhouette score = 0.4600339588086069
In [38]: | 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()
```

Elbow Method for Optimal K

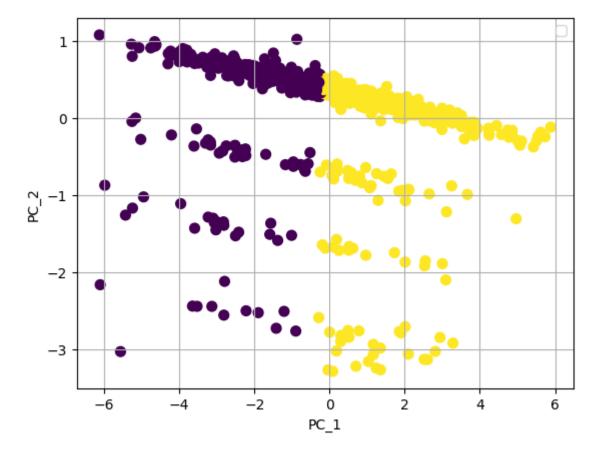


Using silhouette score for each amount of clusters, we se that we achieve a maximum score of 0,473 on 2 clusters. Let's try and visualize them

```
In [39]: kmeans = KMeans(init='k-means++', n_clusters=2, n_init=10)
    prediction = kmeans.fit_predict(df_pca)

In [40]: 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_11022/3703295130.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 [41]: 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.columnset_pca
```

Out[41]:		Aroma	Flavor	Acidity	Body	Balance	Aftertaste	Uniformity	Sweet
	PC_1	0.381225	0.436044	0.392771	0.381476	0.404040	0.428197	0.128396	0.04
	PC_2	0.103547	0.019839	0.057700	0.113975	0.009413	0.009358	0.659328	0.73
	PC_3	0.049970	0.040739	0.022757	0.067166	0.034935	0.002558	0.731547	0.67

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

```
        PC_1
        PC_2
        PC_3

        0
        8.565309
        -0.713374
        -0.498447

        1
        7.920370
        -0.663066
        -0.486764

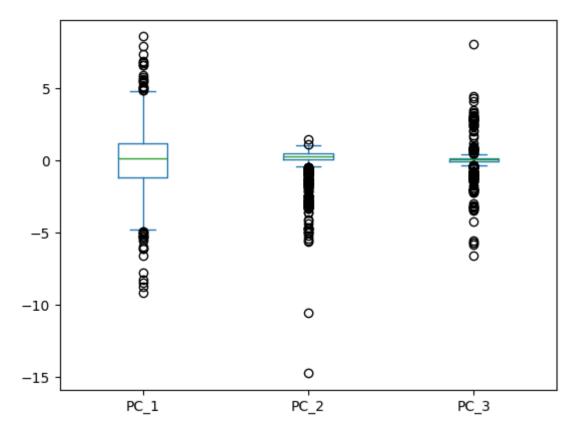
        2
        6.869235
        -0.475166
        -0.403830

        3
        6.696222
        -0.467683
        -0.395929

        4
        6.561643
        -0.466118
        -0.383813
```

```
In [43]: df_pca.plot.box()
```

Out[43]: <Axes: >

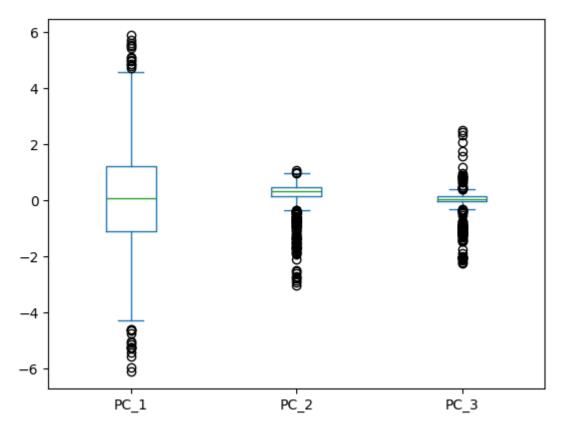


We'll remove the outliers again

```
In [44]: z_scores = np.abs(zscore(df_pca))
    df_pca = df_pca[(z_scores < 3).all(axis=1)]

In [45]: df_pca.plot.box()

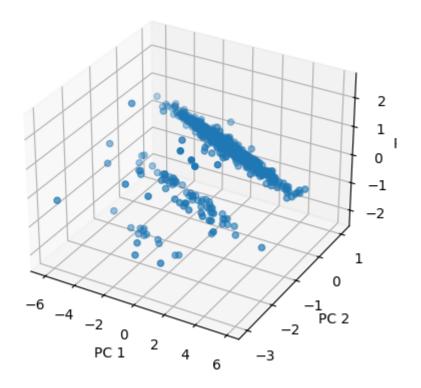
Out[45]: <Axes: >
```



```
In [46]: fig = plt.figure()
    ax = fig.add_subplot(projection='3d')
    ax.scatter(df_pca['PC_1'], df_pca['PC_2'], df_pca['PC_3'])

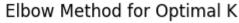
ax.set_xlabel('PC 1')
    ax.set_ylabel('PC 2')
    ax.set_zlabel('PC 3')
```

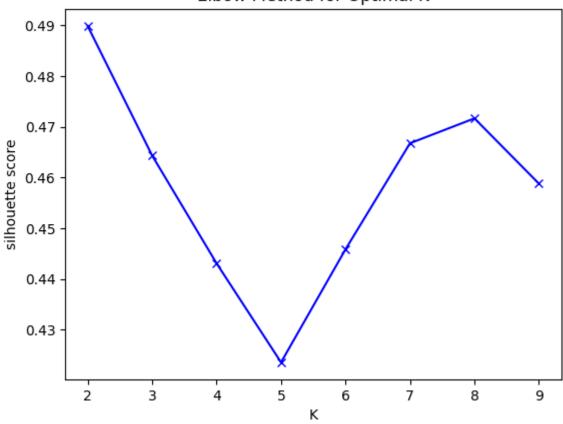
Out[46]: Text(0.5, 0, 'PC 3')



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 [47]: # Calculating optimal number of clusters in a K-means algorithm using sill
         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='euc
             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 = 0.4643237006986533
        Number of clusters = 4
        Silhouette score = 0.4430582641319094
        Number of clusters = 5
        Silhouette score = 0.4235502939312917
        Number of clusters = 6
        Silhouette score = 0.44583337191385314
        Number of clusters = 7
        Silhouette score = 0.46673994176770084
        Number of clusters = 8
        Silhouette score = 0.4716433426294572
        Number of clusters = 9
        Silhouette score = 0.45877396158210904
In [48]: 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 [49]: kmeans = KMeans(init='k-means++', n_clusters=2, n_init=10)
    prediction = kmeans.fit_predict(df_pca)

In [50]: prediction

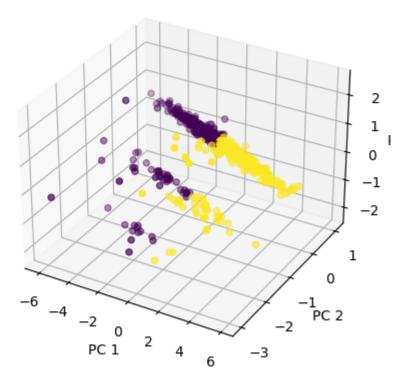
Out[50]: array([1, 1, 1, ..., 1, 1], shape=(1042,), dtype=int32)

In [51]: 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')

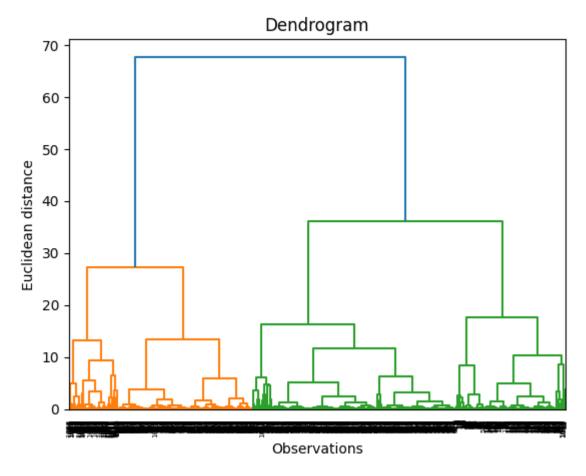
Out[51]: Text(0.5, 0, 'PC 3')
```

K-Means



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

```
In [52]: # 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()
```

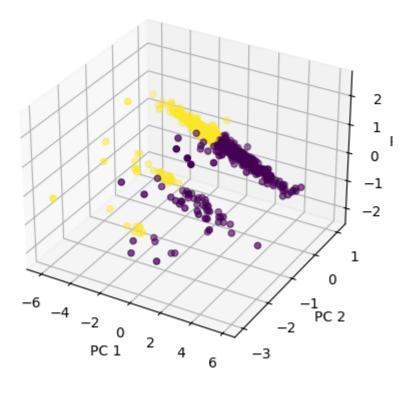


```
In [53]: model = AgglomerativeClustering(2, linkage = 'ward')
    aggmodel_pred = model.fit_predict(df_pca)

In [54]: 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_prediction='3d')
    ax.set_xlabel('PC 1')
    ax.set_ylabel('PC 2')
    ax.set_zlabel('PC 3')
```

Out[54]: Text(0.5, 0, 'PC 3')

Agglomerative Clustering



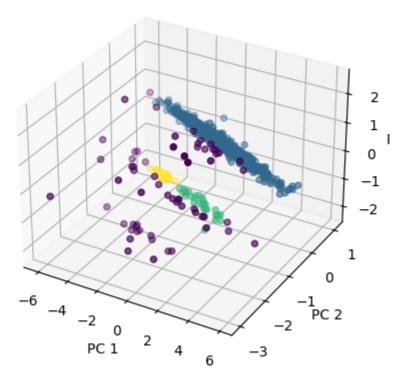
Well that doesn't seem to agree either. Lets try running a DBSCAN

```
In [57]: #DBSCAN for automatically determining amount of clusters
# Tried to play a little around with eps here
# for finding the optimal separation
dbscan = DBSCAN(eps=0.7, min_samples=10)
dbscan_pred = dbscan.fit_predict(df_pca)
dbscan_pred

Out[57]: array([ 0,  0,  0, ..., -1, -1, -1], shape=(1042,))

In [56]: 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[56]: Text(0.5, 0, 'PC 3')
```

DBSCAN



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.

In summary, what we can tell about the dataset is the following:

- The Main quality measures in the coffee seems to be the flavor parameters
- It takes a large amount of defects and quakers to actually worsen the overall quality
- Arabica beans tend to be sweeter than Robusta beans
- There is a very slight indication that higher quality coffee tends to come fom Africa