```
In [59]: %time
    import pandas as pd
    import numpy as np
    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 $\mu s,$ sys: 0 ns, total: 2 μs Wall time: 4.05 μs

In [60]: 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 Arabio	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	30.8			
	16	Arabica	Ethiopia	Ethiopian Yirgacheffe	Natural / Dry	8.17	8.17	8.00			
	17	Arabica	United States	Other	Washed / Wet	8.00	8.25	30.8			
	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]:	df.	columns									
Out[61]:	<pre>Index(['Species', 'Country.of.Origin', 'Variety', 'Processing.Method', 'Aroma',</pre>										
	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]: df.info()

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1103 entries, 0 to 1102
Data columns (total 21 columns):
                           Non-Null Count Dtype
     Column
 0
     Species
                           1103 non-null
                                           object
 1
    Country.of.Origin
                           1103 non-null
                                           object
    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
                                           float64
    Acidity
                           1103 non-null
 8
    Body
                           1103 non-null
                                           float64
                                           float64
 9
     Balance
                           1103 non-null
 10 Uniformity
                           1103 non-null
                                           float64
 11 Clean.Cup
                           1103 non-null
                                           float64
                                           float64
 12
    Sweetness
                           1103 non-null
    Cupper.Points
                           1103 non-null
                                           float64
 14
                           1103 non-null
                                           float64
    Total.Cup.Points
 15
                           1103 non-null
                                           float64
    Moisture
 16
    Category.One.Defects 1103 non-null
                                           int64
 17
    Quakers
                           1103 non-null
                                           float64
 18
    Color
                           1103 non-null
                                           object
```

dtypes: float64(14), int64(2), object(5)
memory usage: 181.1+ KB

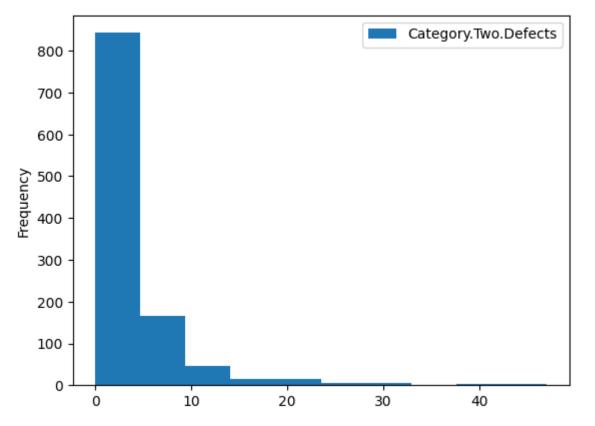
20 altitude_mean_meters 1103 non-null

memory usage: 181.1+ KB

19 Category.Two.Defects

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

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

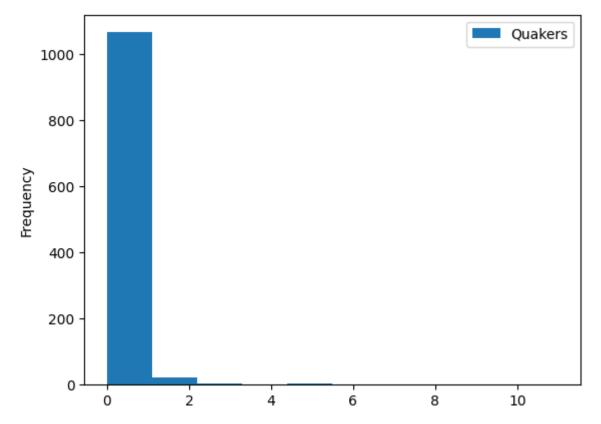


1103 non-null

int64 float64

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

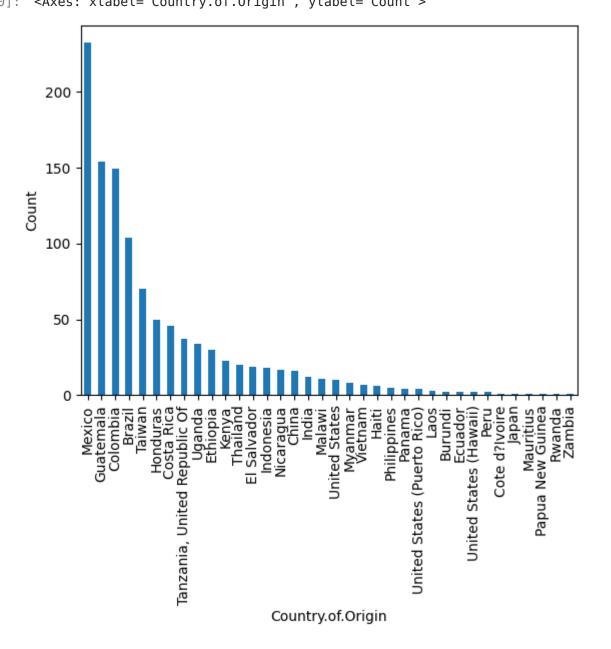
```
In [69]: # lets see which countries can boast the highest cup grades
df.groupby('Country.of.Origin')['Total.Cup.Points'].mean().reset_index().
```

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. 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 [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. About 1/4 of the coffee in the dataset is from Mexico!

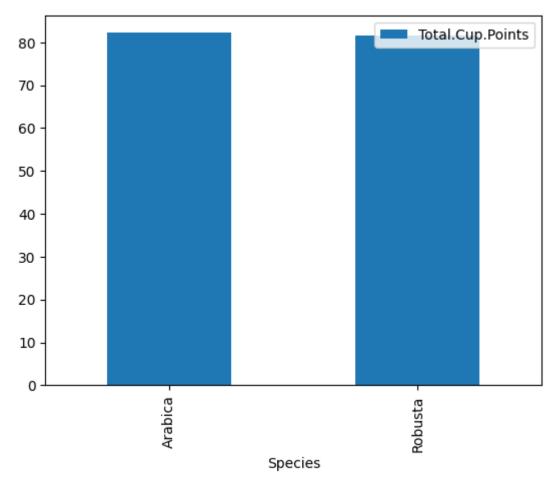
```
In [71]: df.groupby('Country.of.Origin')['Total.Cup.Points'].median().reset_index(
```

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 about the same

```
In [72]: df.groupby('Species')['Total.Cup.Points'].mean().reset_index().sort_value
Out[72]: <Axes: xlabel='Species'>
```

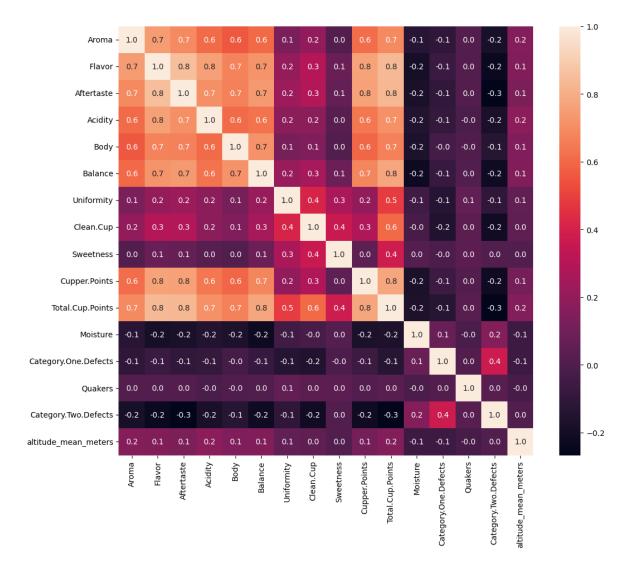


Surprinsingly, The Robusta species does not seem to have a much lower average score than Arabica, which we thought were far superior in taste

```
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	0.72214		
	Aftertaste	0.688130	0.849983	1.000000	0.705410	0.666111	0.73743		
	Acidity	0.606707	0.757027	0.705410	1.000000	0.604118	0.62478		
	Body	0.558217	0.668397	0.666111	0.604118	1.000000	0.71504		
	Balance	0.602133	0.722149	0.737439	0.624788	0.715045	1.00000		
	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	0.08359		
	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	-0.07942		
	Quakers	0.007763	0.009010	0.007843	-0.017353	-0.002792	0.00100		
	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
                                 float64
         Aroma
                                 float64
         Flavor
         Aftertaste
                                 float64
         Acidity
                                 float64
                                 float64
         Body
         Balance
                                 float64
         Uniformity
                                 float64
                                 float64
         Clean.Cup
         Sweetness
                                 float64
         Cupper.Points
                                 float64
         Total.Cup.Points
                                 float64
                                 float64
         Moisture
         Category.One.Defects
                                   int64
                                 float64
         Quakers
         Color
                                 object
         Category.Two.Defects
                                  int64
         altitude mean meters
                                 float64
         dtype: object
```

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

```
In [76]: 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

 $11 {
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```
In [77]: enc df.to csv("../data cleaned/encoded df.csv", index=False)
In [78]: # lets see how much variance it give us
           df.describe()
Out[78]:
                                        Flavor
                                                   Aftertaste
                                                                     Acidity
                                                                                                 Balanc
                         Aroma
                                                                                     Body
                  1103.000000 1103.000000 1103.000000 1103.000000 1103.000000 1103.000000
                       7.578368
                                      7.527824
                                                                   7.535739
                                                                                 7.513654
            mean
                                                    7.401496
                                                                                                7.51266
                       0.309181
                                      0.331268
                                                    0.340065
                                                                   0.313192
                                                                                 0.289467
                                                                                                0.35402
              std
                      5.080000
                                     6.170000
                                                    6.170000
                                                                  5.250000
                                                                                 5.170000
                                                                                               5.250000
             min
            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
                       8.750000
                                     8.830000
                                                    8.670000
                                                                  8.750000
                                                                                 8.580000
                                                                                                8.750000
             max
In [79]:
           enc_corr_mat = enc_df.corr()
           plt.figure(figsize=(12, 10))
           sns.heatmap(enc_corr_mat, annot = True, fmt = ".1f")
Out[79]: <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
                         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
                         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
                 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 0.0 -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 0.0 0.1 0.2 -0.1 -0.1 -0.0 0.0 0.0 1.0
                               Variety
                            Country.of.Origin
                                   Processing.Method
                                                            Clean.Cup
                                                                Sweetness
                                                                   Cupper.Points
                                                                      Total.Cup.Points
                                                                         Moisture
                                                                            Category.One.Defects
                                                                                      Category. Two. Defects
                                                                                Quakers
                                                                                         altitude_mean_meters
```

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

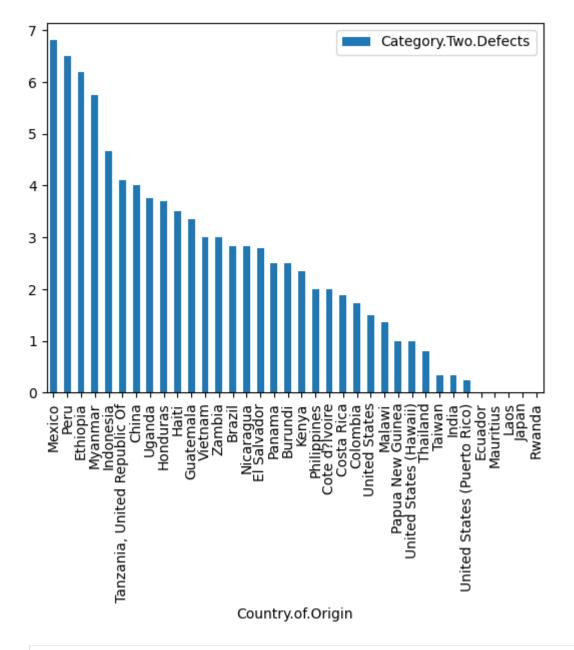
So this is where the Arabica beans stand out!

Arabica

```
In [81]: df.groupby('Country.of.Origin')['Category.Two.Defects'].mean().reset_inde
Out[81]: <Axes: xlabel='Country.of.Origin'>
```

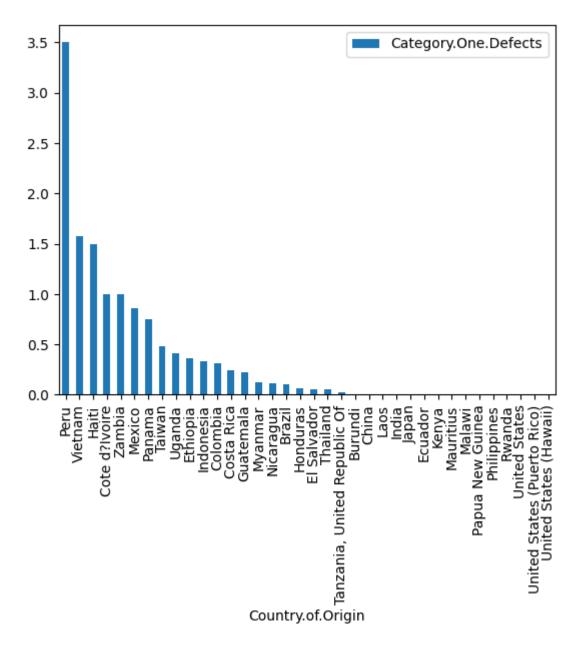
Species

Robusta



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 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 [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)
```

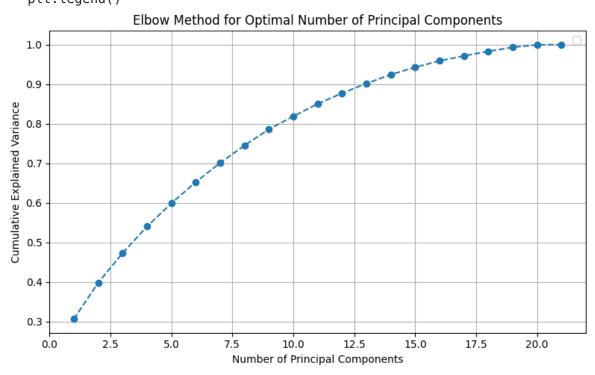
Out[85]:	: Species		Country.of.Origin	Variety	Processing.Method	Aroma	Flavor
	962	-0.152286	-0.441966	-0.958392	0.526081	-0.253585	-1.594069
	307	-0.152286	-1.070443	-0.620082	0.526081	-0.253585	0.157575
	849	-0.152286	0.710241	0.282078	-1.445381	-1.321406	-0.325637
	1002	-0.152286	0.605495	1.635319	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()



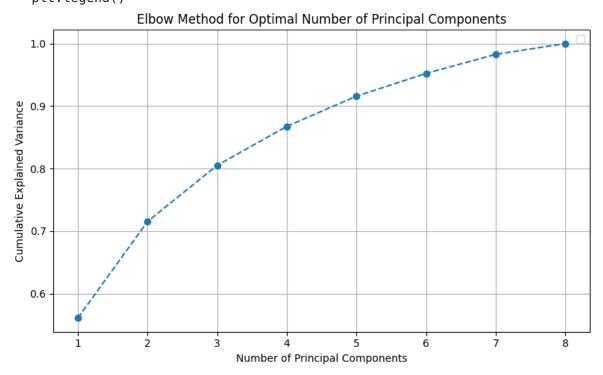
Not as much as we hoped for. For 3 principal components, we get just above 50% explained variance, which is not a lot. Lets try and extract high correlating features and do

 $16 {
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the PCA again

```
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
```

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m 31}$

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	0.04
	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[92]:
        PC_1
        PC_2

        0
        8.565309
        -0.713374

        1
        7.920370
        -0.663066

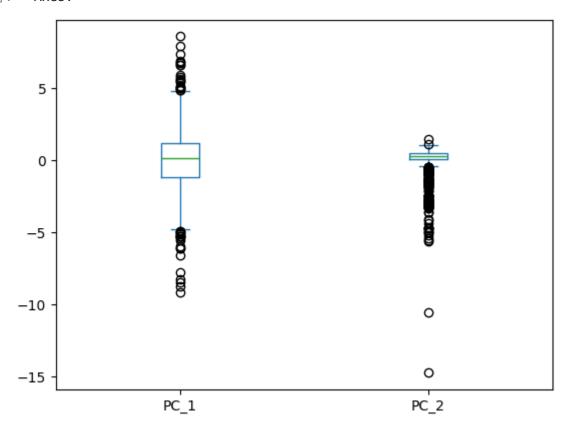
        2
        6.869235
        -0.475166

        3
        6.696222
        -0.467683

        4
        6.561643
        -0.466118
```

```
In [93]: df_pca.plot.box()
```

Out[93]: <Axes: >

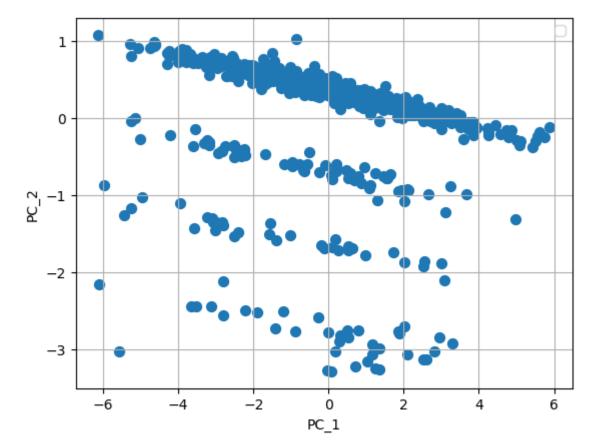


We have also introduced some serious outliers. Lets remove them

```
In [94]: z_scores = np.abs(zscore(df_pca))
df_pca = df_pca[(z_scores < 3).all(axis=1)]</pre>
```

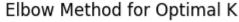
```
In [ ]: fig = plt.figure()
    plt.scatter(df_pca['PC_1'], df_pca['PC_2'], s=50)
    plt.xlabel('PC_1')
    plt.ylabel('PC_2')
    plt.grid(True)
    plt.legend()
    plt.show()
```

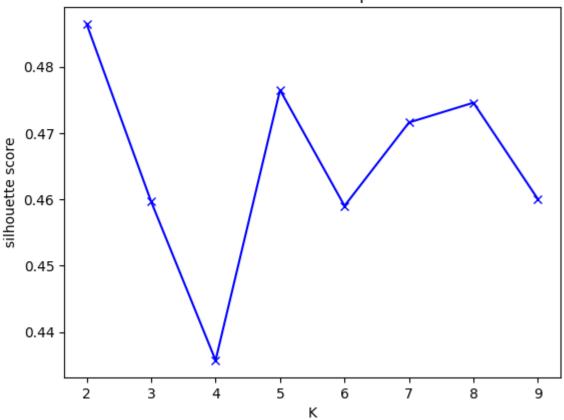
/tmp/ipykernel_12403/519479020.py:2: UserWarning: No data for colormapping
provided via 'c'. Parameters 'cmap' will be ignored
 plt.scatter(df_pca['PC_1'], df_pca['PC_2'], s=50, cmap='viridis')
/tmp/ipykernel_12403/519479020.py:6: UserWarning: No artists with labels f
ound to put in legend. Note that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



```
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()
```

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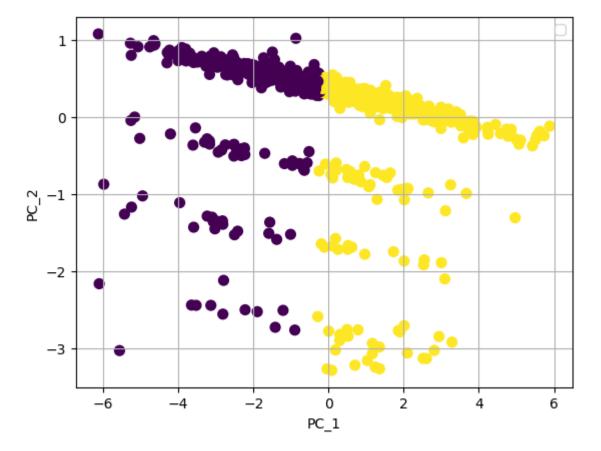


Using silhouette score for each amount of clusters, we se that we achieve a maximum score of 0,473 on 2 clusters. Let's try and visualize them

```
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()
```

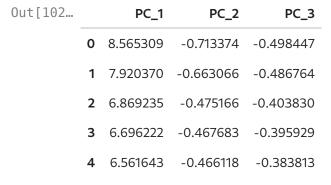
/tmp/ipykernel_12403/3703295130.py:6: UserWarning: No artists with labels
found to put in legend. Note that artists whose label start with an under
score are ignored when legend() is called with no argument.
 plt.legend()



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

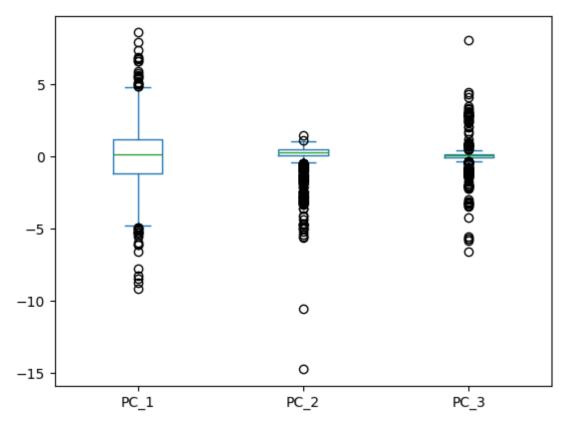
Out[101		Aroma	Flavor	Acidity	Body	Balance	Aftertaste	Uniformity	Swee
	PC_1	0.381225	0.436044	0.392771	0.381476	0.404040	0.428197	0.128396	0.0
	PC_2	0.103547	0.019839	0.057700	0.113975	0.009413	0.009358	0.659328	0.7
	PC_3	0.049970	0.040739	0.022757	0.067166	0.034935	0.002558	0.731547	0.6

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



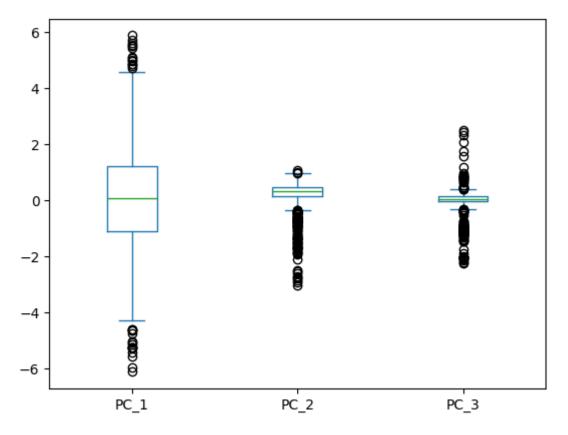
```
In [103... df_pca.plot.box()
```

Out[103... <Axes: >



We'll remove the outliers again

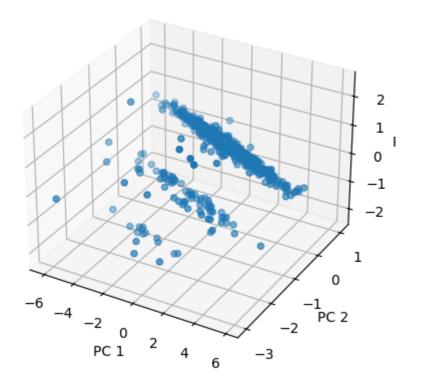
```
In [104... z_scores = np.abs(zscore(df_pca))
    df_pca = df_pca[(z_scores < 3).all(axis=1)]
In [105... df_pca.plot.box()</pre>
Out[105... <Axes: >
```



```
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')
```

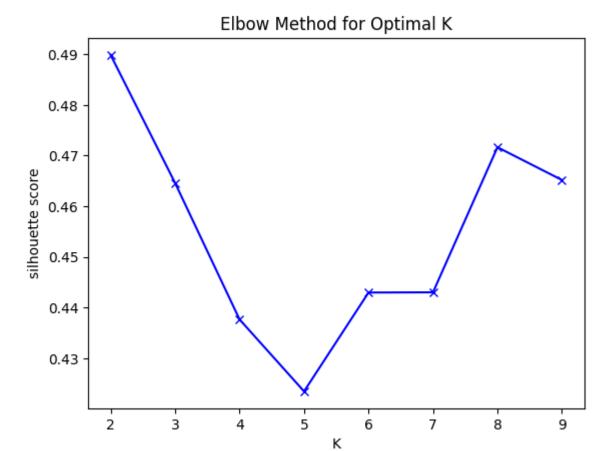
Out[106... Text(0.5, 0, 'PC 3')



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)

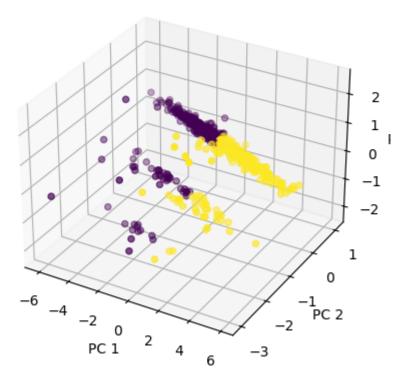
In [111... fig = plt.figure()
    fig.suptitle("K-Means")
    ax = fig.add_subplot(projection='3d')
    ax.scatter(df_pca['PC_1'], df_pca['PC_2'], df_pca['PC_3'], c=prediction)

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

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

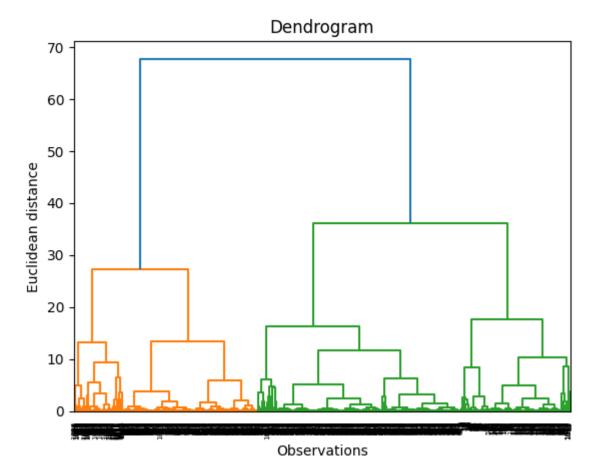
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K-Means



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

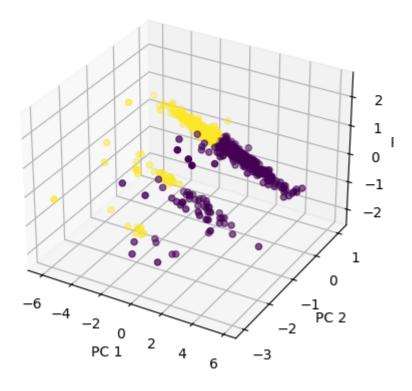
```
In [112... # Dendogram for agglomerative clustering
    plt.figure()
    dendogram = ch.dendrogram(ch.linkage(df_pca, method = 'ward'))
    plt.title('Dendrogram')
    plt.xlabel('Observations')
    plt.ylabel('Euclidean distance')
    plt.show()
```



```
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')
```

Agglomerative Clustering



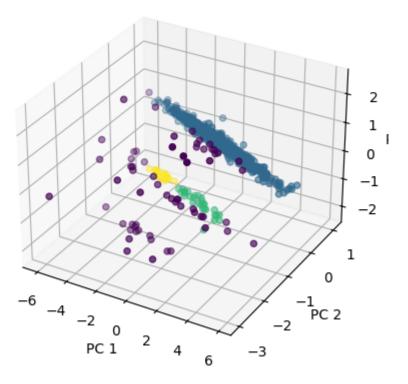
Well that doesn't seem to agree either. Lets try running a DBSCAN

```
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')
```

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

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