Introduction

Research around the human microbiome (the collection of bacteria and microbes that live in and on our bodies) has been growing as a science and field of interest more and more over the last decade (Ursell et al., 2012). Many people experience disruptions to their health that could be attributed to an imbalance of these little organisms that share life with each of us (Ursell et al., 2012). Gastrointestinal (Gl/gut) health is of particular interest, and investigations around how to improve this ecosystem within us are expanding. One approach to achieve this is Fecal Microbiota Transplant (FMT).

FMT is a method of transferring a healthy population (high species quantity and diversity) of microbes from one person to another in hopes of restoring the bacterial colonies in the recipient and thus contributing to greater overall health (Orr, et al. 2018). FMT has been used as a therapy for a limited selection of illnesses (and is not approved for many uses in the USA), but it is gaining relevance as a therapeutic application for a wide variety of infections, gastrointestinal issues, and auto-immune disorders (Gupta et al., 2016). FMT could be an effective intervention for a variety of health issues caused by diet, environment, overuse of antibiotics, and other factors.

In order to successfully implement an intervention such as this, we need to understand the structure of human microbiota. Using data sourced from NIH Human Microbiome Project, I will run an EDA to explore the species types and prevalence. For the EDA portion, I will be roughly following this Kaggle notebook. The dataset utilized for that project is older (as the project is in constant motion), so although it is a great framework, my approach will have to be adjusted. Moving beyond this step, I would like to build models to predict the presence of these microbes to potentially I will likely reference this or this dataset.

According to AWS: "The NIH-funded Human Microbiome Project (HMP) is a collaborative effort of over 300 scientists from more than 80 organizations to comprehensively characterize the microbial communities inhabiting the human body and elucidate their role in human health and disease. To accomplish this task, microbial community samples were isolated from a cohort of 300 healthy adult human subjects at 18 specific sites within five regions of the body (oral cavity, airways, urogenital track, skin, and gut). Targeted sequencing of the 16S bacterial marker gene and/or whole metagenome shotgun sequencing was performed for thousands of these samples. In addition, whole genome sequences were generated for isolate strains collected from human body sites to act as reference organisms for analysis. Finally, 16S marker and whole metagenome sequencing was also done on additional samples from people suffering from several disease conditions."

 Gupta, S., Allen-Vercoe, E., & Petrof, E. O. (2016). Fecal microbiota transplantation: in perspective. Therapeutic Advances in Gastroenterology, 9(2), 229-239. https://doi.org/10.1177/1756283X15607414

- Orr, M. R., Kocurek, K. M., & Young, D. L. (that's me!) (2018). Gut Microbiota and Human Health: Insights From Ecological Restoration. The Quarterly Review of Biology, 93(2), 73–90. https://doi.org/10.1086/698021
- Ursell, L. K., Metcalf, J. L., Parfrey, L. W., & Knight, R. (2012). Defining the Human Microbiome. Nutrition reviews, 70(Suppl 1), S38. https://doi.org/10.1111/j.1753-4887.2012.00493.

Import and Cleaning

```
In [1]: #import libraries and dataset
        import pandas as pd
        import matplotlib.pyplot as plt
        import numpy as np
        import seaborn as sns
        import warnings
        warnings.filterwarnings('ignore')
        #part 2
        from sklearn import metrics
        from sklearn.metrics import accuracy score
        from sklearn.model_selection import train_test_split, GridSearchCV
        from sklearn.preprocessing import StandardScaler, MinMaxScaler
        from sklearn.neighbors import KNeighborsClassifier
        from sklearn.linear_model import LogisticRegression
        from sklearn.pipeline import Pipeline, FeatureUnion
        from sklearn.preprocessing import OneHotEncoder, StandardScaler
        from sklearn.cluster import KMeans
        from sklearn.pipeline import make_pipeline
        from sklearn.compose import ColumnTransformer
        import matplotlib.pyplot as plt
        from sklearn.decomposition import PCA
        microbes=pd.read csv('/Users/debane/Documents/MS Data Science/550 Data Minir
        #####pd.set_option('display.max_rows', None, 'display.max_columns', None)
```

<u> </u>	HMP ID	GOLD ID	Organism Name	Domain	NCBI Superkingdom	HMP Isolation Body Site	Projec [®] Status
0	1	Gi03551	Abiotrophia defectiva ATCC 49176	BACTERIAL	Bacteria	oral	Complete
1	4	Gi03555	Achromobacter piechaudii ATCC 43553	BACTERIAL	Bacteria	airways	Complete
2	5	Gi03554	Achromobacter xylosoxidans C54	BACTERIAL	Bacteria	airways	Complete
3	10	Gi03422	Acinetobacter baumannii ATCC 19606	BACTERIAL	Bacteria	urogenital_tract	Complete
4	12	Gi03421	Acinetobacter calcoaceticus RUH2202	BACTERIAL	Bacteria	skin	Complete
		,					
(29	15,	19)					
			s in dataset				
l',	,	'HMP Isol 'NCBI Sub 'IMG/HMP	ation Body Simission Status	ite', 'Project Status', 'Current Finishing Leve us', 'NCBI Project ID', 'Genbank ID', 'Gene Cou D', 'Sequencing Center', 'Funding Source',			
	0 1 2 3 4 #See mic Ind l',	0 1 1 4 2 5 #Check smicrobes (2915, #See codmicrobes Index([l', nt',	1 4 Gi03555 1 4 Gi03555 2 5 Gi03554 3 10 Gi03422 4 12 Gi03421 #Check shape microbes.shape (2915, 19) #See column name microbes.columns Index(['HMP ID', 'HMP Isolut', 'NCBI Subnt', 'IMG/HMP 'Strain R	Abiotrophia Abiotrophia defectiva ATCC 49176 Achromobacter piechaudii ATCC 43553 Achromobacter piechaudii ATCC 43553 Achromobacter xylosoxidans C54 Acinetobacter baumannii ATCC 19606 Acinetobacter calcoaceticus RUH2202 #Check shape microbes.shape (2915, 19) #See column names in dataset microbes.columns Index(['HMP ID', 'GOLD ID', 'Gold in Body Side of the Body Side of	Abiotrophia defectiva ATCC 49176 Achromobacter piechaudii ATCC 43553 Achromobacter zylosoxidans BACTERIAL C54 Acinetobacter baumannii ATCC 19606 Acinetobacter calcoaceticus BACTERIAL RUH2202 #Check shape microbes.shape (2915, 19) #See column names in dataset microbes.columns Index(['HMP ID', 'GOLD ID', 'Organism Na' HMP Isolation Body Site', 'Projet', 'NCBI Submission Status', 'NCBI Pit', 'IMG/HMP ID', 'HOMD ID', 'Sequency 'Strain Repository ID', 'Unnamed:	Abiotrophia Abiotrophia defectiva ATCC 49176 Achromobacter piechaudii ATCC 43553 Achromobacter xylosoxidans C54 Acinetobacter baumannii ATCC 19606 Acinetobacter calcoaceticus RUH2202 Acinetobacter calcoaceticus BACTERIAL Bacteria RUH2202 Acinetobacter calcoaceticus RUH2202 Acinetobacter calcoaceticus BACTERIAL Bacteria RUH2202 Acinetobacter calcoaceticus RUH2202 Acinetobacter calcoaceticus Calcoaceticus RUH2202 Acinetobacter calcoaceticus BACTERIAL Bacteria RUH2202	Abiotrophia Abiotrophia Gefectiva ATCC 49176 Achromobacter piechaudii ATCC 43553 Achromobacter xylosoxidans C54 Achromobacter baumannii ATCC 19606 Acinetobacter baumannii ATCC 19606 Achromobacter xylosoxidans BACTERIAL Bacteria airways Achromobacter xylosoxidans BACTERIAL Bacteria airways Achromobacter xylosoxidans BACTERIAL Bacteria airways Achromobacter baumannii BACTERIAL Bacteria urogenital_tract Acinetobacter baumannii ATCC 19606 Acinetobacter calcoaceticus BACTERIAL Bacteria wrogenital_tract Acinetobacter calcoaceticus BACTERIAL Bacteria skin RUH2202 #Check shape microbes.shape (2915, 19) #See column names in dataset microbes.columns Index(['HMP ID', 'GOLD ID', 'Organism Name', 'Domain', 'NCBI Superk: 'HMP Isolation Body Site', 'Project Status', 'Current Finish: ', 'NCBI Submission Status', 'NCBI Project ID', 'Genbank ID', 'Gnt', 'IMG/HMP ID', 'HOMD ID', 'Sequencing Center', 'Funding Source 'Strain Repository ID', 'Unnamed: 17', 'Unnamed: 18'],

```
In [5]: #View descriptions of data
microbes.info()
```

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 2915 entries, 0 to 2914
Data columns (total 19 columns):

#	Column	Non-Null Count	Dtype
0	HMP ID	2915 non-null	 int64
1	GOLD ID	1783 non-null	object
2	Organism Name	2915 non-null	object
3	Domain	2712 non-null	object
4	NCBI Superkingdom	2751 non-null	object
5	HMP Isolation Body Site	2915 non-null	object
6	Project Status	2915 non-null	object
7	Current Finishing Level	1579 non-null	object
8	NCBI Submission Status		object
9	NCBI Project ID	2915 non-null	int64
10	Genbank ID	1579 non-null	object
11	Gene Count	2915 non-null	
12	IMG/HMP ID	2915 non-null	
13	HOMD ID	397 non-null	object
14	Sequencing Center	2911 non-null	object
15	Funding Source	2915 non-null	object
16	Strain Repository ID		object
17	Unnamed: 17	0 non-null	float64
18		0 non-null	float64
	es: float64(2), int64(4),	object(13)	
memo	ry usage: 432.8+ KB		

There is a broad range of information here, some of which may be beneficial to study regardless of project status, but for efficacy of this project, I'd like to check how many of the entires are complete.

```
In [6]: microbes['Project Status'].value_counts()
```

Out[6]: Project Status
Complete 1579
In Progress 1336
Name: count, dtype: int64

I'm going to remove any entries that are "in progress" from the main dataframe and place them in a new dataframe so I have it for running later if I want.

```
In [7]: # Split Dataframe using groupby() &
    # grouping by particular dataframe column
    grouped = microbes.groupby(['Project Status'])
    microbes_in_progress = grouped.get_group("In Progress")
    microbes_in_progress.shape
```

Out[7]: (1336, 19)

```
In [8]: # Split Dataframe using groupby() &
    # grouping by particular dataframe column
```

```
grouped = microbes.groupby(['Project Status'])
         microbes_complete = grouped.get_group("Complete")
         microbes complete.shape
Out[8]: (1579, 19)
In [9]: #rename group of "complete" for ease
         micro = microbes_complete
         micro.shape
Out[9]: (1579, 19)
In [10]: micro.info()
       <class 'pandas.core.frame.DataFrame'>
       Index: 1579 entries, 0 to 2914
       Data columns (total 19 columns):
        #
            Column
                                     Non-Null Count
                                                     Dtype
            _____
            HMP ID
                                     1579 non-null
        0
                                                     int64
            GOLD ID
                                     1493 non-null
        1
                                                     object
        2
            Organism Name
                                     1579 non-null
                                                     object
        3
            Domain
                                     1552 non-null
                                                     object
        4
            NCBI Superkingdom
                                     1462 non-null
                                                     object
            HMP Isolation Body Site 1579 non-null
        5
                                                     object
        6
            Project Status
                                     1579 non-null
                                                     object
        7
            Current Finishing Level 1579 non-null
                                                     object
        8
            NCBI Submission Status
                                     1579 non-null
                                                     object
        9
            NCBI Project ID
                                     1579 non-null
                                                     int64
        10 Genbank ID
                                     1579 non-null
                                                     object
        11 Gene Count
                                     1579 non-null
                                                     int64
        12 IMG/HMP ID
                                     1579 non-null
                                                     int64
        13 HOMD ID
                                     386 non-null
                                                     object
        14 Sequencing Center
                                     1579 non-null
                                                     object
        15 Funding Source
                                     1579 non-null
                                                     object
        16 Strain Repository ID
                                     1272 non-null
                                                     object
        17 Unnamed: 17
                                     0 non-null
                                                     float64
        18 Unnamed: 18
                                     0 non-null
                                                     float64
        dtypes: float64(2), int64(4), object(13)
       memory usage: 246.7+ KB
```

I'm curious about some of the columns that have null values. The ones that are important to organism analysis are "Domain", and "NCBI Superkingdom".

Out[12]:		HMP ID	GOLD ID	Organism Name	NCBI Superkingdom	HMP Isolation Body Site	Project Status	Current Finishing Level	Subi
	Domain								
	ARCHAEAL	2	2	2	2	2	2	2	
	BACTERIAL	1541	1487	1541	1440	1541	1541	1541	
	EUKARYAL	4	4	4	4	4	4	4	
	VIRUS	5	0	5	5	5	5	5	

In [13]: micro.groupby('NCBI Superkingdom').count()

Out[13]:		HMP ID	GOLD ID	Organism Name	Domain	HMP Isolation Body Site	Project Status	Current Finishing Level	N Submiss Sta
	NCBI Superkingdom								
	Archaea	2	2	2	2	2	2	2	
	Bacteria	1448	1384	1448	1437	1448	1448	1448	14
	Error!!!	3	3	3	3	3	3	3	
	Eukaryota	4	4	4	4	4	4	4	
	Viruses	5	0	5	5	5	5	5	

There is an "Error!!!" value for Superkingdom, so that's nice to be able to see exactly what I should replace. I'll start by checking those values specifically.

In [14]: micro[micro['NCBI Superkingdom']=='Error!!!']

Out[14]:		HMP ID	GOLD ID	Organism Name	Domain	NCBI Superkingdom	HMP Isolation Body Site	Project Status	ı
	2478	9176	Gi05045	Streptococcus downei F0415	BACTERIAL	Error!!!	oral	Complete	
	2481	9180	Gi05049	Streptococcus peroris ATCC 700780	BACTERIAL	Error!!!	oral	Complete	
	2487	9192	Gi05061	Streptococcus vestibularis F0396	BACTERIAL	Error!!!	oral	Complete	
				·		e their values with			
In [15]:			•	•		!', 'Bacteria'	•		
				pased on the Sup nissing, so I'll ch	•	and vice versa, bu	ut I can't us	se any	
In [16]:	len(m	icro.l	.oc[micro	['Domain'].is	null()& mic	ro['NCBI Supe	rkingdom'].isnull()]
Out[16]:	16								
	There	are 16	values tha	t have both miss	sing so I'm go	oing to drop thos	e.		
In [17]:		=micro .shape	•	cro[(micro['D	omain'].isn	ull()) & (mic	ro['NCBI	Superkingd	C
Out[17]:	(1563	3, 19)							
	In orde	er to re	place the o	other values, I'm	going to trar	nsform them to N	laN first.		
In [18]:	micro	['NCBI	Superki	ngdom'].fillna	a('NaN', in	place= True)			
In [19]:	(micr	o ['NCB	SI Superk	ingdom'] == ""	NaN").value	e_counts()			

```
Out[19]: NCBI Superkingdom
          False
                   1462
          True
                    101
         Name: count, dtype: int64
In [20]: micro['Domain'].fillna('NaN', inplace=True)
In [21]: #check value counts
         (micro['Domain'] == "NaN").value_counts()
Out[21]: Domain
          False
                   1552
          True
                     11
         Name: count, dtype: int64
         I'm going to replace all of the Domain values with their relative Superkingdom name
         where applicable using pandas transform function.
In [22]: #make dataframe containing only rows with NaN in Domain or Superkingdom
         micro_null = micro[(micro['Domain'] == "NaN") | (micro['NCBI Superkingdom']
In [23]: #See which rows have NaN to compare with their Superkingdom value
         micro_null.loc[micro_null['Domain'] == "NaN"]
```

Out[23]:

	HMP ID	GOLD ID	Organism Name	Domain	NCBI Superkingdom	HMP Isolation Body Site	Project Status
1314	1978	NaN	Actinomyces graevenitzii F0530	NaN	Bacteria	oral	Complete
1463	2128	NaN	Arthrobacter albus DNF00011	NaN	Bacteria	urogenital_tract	Complete
1464	2129	NaN	Corynebacterium tuscaniense DNF00037	NaN	Bacteria	urogenital_tract	Complete
1465	2130	NaN	Oligella urethralis DNF00040	NaN	Bacteria	urogenital_tract	Complete
1467	2132	NaN	Prevotella histicola JCM 15637 = DNF00424	NaN	Bacteria	urogenital_tract	Complete
1469	2134	NaN	Peptoniphilus lacrimalis DNF00528	NaN	Bacteria	urogenital_tract	Complete
1470	2135	NaN	Staphylococcus haemolyticus DNF00585	NaN	Bacteria	urogenital_tract	Complete
1471	2136	NaN	Prevotella bivia DNF00650	NaN	Bacteria	urogenital_tract	Complete

		HMP ID	GOLD ID	Organism Name	Domain	NCBI Superkingdom	HMP Isolation Body Site	Project Status
	1472	2137	NaN	Prevotella buccalis DNF00853	NaN	Bacteria	urogenital_tract	Complete
	1474	2139	NaN	Prevotella denticola DNF00960	NaN	Bacteria	urogenital_tract	Complete
	1475	2140	NaN	Prevotella buccalis DNF00985	NaN	Bacteria	urogenital_tract	Complete
In [24]:				ompare == "NaN").sum()				
Out[24]:	11							
In [25]:				es with "BACTER micro['Domain'		e(["NaN"], "B <i>A</i>	ACTERIAL")	

Out[25]:

:		HMP ID	GOLD ID	Organism Name	Domain	NCBI Superkingdom	HMP Isolation Body Si
	0	1	Gi03551	Abiotrophia defectiva ATCC 49176	BACTERIAL	Bacteria	Ol
	1	4	Gi03555	Achromobacter piechaudii ATCC 43553	BACTERIAL	Bacteria	airwa
	2	5	Gi03554	Achromobacter xylosoxidans C54	BACTERIAL	Bacteria	airwa
	3	10	Gi03422	Acinetobacter baumannii ATCC 19606	BACTERIAL	Bacteria	urogenital_tra
	4	12	Gi03421	Acinetobacter calcoaceticus RUH2202	BACTERIAL	Bacteria	sł
	•••						
	2910	9995	Gi08654	Staphylococcus epidermidis NIHLM095	BACTERIAL	Bacteria	unknov
	2911	9996	Gi09593	Aggregatibacter actinomycetemcomitans Y4	BACTERIAL	Bacteria	O
	2912	9997	Gi09594	Corynebacterium durum F0235	BACTERIAL	Bacteria	Ol

		HMP ID	GOLD ID	Organism Name	Domain	NCBI Superkingdom	HMP Isolation Body Si
	2913	9998	Gi09595	Peptostreptococcus anaerobius VPI 4330	BACTERIAL	Bacteria	Ol
	2914	9999	Gi09596	Prevotella sp. oral taxon 473 str. F0040	BACTERIAL	Bacteria	Ol
	1563 rd	ows × 1	9 columns				
In [26]:			values r ain'] ==	replaced "NaN").sum()			
Out[26]:	0						
				e Superkingdom values v stransform function.	with their Dor	main name where	
In [27]:	kingd	om = m	icro_null	omain in regard to Su loc[micro_null['NCB alue_counts()			1
Out[27]:	BACTE	RIAL	101 , dtype:	int64			
				kingdom values are in the alue of "Bacteria".	e Bacterial do	omain, so we can r	replace
In [28]:			s to comp ['NCBI Su	pare uperkingdom'] == "NaN	").sum()		
Out[28]:	101						
In [29]:		["NCBI		<pre>with "BACTERIAL" ngdom"] = micro['NCBI</pre>	Superkingo	dom'].replace(['NaN'], 'Ba

Out[29]:

:		HMP ID	GOLD ID	Organism Name	Domain	NCBI Superkingdom	HMP Isolation Body Si
	0	1	Gi03551	Abiotrophia defectiva ATCC 49176	BACTERIAL	Bacteria	Ol
	1	4	Gi03555	Achromobacter piechaudii ATCC 43553	BACTERIAL	Bacteria	airwa
	2	5	Gi03554	Achromobacter xylosoxidans C54	BACTERIAL	Bacteria	airwa
	3	10	Gi03422	Acinetobacter baumannii ATCC 19606	BACTERIAL	Bacteria	urogenital_tra
	4	12	Gi03421	Acinetobacter calcoaceticus RUH2202	BACTERIAL	Bacteria	sł
	•••						
	2910	9995	Gi08654	Staphylococcus epidermidis NIHLM095	BACTERIAL	Bacteria	unknov
	2911	9996	Gi09593	Aggregatibacter actinomycetemcomitans Y4	BACTERIAL	Bacteria	Ol
	2912	9997	Gi09594	Corynebacterium durum F0235	BACTERIAL	Bacteria	O

LMD

COLD

Body Si	Superkingdom	Domain	Organism Name	ID	ID	
O	Bacteria	BACTERIAL	Peptostreptococcus anaerobius VPI 4330	Gi09595	9998	2913
O	Bacteria	BACTERIAL	Prevotella sp. oral taxon 473 str. F0040	Gi09596	9999	2914

NODI

HMD Isolation

1563 rows × 19 columns

```
In [30]: #Check that values replaced
  (micro['NCBI Superkingdom'] == "NaN").sum()
```

Out[30]: 0

Exploration

Now that those are cleaned up, I'm going to review the full dataset based on Gene Count to start.

```
In [31]: micro['Gene Count'].describe()
Out[31]: count
                   1563.000000
                   2729.550864
          mean
          std
                   1288.903478
          min
                      0.000000
          25%
                   1956,000000
          50%
                   2411.000000
          75%
                   3176.000000
                   8490.000000
          max
          Name: Gene Count, dtype: float64
         There are no null values for "Gene Count", but some are counted as 0.
In [32]: micro_gene_count=micro[micro['Gene Count']==0]
         micro_gene_count['NCBI Superkingdom'].value_counts()
```

Out[32]: NCBI Superkingdom

Bacteria 47 Viruses 5 Eukaryota 4

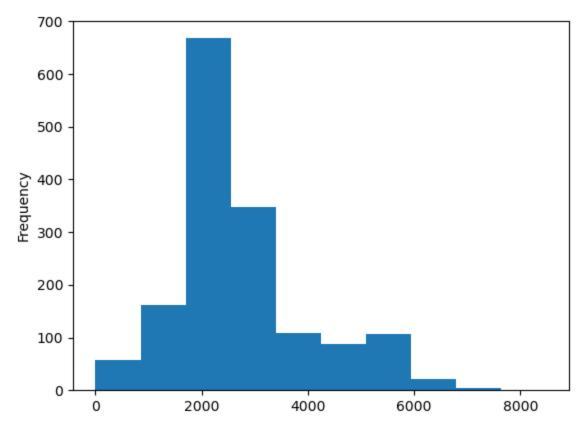
Name: count, dtype: int64

There are 47 bacteria, 5 viruses, and 4 eukaryota absent from the count. Because these may be based on a reporting error, I may want to drop these later to improve the model, but I'll keep them for now.

There are many species listed in this project, so I want to look at their distribution of gene count frequency.

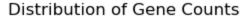
```
In [33]: micro["Gene Count"].plot(kind='hist')
```

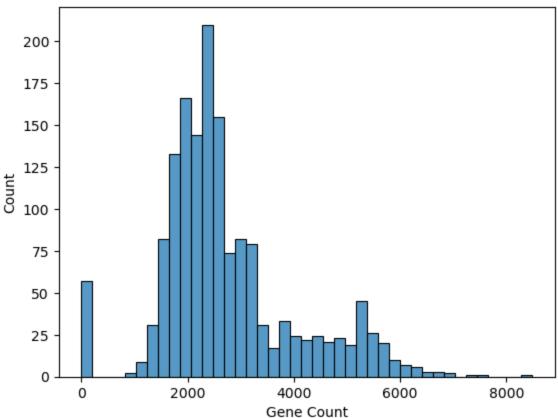
Out[33]: <Axes: ylabel='Frequency'>



```
In [152... sns.histplot(data=micro, x="Gene Count")
   plt.title('Distribution of Gene Counts')
```

Out[152... Text(0.5, 1.0, 'Distribution of Gene Counts')





Interestingly, there is an almost normal distribution, skewed right, but we can see that the species with gene counts in the middle range have the highest frequency.

I'm curious about the microbe with the highest gene count (max value from the descriptive statistics), with a value of 8490.

In [35]:	micro	[micr	o['Gene	Count']==849	0]			
Out[35]:		HMP ID	GOLD ID	Organism Name	Domain	NCBI Superkingdom	HMP Isolation Body Site	P
	679	1211	Gi10716	Streptomyces sp. HGB0020	BACTERIAL	Bacteria	gastrointestinal_tract	Соі

I want to check to see if there is another Streptomyces species with high prevalence.

```
In [36]: micro[micro['Organism Name'].str.contains("Streptomyces")]
```

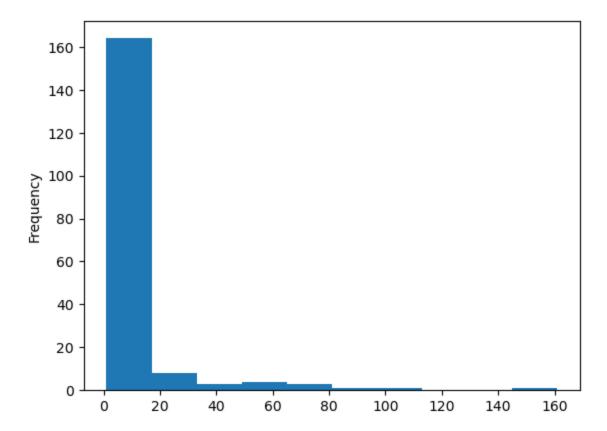
Out[36]:		HMP ID	GOLD ID	Organism Name	Domain	NCBI Superkingdom	HMP Isolation Body Site	F
	679	1211	Gi10716	Streptomyces sp. HGB0020	BACTERIAL	Bacteria	gastrointestinal_tract	Со
	934	1486	Gi16997	Streptomyces sp. HPH0547	BACTERIAL	Bacteria	gastrointestinal_tract	Со

The presences of another Streoptomyces with a high gene count makes me think that it may be beneficial to sort organisms on their genus. I'm going make a new dataframe and attempt to add a column for genus by extracting the first word of the Organism Name.

```
In [37]: df = micro
    df['Genus'] = df['Organism Name'].str.split(' ').str[0]
    df['Genus'].nunique()

Out[37]: 185
In [38]: df["Genus"].value_counts().plot(kind='hist')

Out[38]: <Axes: ylabel='Frequency'>
```



Since there are so many distributed around 0-15, I'm going to exclude those and print the value counts of the higher ones.

Out[40]:		161
	Streptococcus Enterococcus	110
	Propionibacterium	92
	Lactobacillus	73
	Helicobacter	70
	Prevotella	65
	Staphylococcus	64
	Bacteroides	63
	Escherichia	61
	Clostridium	58
	Corynebacterium	38
	Fusobacterium	36
	Actinomyces	34
	Bifidobacterium	31
	Treponema	25
	Gardnerella	22
	Klebsiella	21
	Eubacterium	21

Neisseria

Porphyromonas

Veillonella

Out[41]: Genus

Capnocytophaga

Name: count, dtype: int64

Since the list is limited, I probably could have just guessed the index number until I got to the value I wanted.

In [41]: df['Genus'].value_counts(ascending=False)[:22]

19

17

17

16

21

21

19

17

17

16

```
Streptococcus
                     161
Enterococcus
                     110
Propionibacterium
                      92
Lactobacillus
                      73
Helicobacter
                      70
Prevotella
                      65
Staphylococcus
                      64
Bacteroides
                      63
Escherichia
                      61
                      58
Clostridium
Corynebacterium
                      38
Fusobacterium
                      36
Actinomyces
                      34
Bifidobacterium
                      31
                      25
Treponema
                      22
Gardnerella
```

Klebsiella

Neisseria

Eubacterium

Capnocytophaga

Name: count, dtype: int64

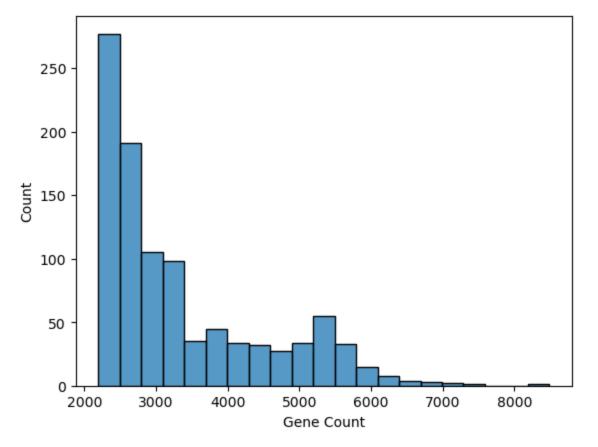
Porphyromonas

Veillonella

Let's see if this changes based on a subset of the most prevalent organisms.

```
In [42]: top_organisms=micro.sort_values(by='Gene Count', ascending = False)[:1000]
In [43]: sns.histplot(data=top_organisms, x="Gene Count")
```

Out[43]: <Axes: xlabel='Gene Count', ylabel='Count'>



```
In [44]: # add genus column to the top_organisms
top = top_organisms
top['Genus'] = top['Organism Name'].str.split(' ').str[0]
```

In [45]: top['Genus'].value_counts()[:22]

Out[45]:	Genus	
	Enterococcus	109
	Propionibacterium	91
	Staphylococcus	62
	Bacteroides	62
	Escherichia	60
	Clostridium	57
	Streptococcus	53
	Prevotella	51
	Corynebacterium	32
	Treponema	24
	Lactobacillus	22
	Klebsiella	21
	Fusobacterium	20
	Actinomyces	17
	Neisseria	17
	Capnocytophaga	16
	Parabacteroides	15
	Acinetobacter	14
	Bifidobacterium	12
	Providencia	11
	Eubacterium	9
	Selenomonas	8
	Name: count, dtype:	int64

In the original histogram, we saw that the highest frequency of species was between 1800-2400 gene count, so I am going to make a dataframe around that.

```
In [46]: mid_microbe = micro[(micro['Gene Count'].values >= 1800) & (micro['Gene Cour
In [47]: mid_microbe['Genus'] = mid_microbe['Organism Name'].str.split(' ').str[0]
In [48]: mid_microbe["Genus"].value_counts().sort_values(ascending=False)[:22]
```

Out[48]:	Genus					
	Streptococcus	142				
	Lactobacillus	30				
	Staphylococcus	27				
	Prevotella	25				
	Corynebacterium	23				
	Bifidobacterium	21				
	Propionibacterium	20				
	Fusobacterium					
	Actinomyces					
	Veillonella					
	Porphyromonas					
	Selenomonas					
	Haemophilus					
	Mobiluncus	8				
	Capnocytophaga					
	Anaerococcus	5				
	Neisseria	4				
	Peptostreptococcaceae					
	Helicobacter	4				
	Oribacterium	4				
	Leptotrichia	4				
	Peptoniphilus	4				
	Name: count, dtype: int64					

Now that I'm comfortable with having added "Genus" to my dataframes, I'm going to replace the main dataframe with the amended one.

```
In [49]: df = micro
```

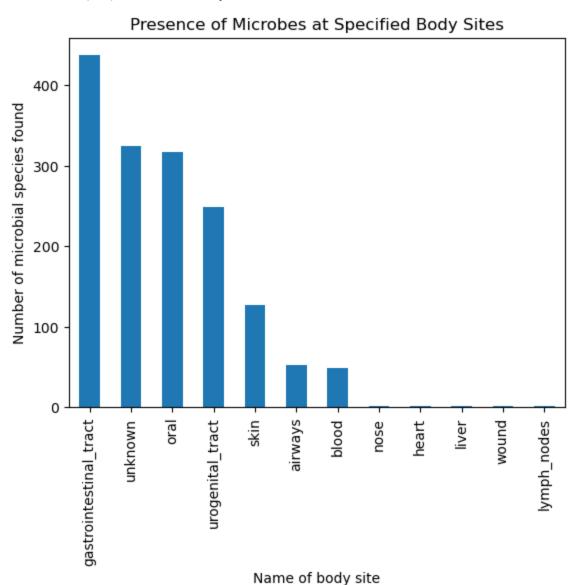
I want to know how many unique sites on the human body were researched.

```
In [50]: micro['HMP Isolation Body Site'].nunique()
Out[50]: 12
In [51]: micro['HMP Isolation Body Site'].value_counts()
Out[51]: HMP Isolation Body Site
          gastrointestinal_tract
                                     437
                                     324
          unknown
          oral
                                     317
          urogenital_tract
                                     249
          skin
                                     127
          airways
                                     53
                                      49
          blood
                                      2
          nose
                                      2
          heart
          liver
                                      1
          wound
                                      1
          lymph_nodes
                                       1
         Name: count, dtype: int64
```

Here is a chart of the species diversity at the different sites.

```
In [52]: micro['HMP Isolation Body Site'].value_counts().plot(kind='bar')
   plt.title('Presence of Microbes at Specified Body Sites')
   plt.ylabel('Number of microbial species found')
   plt.xlabel('Name of body site')
```

Out[52]: Text(0.5, 0, 'Name of body site')

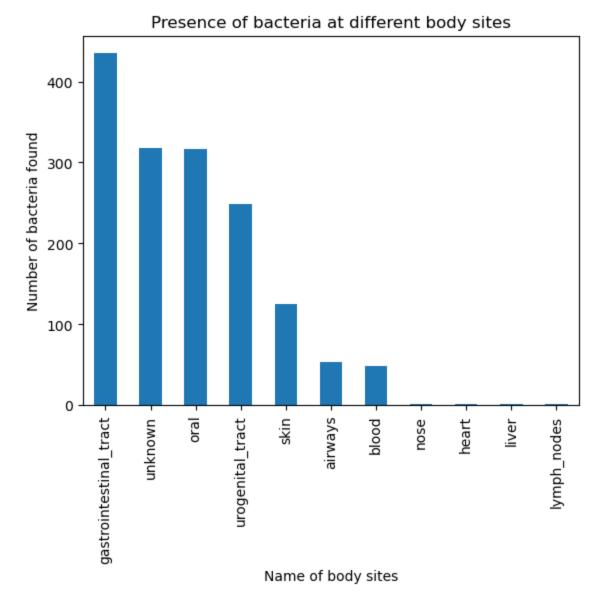


To find out more about the kingdom variance throughout the body, I'll look into those values.

```
In [53]: micro.groupby('NCBI Superkingdom')['HMP Isolation Body Site'].nunique().sort
Out[53]: NCBI Superkingdom
Bacteria 11
Eukaryota 3
Archaea 1
Viruses 1
Name: HMP Isolation Body Site, dtype: int64
```

The Bacteria Kingdom is most prevelent throughout the body, so I'm going to look more closely that their locations by making a dataframe with the values from the "bacterial" domain.

Out[55]: Text(0.5, 1.0, 'Presence of bacteria at different body sites')



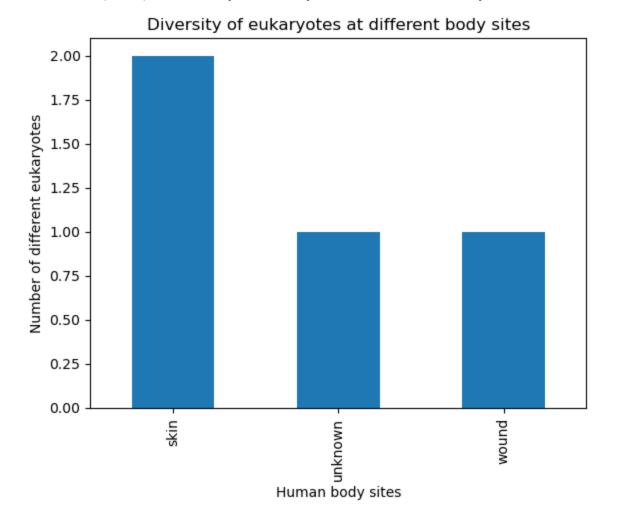
The greatest amount of bacteria are found in the gastrointestinal tract. Let's look at the other kingdoms.

```
In [56]: #Select Eukaryal domain and check body sites
    euk=micro.loc[micro['Domain']=='EUKARYAL']
    euk['HMP Isolation Body Site'].unique()

Out[56]: array(['unknown', 'skin', 'wound'], dtype=object)

In [57]: #plot
    euk['HMP Isolation Body Site'].value_counts(ascending=False).plot(kind='bar')
    plt.ylabel('Number of different eukaryotes')
    plt.xlabel('Human body sites')
    plt.title('Diversity of eukaryotes at different body sites')
```

Out[57]: Text(0.5, 1.0, 'Diversity of eukaryotes at different body sites')



The greatest amount of eukaryotes are found on the skin.

```
In [58]: vir=micro.loc[micro['Domain']=='VIRUS']
vir['HMP Isolation Body Site'].unique()
```

Out[58]: array(['unknown'], dtype=object)

From the data that we have, we are unable to determine where the greatest number of viruses are located. I'm guessing this is because viruses infect and replicate in cells, sometimes mainly infecting neighboring cells, but often spreading throughout the body.

```
In [59]: arc=micro.loc[micro['Domain']=='ARCHAEAL']
arc['HMP Isolation Body Site'].unique()
```

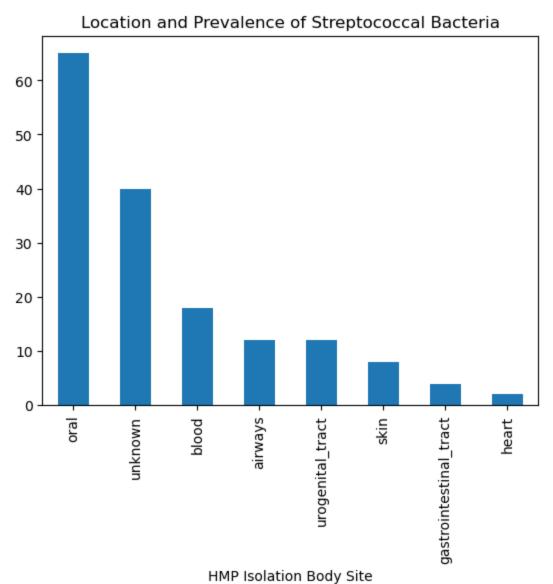
Out[59]: array(['gastrointestinal_tract'], dtype=object)

Based on this project, archaea are found solely in the Gastrointestinal Tract.

Streptococcus are the most prevalent throughout the body. Let's look further into this.

```
In [60]: strep=micro.loc[micro['Genus']=='Streptococcus']
    strep['HMP Isolation Body Site'].value_counts().plot(kind='bar')
    plt.title("Location and Prevalence of Streptococcal Bacteria")
```

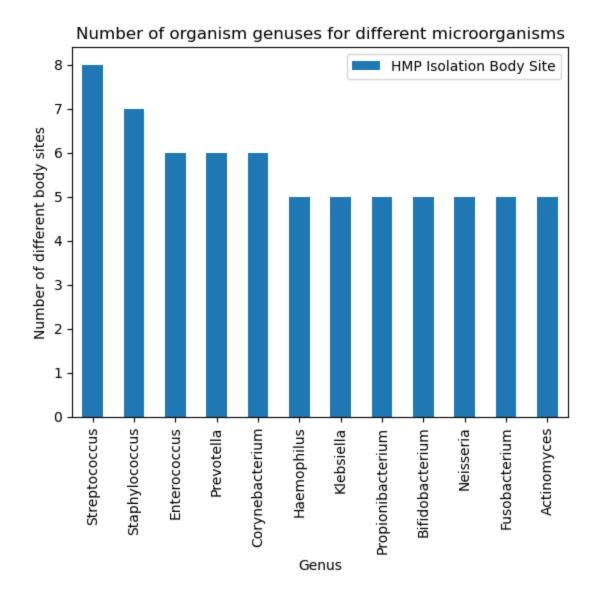
Out[60]: Text(0.5, 1.0, 'Location and Prevalence of Streptococcal Bacteria')



Let's see how other top genuses compare.

HMP Isolation Body Site Genus Streptococcus 8 7 Staphylococcus Enterococcus 6 Prevotella 6 Corynebacterium 6 5 Haemophilus 5 Klebsiella 5 Propionibacterium Bifidobacterium 5 5 Neisseria 5 Fusobacterium 5 Actinomyces

Out[61]: Text(0.5, 1.0, 'Number of organism genuses for different microorganisms')



Because viruses are limited, we can print all of their names.

```
In [62]: viruses= micro[micro['NCBI Superkingdom'] == 'Viruses']
          viruses['Organism Name']
Out[62]:
          2852
                  Pseudomonas phage F_HA0480sp/Pa1651
                               Pseudomonas phage JBD18
          2853
          2854
                               Pseudomonas phage JBD25
          2855
                               Pseudomonas phage JBD26
          2856
                               Pseudomonas phage JBD67
          Name: Organism Name, dtype: object
         Because eukaryotes are limited, we can print all of their names.
In [63]: eukaryotes= micro[micro['NCBI Superkingdom']=='Eukaryota']
         eukaryotes['Organism Name']
```

```
Out[63]: 601 Exophiala dermatitidis NIH/UT8656
983 Phialophora europaea CBS 101466
985 Mucor circinelloides f. circinelloides 1006PhL
1065 Sporothrix schenckii ATCC 58251
Name: Organism Name, dtype: object
```

Because archaea are limited, we can print all of their names.

```
In [64]: archaea= micro[micro['NCBI Superkingdom']=='Archaea']
         archaea['Organism Name']
         302
Out[64]:
                Methanobrevibacter smithii DSM 2374
         303
                Methanobrevibacter smithii DSM 2375
         Name: Organism Name, dtype: object
In [65]: micro['NCBI Superkingdom'].value_counts()
Out[65]: NCBI Superkingdom
         Bacteria
                       1552
                          5
         Viruses
         Eukaryota
                          4
                          2
         Archaea
         Name: count, dtype: int64
```

Observations from this EDA:

- Gastrointestinal system shows most diversity of microbes
- Streptomyces sp. HGB0020 shows the maximum gene count in human
- Streptococcus is most common genus

```
In [66]: # change df name for transformations
df = micro
```

In [67]: # df.head() #commented out for brevity

Out[67]:		HMP ID	GOLD ID	Organism Name	Domain	NCBI Superkingdom	HMP Isolation Body Site	Projec Status
	0	1	Gi03551	Abiotrophia defectiva ATCC 49176	BACTERIAL	Bacteria	oral	Complete
	1	4	Gi03555	Achromobacter piechaudii ATCC 43553	BACTERIAL	Bacteria	airways	Complete
	2	5	Gi03554	Achromobacter xylosoxidans C54	BACTERIAL	Bacteria	airways	Complete
	3	10	Gi03422	Acinetobacter baumannii ATCC 19606	BACTERIAL	Bacteria	urogenital_tract	Complete
	4	12	Gi03421	Acinetobacter calcoaceticus RUH2202	BACTERIAL	Bacteria	skin	Complete
In [68]:			values).sum()					

P3Code-HMP 2/29/24, 5:57 PM

```
Out[68]: HMP ID
                                         0
          GOLD ID
                                        70
          Organism Name
                                         0
          Domain
                                         0
          NCBI Superkingdom
                                         0
          HMP Isolation Body Site
                                         0
          Project Status
                                         0
          Current Finishing Level
                                         0
          NCBI Submission Status
                                         0
          NCBI Project ID
                                         0
          Genbank ID
                                         0
          Gene Count
                                         0
          IMG/HMP ID
                                         0
          HOMD ID
                                      1177
          Sequencing Center
                                         0
          Funding Source
                                         0
          Strain Repository ID
                                       296
          Unnamed: 17
                                      1563
          Unnamed: 18
                                      1563
          Genus
                                         0
          dtype: int64
In [69]: #check percentage missing values
         round((df.isnull().sum() * 100/ len(df)),2).sort_values(ascending=False)
Out[69]: Unnamed: 18
                                      100.00
          Unnamed: 17
                                      100.00
          HOMD ID
                                       75.30
          Strain Repository ID
                                       18.94
                                        4.48
          GOLD ID
          HMP ID
                                        0.00
                                        0.00
          Funding Source
          Sequencing Center
                                        0.00
          IMG/HMP ID
                                        0.00
          Gene Count
                                        0.00
          Genbank ID
                                        0.00
          NCBI Project ID
                                        0.00
         NCBI Submission Status
                                        0.00
          Current Finishing Level
                                        0.00
                                        0.00
          Project Status
          HMP Isolation Body Site
                                        0.00
          NCBI Superkingdom
                                        0.00
          Domain
                                        0.00
          Organism Name
                                        0.00
          Genus
                                        0.00
          dtype: float64
In [70]: # HOMD ID has 75% missing values so I'm checking it
```

```
df['HOMD ID']
```

```
Out[70]: 0
                   HOMD: tax 389
          1
                             NaN
          2
                   HOMD: tax 343
          3
                   HOMD: tax_554
          4
                       . . .
          2910
                             NaN
          2911
                             NaN
                             NaN
          2912
          2913
                             NaN
          2914
                             NaN
          Name: HOMD ID, Length: 1563, dtype: object
```

The unnamed columns provide no information so they can be removed. HOMD ID isn't necessary for analysis so it can be removed as well.

```
In [71]: df2 = df.drop(['Unnamed: 18', 'Unnamed: 17', 'HOMD ID'], axis=1)
In [72]: #check percentage missing values
          round((df2.isnull().sum() * 100/ len(df2)),2).sort_values(ascending=False)
Out[72]: Strain Repository ID
                                      18.94
          GOLD ID
                                       4.48
          HMP ID
                                       0.00
          NCBI Project ID
                                       0.00
          Funding Source
                                       0.00
          Sequencing Center
                                       0.00
          IMG/HMP ID
                                       0.00
          Gene Count
                                       0.00
          Genbank ID
                                       0.00
          NCBI Submission Status
                                       0.00
          Current Finishing Level
                                       0.00
          Project Status
                                       0.00
          HMP Isolation Body Site
                                       0.00
          NCBI Superkingdom
                                       0.00
          Domain
                                       0.00
          Organism Name
                                       0.00
          Genus
                                       0.00
          dtype: float64
In [73]: df['Strain Repository ID']
Out[73]: 0
                           ATCC 49176, CIP 103242
                  ATCC 43553, CIP 55774, LMG 6100
          1
          2
                                        BEI HM-235
          3
                             ATCC 19606, DSM 6974
          4
                                         LMG 10517
                                . . .
          2910
                                        BEI HM-909
          2911
                                        ATCC 43718
          2912
                                        BEI HM-755
          2913
                                        ATCC 27337
          2914
                                        BEI HM-756
          Name: Strain Repository ID, Length: 1563, dtype: object
```

```
In [74]: df["GOLD ID"]
Out[74]: 0
                  Gi03551
                  Gi03555
          1
          2
                  Gi03554
          3
                  Gi03422
          4
                  Gi03421
                   . . .
          2910
                  Gi08654
          2911
                  Gi09593
          2912
                  Gi09594
          2913
                  Gi09595
          2914
                  Gi09596
         Name: GOLD ID, Length: 1563, dtype: object
In [75]: #HOMD ID and Strain Repository ID are not necessary for analysis so they can
         df2 = df2.drop(['Strain Repository ID', 'GOLD ID'], axis=1)
In [76]: df2.columns.tolist()
Out[76]: ['HMP ID',
           'Organism Name',
           'Domain',
           'NCBI Superkingdom',
           'HMP Isolation Body Site',
           'Project Status',
           'Current Finishing Level',
           'NCBI Submission Status',
           'NCBI Project ID',
           'Genbank ID',
           'Gene Count',
           'IMG/HMP ID',
           'Sequencing Center',
           'Funding Source',
           'Genus'l
In [77]: #removing the rest of the ID columns
         df2 = df2.drop(['NCBI Project ID',
          'Genbank ID', 'IMG/HMP ID'], axis=1)
In [78]: #new df name to preserve previous
         df = df2
In [79]: df.columns.tolist()
```

```
Out[79]: ['HMP ID',
           'Organism Name',
           'Domain',
           'NCBI Superkingdom',
           'HMP Isolation Body Site',
           'Project Status',
           'Current Finishing Level',
           'NCBI Submission Status',
           'Gene Count',
           'Sequencing Center',
           'Funding Source',
           'Genus']
In [80]: # subset of df
         test_df = df[['HMP ID',
           'Organism Name',
          'Domain',
          'NCBI Superkingdom',
          'HMP Isolation Body Site',
          'Gene Count',
          'Genus']]
In [81]: test_df.shape
Out[81]: (1563, 7)
In [82]: #checking size and unique values of columns
         df['Genus'].value_counts()
Out[82]: Genus
          Streptococcus
                               161
          Enterococcus
                               110
          Propionibacterium
                                92
                                73
          Lactobacillus
         Helicobacter
                                70
          Pediococcus
                                 1
         Mycobacterium
                                 1
         Micrococcus
                                 1
                                 1
          Leuconostoc
         Acetobacteraceae
                                 1
         Name: count, Length: 185, dtype: int64
In [83]: # rename for to preserve previous
         new_df = test_df
In [84]: new_df
```

\cap	111	+	Γ	0	/	1	
U	u	L	L	O	+	J.	1

	HMP ID	Organism Name	Domain	NCBI Superkingdom	HMP Isolation Body Site	Gene Count
0	1	Abiotrophia defectiva ATCC 49176	BACTERIAL	Bacteria	oral	1950
1	4	Achromobacter piechaudii ATCC 43553	BACTERIAL	Bacteria	airways	5755
2	5	Achromobacter xylosoxidans C54	BACTERIAL	Bacteria	airways	6010
3	10	Acinetobacter baumannii ATCC 19606	BACTERIAL	Bacteria	urogenital_tract	3832
4	12	Acinetobacter calcoaceticus RUH2202	BACTERIAL	Bacteria	skin	3632
•••			•••	•••		
2910	9995	Staphylococcus epidermidis NIHLM095	BACTERIAL	Bacteria	unknown	2300
2911	9996	Aggregatibacter actinomycetemcomitans Y4	BACTERIAL	Bacteria	oral	2343
2912	9997	Corynebacterium durum F0235	BACTERIAL	Bacteria	oral	2823
2913	9998	Peptostreptococcus anaerobius VPI 4330	BACTERIAL	Bacteria	oral	1933
2914	9999	Prevotella sp. oral taxon 473 str. F0040	BACTERIAL	Bacteria	oral	2317

1563 rows × 7 columns

I want to remove Domain or Superkingdom because they seem to have the same information, but first I need to check that. I'm going to convert the strings to lowercase so I may make a clean comparison. Then I'll search for the root words in the other column and see if any are not the same (check if they are all duplicated).

```
In [85]: # Convert to lowercase for sorting
   new_df['Domain'] = new_df['Domain'].str.lower()
   new_df['Domain']
```

```
Out[85]: 0
                  bacterial
         1
                  bacterial
          2
                  bacterial
          3
                  bacterial
                  bacterial
                    . . .
          2910
                  bacterial
          2911
                  bacterial
          2912
                  bacterial
          2913
                  bacterial
          2914
                  bacterial
         Name: Domain, Length: 1563, dtype: object
In [86]: # Convert to lowercase for sorting
         new df['NCBI Superkingdom'] = new df['NCBI Superkingdom'].str.lower()
         new df['NCBI Superkingdom']
Out[86]: 0
                  bacteria
          1
                  bacteria
          2
                  bacteria
          3
                  bacteria
          4
                  bacteria
          2910
                  bacteria
          2911
                  bacteria
          2912
                  bacteria
          2913
                  bacteria
          2914
                  bacteria
         Name: NCBI Superkingdom, Length: 1563, dtype: object
In [87]: # use apply to find if the "superkingdom" string is in "domain", if it is no
         new df['New'] = new df.apply(lambda x: x['NCBI Superkingdom'] if x['NCBI Superkingdom']
                               x['Domain'] else np.nan, axis=1)
In [88]: #check NA value total
         new_df['New'].isna().sum()
Out[88]: 9
In [89]: #There are 9 null values so we can see review the entries manually
         new_df[new_df['New'].isna()]
```

Out[89]:

Ger	Gene Count	Isolation Body Site	NCBI Superkingdom	Domain	Organism Name	HMP ID	
Exophi	0	unknown	eukaryota	eukaryal	Exophiala dermatitidis NIH/UT8656	1120	601
Phialoph	0	skin	eukaryota	eukaryal	Phialophora europaea CBS 101466	1541	983
Mu	0	skin	eukaryota	eukaryal	Mucor circinelloides f. circinelloides 1006PhL	1544	985
Sporoth	0	wound	eukaryota	eukaryal	Sporothrix schenckii ATCC 58251	1624	1065
Pseudomor	0	unknown	viruses	virus	Pseudomonas phage F_HA0480sp/Pa1651	9774	2852
Pseudomor	0	unknown	viruses	virus	Pseudomonas phage JBD18	9843	2853
Pseudomor	0	unknown	viruses	virus	Pseudomonas phage JBD25	9847	2854
Pseudomor	0	unknown	viruses	virus	Pseudomonas phage JBD26	9848	2855
Pseudomor	0	unknown	viruses	virus	Pseudomonas phage JBD67	9886	2856

HMP

I see that these are duplicates as well, so all of the values between "NCBI Superkingdom" and "Domain" are the same. I can remove one of them. I am choosing to drop "NCBI Superkingdom" as well as the "new" column I used for comparison purposes.

In [93]: new_df["Organism Name"].nunique()

Out [93]: 1557

In [94]: new_df["Genus"].nunique()

Out [94]: 185

In [95]: new_df.columns

new_df.head() #commented out for brevity

Out [95]:

	HMP ID	Organism Name	Domain	HMP Isolation Body Site	Gene Count	Genus
0	1	Abiotrophia defectiva ATCC 49176	bacterial	oral	1950	Abiotrophia
1	4	Achromobacter piechaudii ATCC 43553	bacterial	airways	5755	Achromobacter
2	5	Achromobacter xylosoxidans C54	bacterial	airways	6010	Achromobacter
3	10	Acinetobacter baumannii ATCC 19606	bacterial	urogenital_tract	3832	Acinetobacter
4	12	Acinetobacter calcoaceticus RUH2202	bacterial	skin	3632	Acinetobacter

Upcoming process:

- 1. ColumnTransformer Creation:
- A ColumnTransformer is instantiated, which applies different preprocessing to different subsets of features: StandardScaler for numerical features and OneHotEncoder for categorical features.
- 2. Data Transformation:
- The fit_transform method is called on the model_df DataFrame, standardizing the numerical features and encoding the categorical features into a format suitable for clustering.
- 3. Elbow Method:
- The elbow method is used to determine the optimal number of clusters (k) by plotting the within-cluster sum of squares (WCSS) against the number of clusters. The "elbow" point in the graph indicates the optimal k.
- 4. K-Means Clustering:

• K-Means clustering is applied to the processed data with the chosen number of clusters (in this case, 7).

- 5. Cluster Analysis:
- The resulting clusters are then added as a new column to the model_df, and the count of data points in each cluster is outputted to give an initial understanding of the cluster distribution.

```
In [96]: # First, save the identifiers in their own dataframe
identifiers_df = new_df[['HMP ID', 'Organism Name']]
identifiers_df.head()
```

Out[96]:	HMP ID		Organism Name		
	0	1	Abiotrophia defectiva ATCC 49176		
	1	4	Achromobacter piechaudii ATCC 43553		
	2	5	Achromobacter xylosoxidans C54		
	3	10	Acinetobacter baumannii ATCC 19606		
	4	12	Acinetobacter calcoaceticus RUH2202		

```
In [97]: # Removing the identifiers ('HMP ID' and 'Organism Name')
model_df = new_df.drop(['HMP ID', 'Organism Name'], axis=1)
model_df.head()
```

1950

Abiotrophia

Out [97]: Domain HMP Isolation Body Site Gene Count Genus

oral

```
1bacterialairways5755Achromobacter2bacterialairways6010Achromobacter3bacterialurogenital_tract3832Acinetobacter
```

4 bacterial skin 3632 Acinetobacter

```
In [153... # Feature Encoding for cluster modeling includes specifying the numerical an
# Assign features for clustering
features = ['HMP Isolation Body Site', 'Gene Count', 'Genus']

# Separate features for encoding and scaling
categorical_features = ['HMP Isolation Body Site', 'Genus']
numerical_features = ['Gene Count']
```

0 bacterial

```
In [154...
         # Create the ColumnTransformer
          preprocessor = ColumnTransformer(
              transformers=[
                   ('num', StandardScaler(), numerical features),
                   ('cat', OneHotEncoder(), categorical_features)])
In [155... # Fit and transform the data
          X_processed = preprocessor.fit_transform(model_df)
In [156... # Use the elbow method to choose the optimal number of clusters k
          distortions = []
          K = range(1, 100)
          for k in K:
              kmeanModel = KMeans(n clusters=k)
              kmeanModel.fit(X_processed)
              distortions.append(kmeanModel.inertia_)
In [157... # Plot the elbow graph
          plt.figure(figsize=(16,8))
          plt.plot(K, distortions, 'bx-')
          plt.xlabel('k')
          plt.ylabel('Distortion')
          plt.title('The Elbow Method showing the optimal k')
          plt.show()
                                         The Elbow Method showing the optimal k
          3000
         2500
         2000
        Distortion
1500
          1000
          500
```

"The elbow method is a graphical representation of finding the optimal 'K' in a K-means clustering. It works by finding WCSS (Within-Cluster Sum of Square) i.e. the sum of the square distance between points in a cluster and the cluster centroid." "Now we will use Euclidean distance or Manhattan distance as the metric to calculate the distance of the points from the nearest centroid and assign the points to that nearest cluster centroid, thus creating K clusters." https://www.analyticsvidhya.com/blog/2021/01/in-depth-intuition-of-k-means-clustering-algorithm-in-machine-learning/

```
In [158... # Apply k-means clustering with optimal k (based on elbow method)
         kmeans = KMeans(n clusters=7)
         clusters = kmeans.fit_predict(X_processed)
In [159... # Add cluster labels to DataFrame
         model df['Cluster'] = clusters
In [160... # Analyze the clusters
         # For example, you can see how many organisms fall into each cluster
         print(model_df['Cluster'].value_counts())
        Cluster
             551
        6
        2
             286
        3
             229
        1
             219
        5
             127
        0
              92
              59
        Name: count, dtype: int64
```

```
In [161... X processed
```

```
Out[161... <1563x186 sparse matrix of type '<class 'numpy.float64'>'
                  with 3126 stored elements in Compressed Sparse Row format>
```

PCA does not support sparse input with the solver set to "auto" when dealing with sparse matrices. The PCA implementation in scikit-learn requires dense input or, if using sparse input, the solver must be explicitly set to "arpack". However, PCA is generally not recommended for sparse data due to the densification process, which can be very memory intensive. Instead, using TruncatedSVD is often recommended for dimensionality reduction on sparse datasets because it is designed to handle sparse matrices more efficiently.

Cluster Profiling: For each cluster, calculate the mean or median of the numerical features and the mode of the categorical features. This will give you an insight into what each cluster represents or characterizes.

Statistical Tests: If your dataset has labeled data or you want to understand the statistical significance of the clusters with respect to some numerical attributes, you can perform ANOVA or other relevant tests to see if the mean of the numerical features significantly differs between clusters.

Visualize Clusters: Use dimensionality reduction techniques like PCA or t-SNE to visualize the clusters in two or three dimensions. This can give you a visual understanding of how well-separated the clusters are.

Interpret Clusters: Based on the profiles and visualizations, interpret what each cluster might represent. If you have domain knowledge, use it to label each cluster meaningfully.

Evaluate Cluster Quality: Beyond the elbow method, use metrics like silhouette score, Davies-Bouldin index, or the Calinski-Harabasz index to evaluate the quality of the clusters.

	Gene Count	Genus
Cluster		
0	2525.239130	Propionibacterium
1	5268.652968	Escherichia
2	3364.475524	Enterococcus
3	1955.414847	Streptococcus
4	34.033898	Lactobacillus
5	2246.196850	Lactobacillus
6	2146.689655	Staphylococcus

The cluster summary table reveals distinct microbial community profiles based on gene count and predominant isolation body site. For instance, Cluster 0, with the highest gene count, predominantly comprises Escherichia from the gastrointestinal tract, indicating a robust gene diversity in this environment. Conversely, Cluster 5, associated with the gastrointestinal tract, features Helicobacter with a lower gene count, suggesting variation in gene complexity within the same body site. Clusters also highlight specific microbial presences, like Lactobacillus in the urogenital tract and Propionibacterium on the skin, reflecting their ecological niches and potential roles in health and disease.

```
In [165... from scipy.stats import f_oneway

# Perform ANOVA across clusters for a numerical attribute
f_oneway(*(model_df[model_df['Cluster'] == cluster]['Gene Count'] for cluste
```

Out [165... F_onewayResult(statistic=2134.7271638526618, pvalue=0.0)

The ANOVA test result with a statistic of 1084.1518968807904 and a p-value of 0.0 suggests that there is a statistically significant difference in the mean gene counts across different clusters. The high F-statistic value indicates a strong between-group variance compared to within-group variance, reinforcing the significance of the clusters in terms of gene count variation. The p-value being 0 (or very close to 0) means this result is highly significant, rejecting the null hypothesis that all group means are equal.

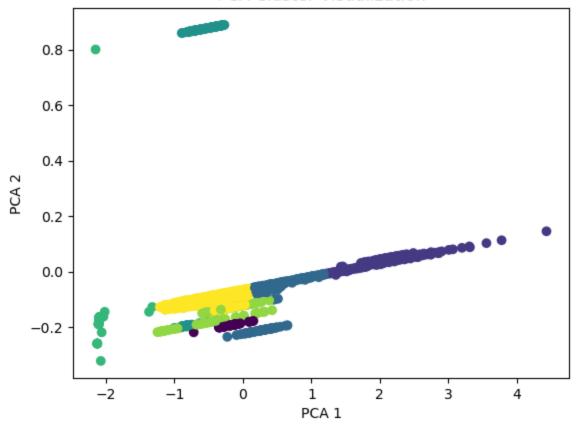
This suggests that the clusters formed have distinct microbial characteristics based on their gene counts.

```
In [166... from sklearn.decomposition import PCA
import matplotlib.pyplot as plt

# PCA for 2D visualization
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_processed.toarray()) # Convert sparse matrix to

plt.scatter(X_pca[:, 0], X_pca[:, 1], c=clusters)
plt.xlabel('PCA 1')
plt.ylabel('PCA 2')
plt.title('PCA Cluster Visualization')
plt.show()
```

PCA Cluster Visualization



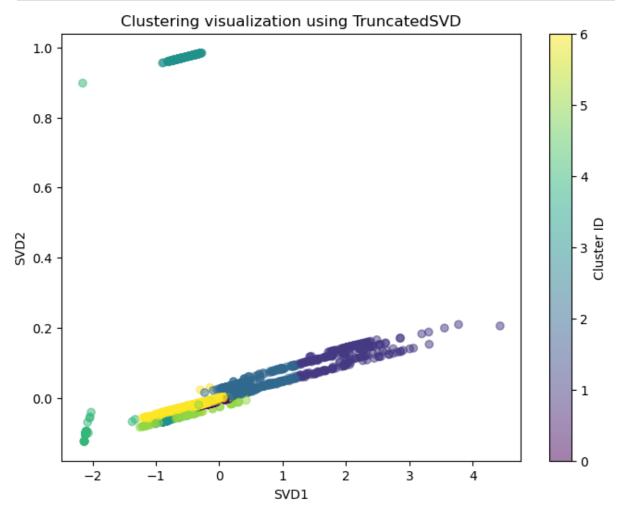
```
In [167... from sklearn.decomposition import TruncatedSVD
import matplotlib.pyplot as plt

# Perform TruncatedSVD
svd = TruncatedSVD(n_components=2)
X_reduced = svd.fit_transform(X_processed)
In [168... # Plot the transformed data
plt.figure(figsize=(8, 6))
```

plt.scatter(X_reduced[:, 0], X_reduced[:, 1], c=clusters, cmap='viridis', al

plt.xlabel('SVD1')

```
plt.ylabel('SVD2')
plt.title('Clustering visualization using TruncatedSVD')
plt.colorbar(label='Cluster ID')
plt.show()
```



```
In [169... from sklearn.metrics import silhouette_score

# Evaluate silhouette score
silhouette_avg = silhouette_score(X_processed, clusters)
print(f'Silhouette Score: {silhouette_avg}')
```

Silhouette Score: 0.24429453257794126

A silhouette score of 0.25275623208645914 suggests that the cluster separation is fair but not strong. Silhouette scores range from -1 (poor clustering) to +1 (perfect clustering), with scores around 0 indicating overlapping clusters. Your score indicates that while there is some structure to the clusters, there might be room for improvement either by adjusting the number of clusters, reconsidering the features used, or applying a different clustering technique.

This project applies machine learning techniques to analyze the human microbiome, focusing on clustering microbial species based on their genetic characteristics and isolation sites. The model leverages k-means clustering to group organisms, revealing

patterns and associations between microbial genuses, gene counts, and their prevalence in different body sites. The statistical analysis, including ANOVA, confirms significant differences among clusters, enhancing our understanding of the microbiome's composition and its potential health implications. The silhouette score indicates moderate cluster separation, suggesting room for model refinement but affirming its utility in microbiome research. This approach offers insights into microbial diversity and its role in human health, paving the way for targeted therapeutic interventions.

This project employs a microbiome-focused approach to examine the human microbiota's composition, aiming to uncover patterns and correlations with health conditions. Through advanced machine learning techniques, including k-means clustering and PCA, the project analyzes microbial diversity and gene count data to identify distinct microbial clusters associated with different body sites. The findings reveal significant microbial community variations, highlighting potential implications for diagnosing and treating health issues. The analysis underscores the microbiome's complexity and its potential as a biomarker for health, paving the way for personalized medicine strategies that consider microbial composition.