About the Project

Case Study 1.1.1: Genetic Codes

Instructor: Tamara Broderick Activity Type: Optional Case Study Description: Using K-means to help figure out that DNA is composed of 3-letter words. Self-Help Documentation: From this document, you will learn how data visualization can help in genomic sequence analysis and start with a fragment of genetic text of a bacterial genome and analyze its structure. Download Self-Help Documentation

Time Required: The time required to do this activity varies depending on your experience in the required programming background. We suggest planning somewhere between 1 & 3 hours. Remember, this is an optional activity for participants looking for hands-on experience. Have questions? Feel free to discuss the case study with other participants in the Discussion Forum under Module 1 - Case Studies Section.

Pre-Processing

In [1]:

```
# Importing libraries
import re
import matplotlib.pyplot as plt
from itertools import product
import numpy as np
import pandas as pd
from pandas import *

# Pretty display for notebooks
%matplotlib inline
```

In [2]:

```
txt = ""
with open("gene.txt", 'r') as reader:
    for line in reader:
        txt = txt + line.rstrip()

reader.close()
```

In [3]:

```
permutationHeaders = [''.join(p) for p in product('acgt', repeat=3)]
data = pd.DataFrame(columns = permutationHeaders)
```

In [4]:

```
n  = 300
n_codons = 3
splitted_codons = []
txtCodons = ""
line = ""
countLine = 0
for index in range(0, len(txt), n):
    line = txt[index : index + n]

    txtCodons =  (re.sub("(.{3})", "\\1 ",line).split())

    #splitted_codons.append(txtCodons)

    wordfreq = []
    for token in permutationHeaders:
        wordfreq.append(txtCodons.count(token))
    data.loc[countLine] = wordfreq

    countLine +=1
```

Exploring and Visualising Data

In [5]:

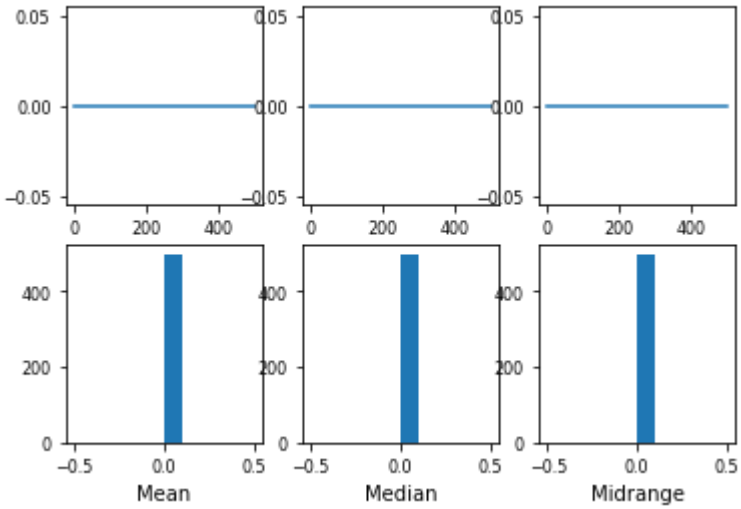
```
# Display a description of the dataset
display(data.describe())
```

	aaa	aac	aag	aat	aca	acc	acg	act	aga	agc	...	tcg	tct	t
count	1018	1018	1018	1018	1018	1018	1018	1018	1018	1018	...	1018	1018	10
unique	6	8	12	5	10	12	12	8	10	11	...	15	9	9
top	0	0	0	0	0	0	0	0	0	1	...	0	0	0
freq	738	551	455	782	600	357	318	684	508	264	...	219	482	43

4 rows × 64 columns

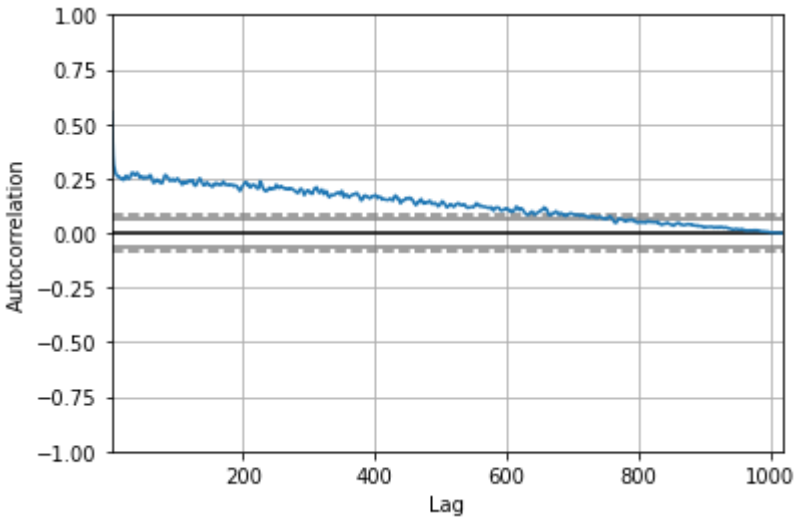
In [6]:

```
plotting.bootstrap_plot(data.all());
```



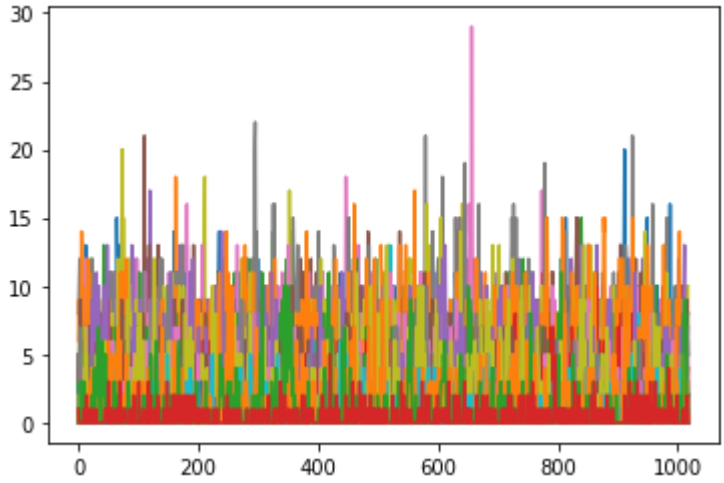
In [7]:

```
plotting.autocorrelation_plot(data);
```



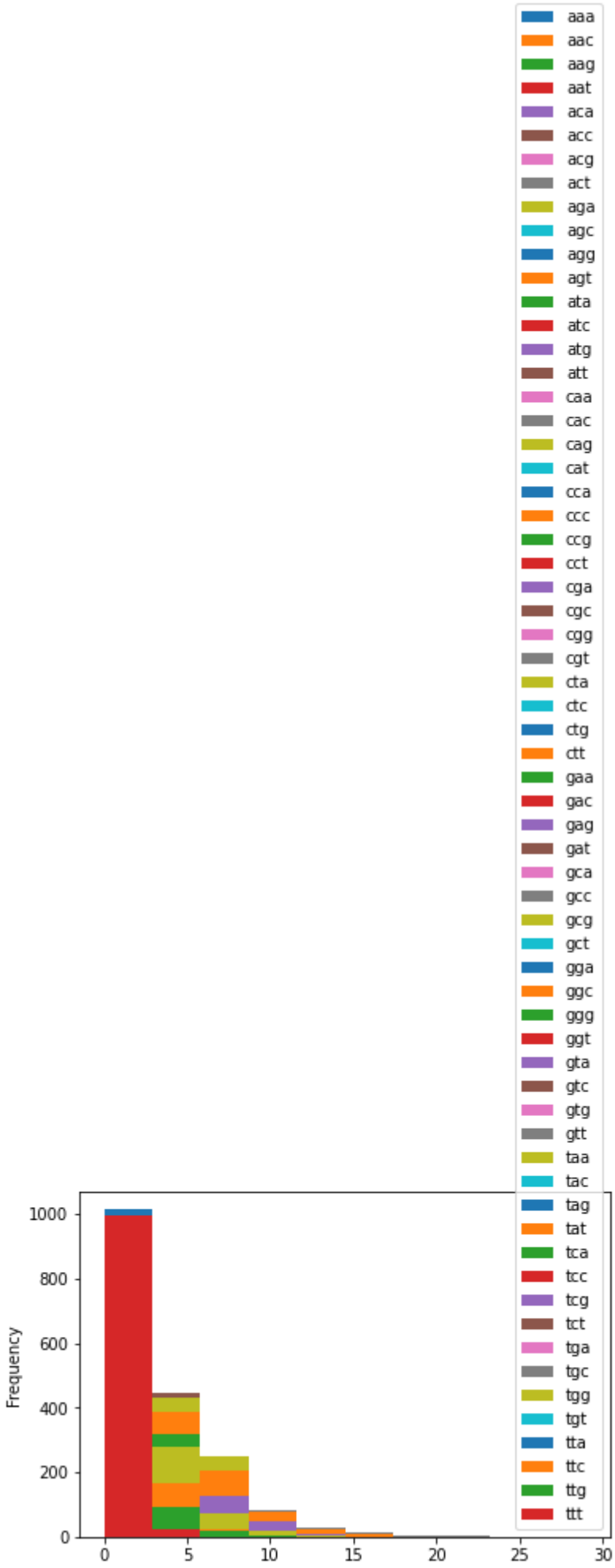
In [8]:

```
plt.plot(data);
```



In [9]:

```
data.plot.hist(legend='center left');
```


aaa
aac
aag
aat
aca
acc
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act
aga
agc
agg
agt
ata
atc
atg
att
caa
cac
cag
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gac
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gat
gca
gcc
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gta
gtc
gtg
gtt
taa
tac
tag
tat
tca
tcc
tcg
tct
tga
tgc
tgg
tgt
tta
ttc
ttg
ttt
Frequency
0
200
400
600
800
1000
0
5
10
15
20
25
30

Applying Clustering and PCA

In [10]:

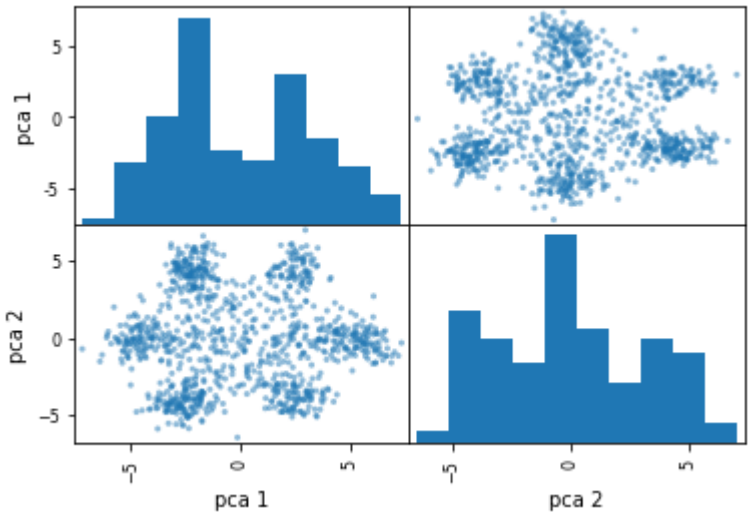
```
from sklearn.preprocessing import StandardScaler
data_scaled = StandardScaler().fit_transform(data)
```

In [11]:

```
from sklearn.decomposition import PCA

# Transform the scaled data using the PCA fit above
pca = PCA(n_components=2 ,random_state=2).fit(data_scaled)

reduced_data = pca.transform(data_scaled)

pca_samples = pd.DataFrame(data = reduced_data, columns = ['pca 1', 'pca 2'])
```

In [16]:

```
plotting.scatter_matrix(pca_samples);
```

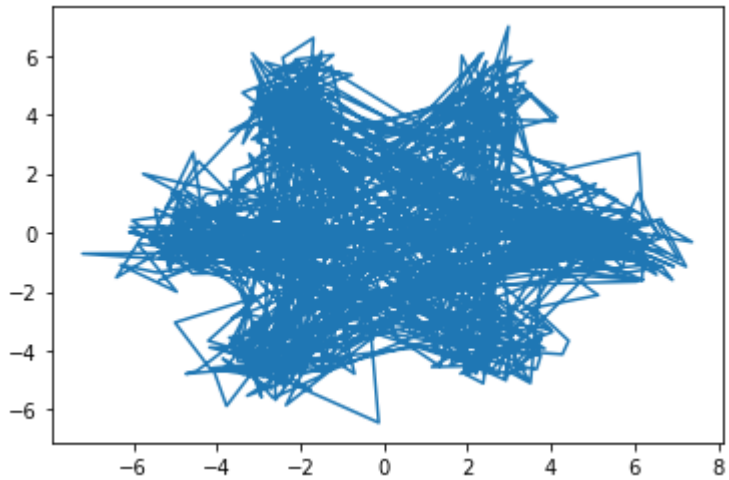


In [13]:

```
plt.plot(pca_samples['pca 1'], pca_samples['pca 2'])
```

Out[13]:

```
[<matplotlib.lines.Line2D at 0x120478668>]
```



Conclusion

In [14]:

```
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_score

n_clusters = 7

clusterer = KMeans(n_clusters = n_clusters, random_state=42).fit(pca_samples)
#Predict the cluster for each data point
preds = clusterer.predict(pca_samples)

#Find the cluster centers
centers = clusterer.cluster_centers_

#Predict the cluster for each transformed sample data point
sample_preds = clusterer.predict(pca_samples)

# TODO: Calculate the mean silhouette coefficient for the number of clusters cho
sen
score = silhouette_score(pca_samples, clusterer.labels_, metric='euclidean')
print ("K-means score: ", score)


plt.scatter(pca_samples['pca 1'], pca_samples['pca 2'], c = sample_preds, s = 20
0, cmap = 'Accent')


plt.scatter(centers[:, 0], centers[:, 1], c='black', s=200, alpha=0.5);
```

```
K-means score:  0.5426067388886062
```