

clustering_titanic

November 11, 2025

```
[41]: import math
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.preprocessing import StandardScaler, MinMaxScaler
from scipy.cluster.hierarchy import linkage, dendrogram, fcluster
import seaborn as sns
from scipy.spatial.distance import pdist, squareform
```

```
[42]: df = pd.read_csv("data/titanic.csv")
df.head()
```

```
[42]:   PassengerId  Survived  Pclass \
0            1         0       3
1            2         1       1
2            3         1       3
3            4         1       1
4            5         0       3

                                                Name     Sex   Age  SibSp \
0          Braund, Mr. Owen Harris    male  22.0      1
1  Cumings, Mrs. John Bradley (Florence Briggs Th...  female  38.0      1
2           Heikkinen, Miss. Laina  female  26.0      0
3    Futrelle, Mrs. Jacques Heath (Lily May Peel)  female  35.0      1
4            Allen, Mr. William Henry    male  35.0      0

   Parch      Ticket     Fare Cabin Embarked
0    0        A/5 21171  7.2500   NaN      S
1    0         PC 17599  71.2833   C85      C
2    0    STON/O2. 3101282  7.9250   NaN      S
3    0        113803  53.1000  C123      S
4    0        373450  8.0500   NaN      S
```

0.0.1 Preprocessing

```
[43]: #from google.colab import drive  
#drive.mount('/content/drive')
```

Fill missing values and convert to numerical (where possible)

```
[44]: sexes = sorted(df['Sex'].unique())  
sexes_mapping = dict(zip(sexes, range(0, len(sexes) + 1)))  
df['Sex_Val'] = df['Sex'].map(sexes_mapping).astype(int)
```

```
[45]: df['Embarked'] = df['Embarked'].fillna(df['Embarked'].mode()[0])  
embarked_locs = sorted(df['Embarked'].unique())  
embarked_locs_mapping = dict(zip(embarked_locs, range(0, len(embarked_locs) + 1)))  
df['Embarked_Val'] = df['Embarked'].map(embarked_locs_mapping).astype(int)
```

```
[46]: df['AgeFill'] = df.groupby(['Sex', 'Pclass'])['Age'].transform(lambda x: x.fillna(x.median()))
```

```
[47]: df['FamilySize'] = df['SibSp'] + df['Parch']
```

```
[48]: df.head()
```

```
[48]:  PassengerId  Survived  Pclass  \  
0            1        0      3  
1            2        1      1  
2            3        1      3  
3            4        1      1  
4            5        0      3  
  
                                         Name     Sex   Age  SibSp  \  
0           Braund, Mr. Owen Harris    male  22.0      1  
1  Cumings, Mrs. John Bradley (Florence Briggs Th...  female  38.0      1  
2           Heikkinen, Miss. Laina  female  26.0      0  
3    Futrelle, Mrs. Jacques Heath (Lily May Peel)  female  35.0      1  
4             Allen, Mr. William Henry    male  35.0      0  
  
      Parch      Ticket      Fare Cabin Embarked  Sex_Val  Embarked_Val  \  
0      0       A/5 21171    7.2500   NaN      S         1             2  
1      0        PC 17599   71.2833   C85         C         0             0  
2      0  STON/O2. 3101282   7.9250   NaN      S         0             2  
3      0          113803  53.1000  C123         S         0             2  
4      0          373450   8.0500   NaN      S         1             2  
  
      AgeFill  FamilySize  
0      22.0          1  
1      38.0          1
```

```
2      26.0      0
3      35.0      1
4      35.0      0
```

Check categorical variables

```
[49]: df.dtypes[df.dtypes.map(lambda x: x == 'object')]
```

```
[49]: Name      object
Sex       object
Ticket    object
Cabin     object
Embarked  object
dtype: object
```

```
[50]: df_train = df.drop(['Name', 'Sex', 'Ticket', 'Cabin', 'Embarked'], axis=1)
df_train.drop(['Survived', 'Age', 'SibSp', 'Parch', 'PassengerId', ↴
    'Embarked_Val', 'Sex_Val'], axis=1, inplace=True)
df_train.dtypes
```

```
[50]: Pclass        int64
Fare         float64
AgeFill      float64
FamilySize   int64
dtype: object
```

```
[51]: df_train.head()
```

```
[51]:   Pclass      Fare  AgeFill  FamilySize
  0      3    7.2500    22.0      1
  1      1   71.2833    38.0      1
  2      3    7.9250    26.0      0
  3      1   53.1000    35.0      1
  4      3    8.0500    35.0      0
```

```
[52]: scaler = MinMaxScaler()
train_data = scaler.fit_transform(df_train)
```

0.0.2 Clustering

```
[53]: from sklearn.metrics import *
from sklearn.cluster import KMeans, DBSCAN, AgglomerativeClustering
from sklearn.neighbors import kneighbors_graph
```

```
[17]: %%time
sse_list = []
sil_list = []
```

```

for k in range(2, 51):
    kmeans = KMeans(init='k-means++', n_clusters=k, n_init=10, max_iter=100)
    kmeans.fit(train_data)
    sse_list.append(kmeans.inertia_)
    sil_list.append(silhouette_score(train_data, kmeans.labels_))

```

CPU times: user 9.45 s, sys: 44.5 ms, total: 9.5 s
Wall time: 5.31 s

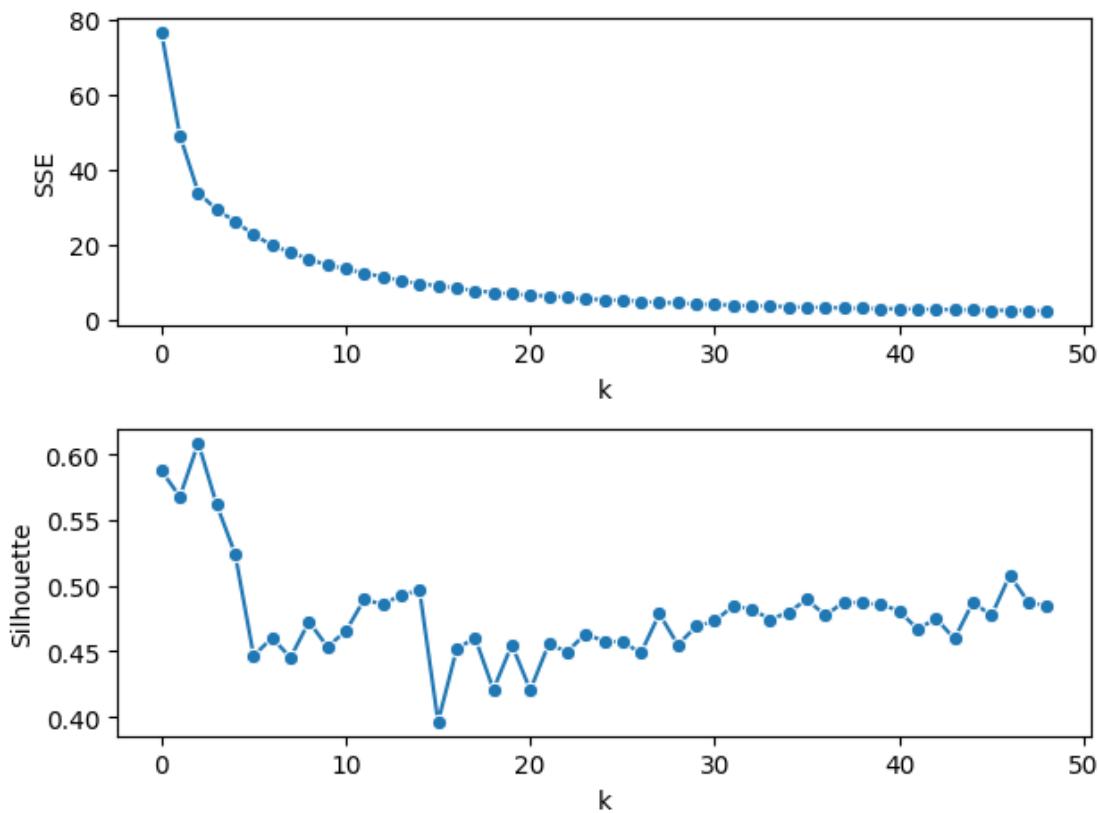
```

[18]: fig, axs = plt.subplots(2) # 1 row, 2 columns

sns.lineplot(x=range(len(sse_list)), y=sse_list, marker='o', ax=axs[0])
axs[0].set(xlabel='k', ylabel='SSE')
sns.lineplot(x=range(len(sil_list)), y=sil_list, marker='o', ax=axs[1])
axs[1].set(xlabel='k', ylabel='Silhouette')

plt.tight_layout() # Adjust the padding between and around subplots

```



```

[22]: kmeans = KMeans(init='k-means++', n_clusters=5, n_init=10, max_iter=100)
kmeans.fit(train_data)

```

```
[22]: KMeans(max_iter=100, n_clusters=5, n_init=10)

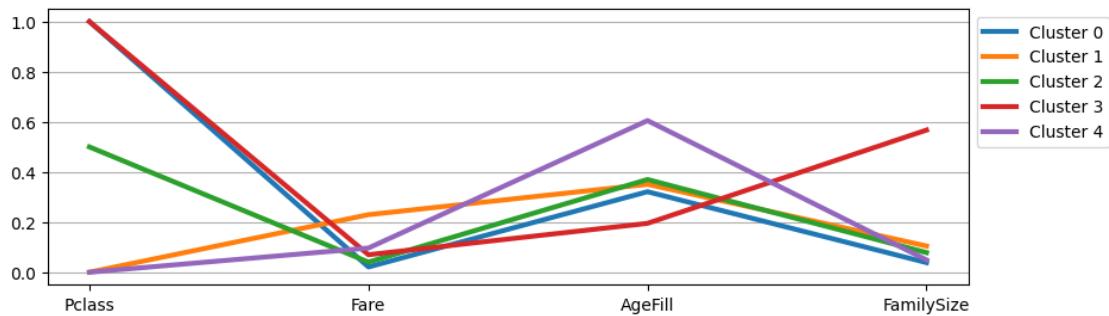
[23]: print('labels', np.unique(kmeans.labels_, return_counts=True))
print('sse', kmeans.inertia_)
print('silhouette', silhouette_score(train_data, kmeans.labels_))

labels (array([0, 1, 2, 3, 4], dtype=int32), array([433, 109, 184, 58, 107]))
sse 29.169946054563958
silhouette 0.5614640538880703
```

[23]:

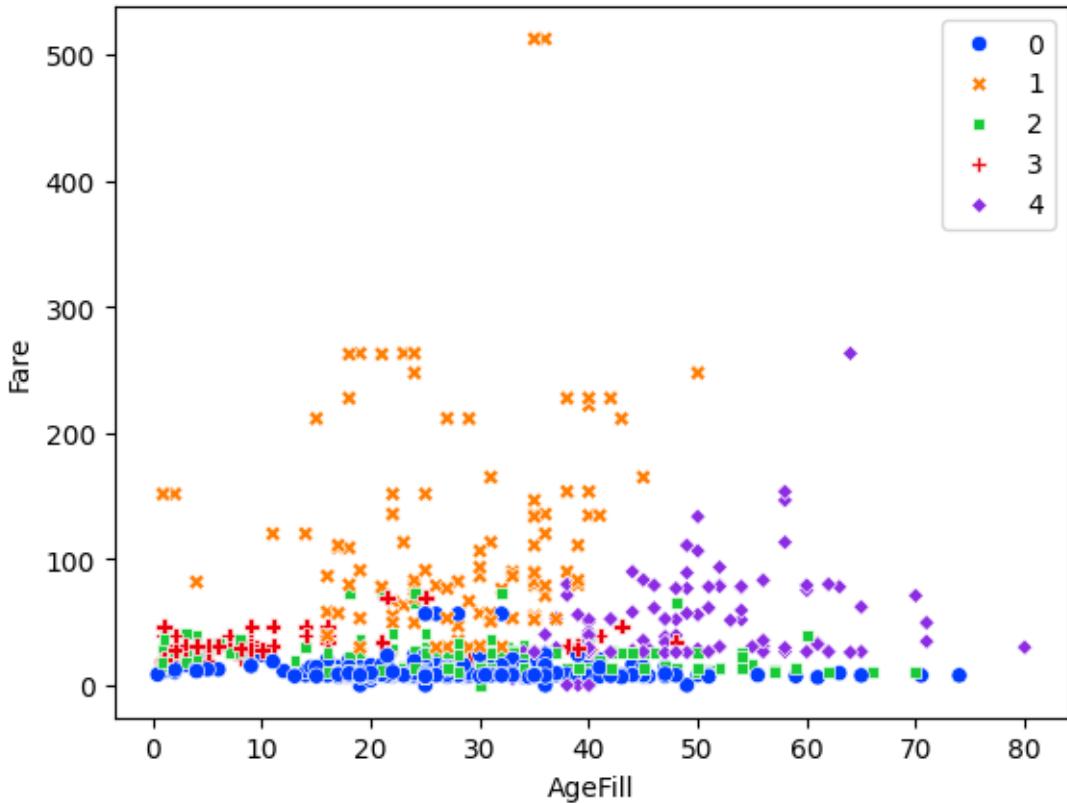
```
[24]: plt.figure(figsize=(10, 3))

for i in range(len(kmeans.cluster_centers_)):
    plt.plot(range(0, 4), kmeans.cluster_centers_[i], label='Cluster %s' % i, linewidth=3)
plt.xticks(range(0, 4), list(df_train.columns))
plt.legend(bbox_to_anchor=(1,1))
plt.grid(axis='y')
plt.show()
```



```
[25]: df_clusters = df_train.copy()
df_clusters['Labels'] = kmeans.labels_
```

```
[26]: sns.scatterplot(data=df_clusters,
                     x="AgeFill",
                     y="Fare",
                     hue=kmeans.labels_,
                     style=kmeans.labels_,
                     palette="bright")
plt.show()
```



```
[27]: df_clusters.head()
```

```
[27]:   Pclass      Fare  AgeFill  FamilySize  Labels
0       3    7.2500     22.0          1        0
1       1   71.2833     38.0          1        4
2       3    7.9250     26.0          0        0
3       1   53.1000     35.0          1        1
4       3    8.0500     35.0          0        0
```

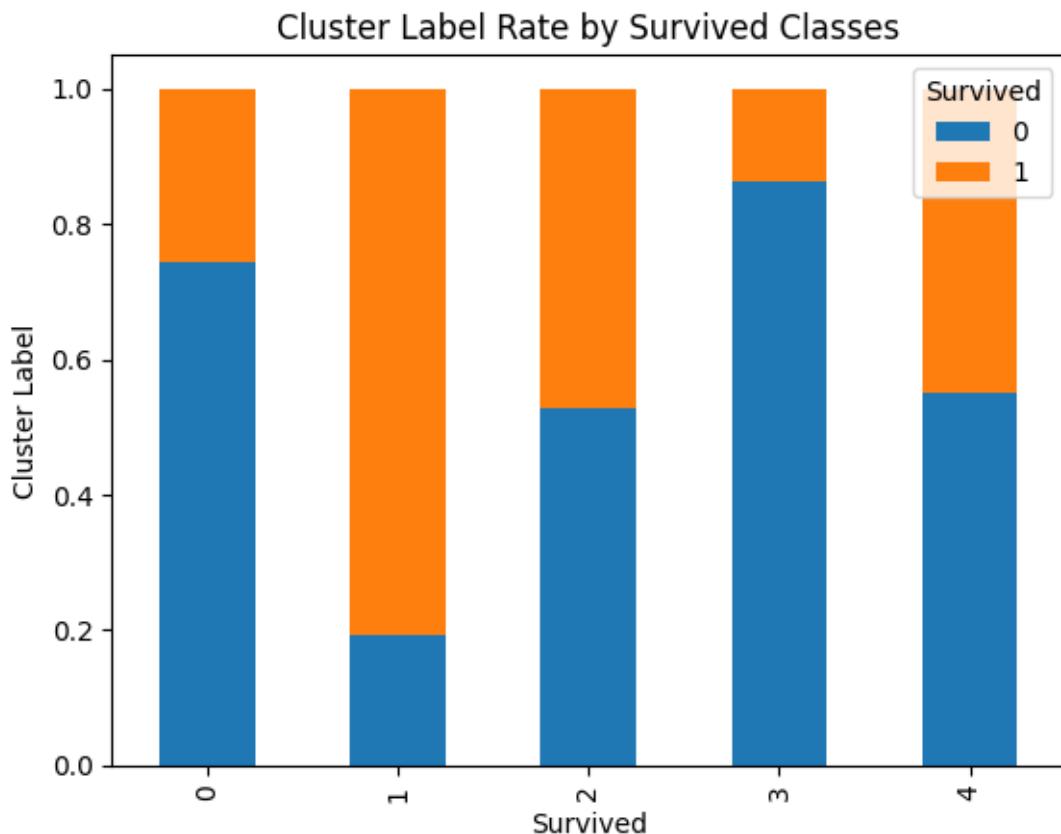
```
[28]: pclass_xt = pd.crosstab(df_clusters['Pclass'], df_clusters['Labels'])
pclass_xt
```

```
[28]: Labels      0      1      2      3      4
Pclass
1          0  109      0      0  107
2          0      0  184      0      0
3        433      0      0  58      0
```

```
[29]: psurv_xt = pd.crosstab(df_clusters['Labels'], df['Survived'])
psurv_xt
```

```
[29]: Survived      0      1
Labels
0            322   111
1             21    88
2             97    87
3             50     8
4             59    48
```

```
[30]: psurv_xt_pct = psurv_xt.div(psurv_xt.sum(1).astype(float), axis=0)
psurv_xt_pct.plot(kind='bar', stacked=True, title='Cluster Label Rate by Survived Classes')
plt.xlabel('Survived')
plt.ylabel('Cluster Label')
plt.show()
```

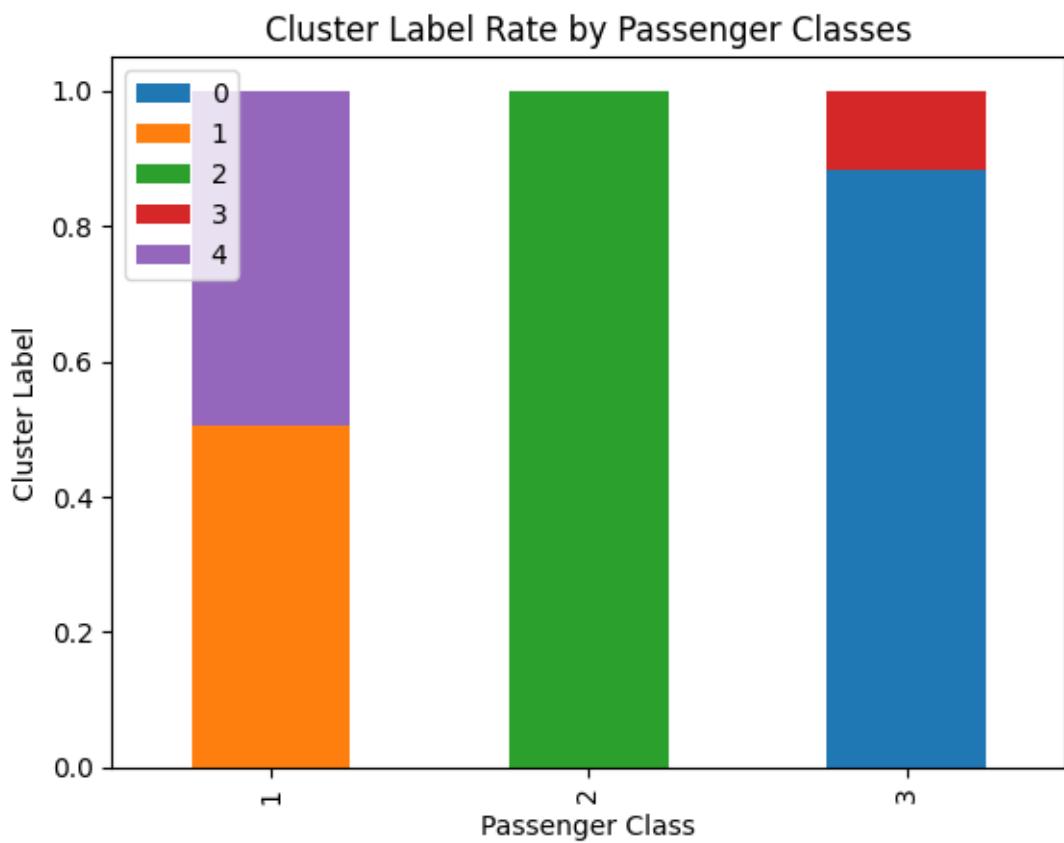


```
[31]: df_clusters[df_clusters['Labels']==1].describe()
```

```
[31]:      Pclass          Fare       AgeFill  FamilySize  Labels
count    109.0  109.000000  109.000000  109.000000  109.0
mean     1.0   118.044533   28.256147    1.045872    1.0
```

std	0.0	92.682510	9.034489	1.173672	0.0
min	1.0	26.283300	0.920000	0.000000	1.0
25%	1.0	56.929200	22.000000	0.000000	1.0
50%	1.0	86.500000	29.000000	1.000000	1.0
75%	1.0	146.520800	35.000000	1.000000	1.0
max	1.0	512.329200	50.000000	5.000000	1.0

```
[32]: pclass_xt_pct = pclass_xt.div(pclass_xt.sum(1).astype(float), axis=0)
pclass_xt_pct.plot(kind='bar', stacked=True, title='Cluster Label Rate by Passenger Classes')
plt.xlabel('Passenger Class')
plt.ylabel('Cluster Label')
plt.legend(loc='best')
plt.show()
```



0.0.3 DBScan

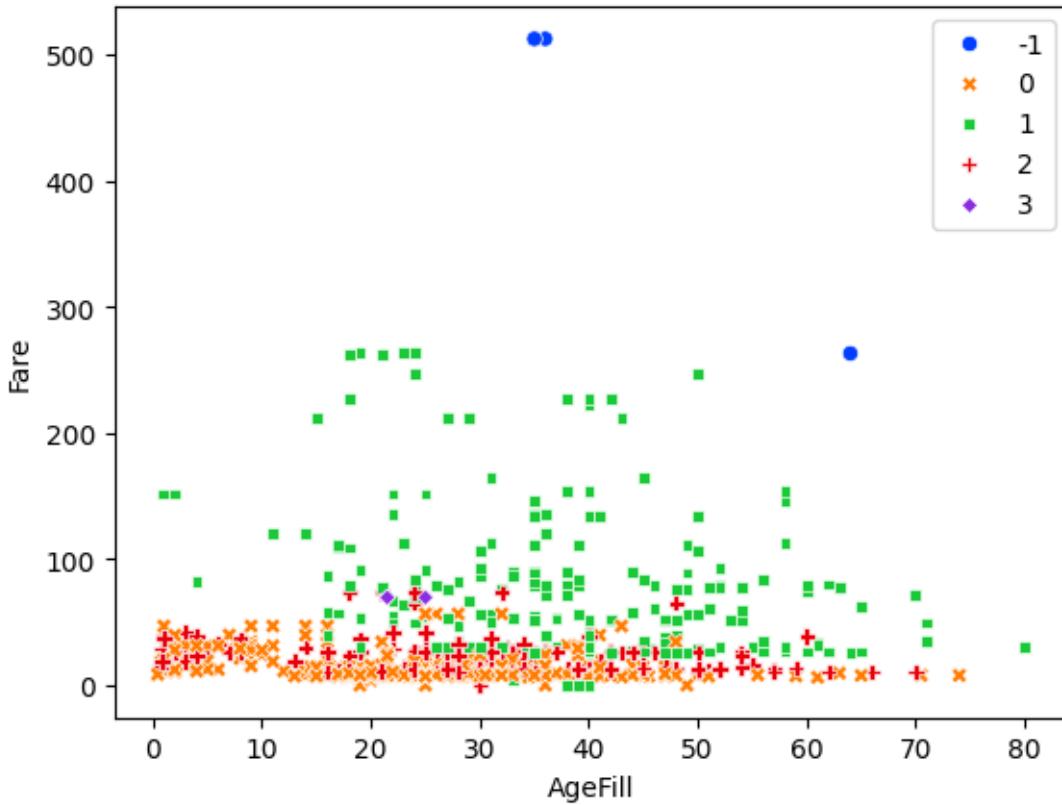
```
[34]: # density based clustering
print('dbscan')

dbscan = DBSCAN(eps=0.3, min_samples=5, metric='euclidean')
dbscan.fit(train_data)

hist, bins = np.histogram(dbscan.labels_, bins=range(-1, len(set(dbscan.
    ↴labels_)) + 1))
print('labels', dict(zip(bins, hist)))
print('silhouette', silhouette_score(train_data[dbscan.labels_ != -1], dbscan.
    ↴labels_[dbscan.labels_ != -1]))
```

```
dbscan
labels {np.int64(-1): np.int64(4), np.int64(0): np.int64(484), np.int64(1):
np.int64(212), np.int64(2): np.int64(184), np.int64(3): np.int64(7),
np.int64(4): np.int64(0)}
silhouette 0.5728928528267885
```

```
[35]: sns.scatterplot(data=df_clusters,
                     x="AgeFill",
                     y="Fare",
                     hue=dbscan.labels_,
                     style=dbscan.labels_,
                     palette="bright")
plt.show()
```



0.0.4 Hierarchical

```
[36]: def get_linkage_matrix(model):
    # Create linkage matrix

    # create the counts of samples under each node
    counts = np.zeros(model.children_.shape[0])
    n_samples = len(model.labels_)
    for i, merge in enumerate(model.children_):
        current_count = 0
        for child_idx in merge:
            if child_idx < n_samples:
                current_count += 1    # leaf node
            else:
                current_count += counts[child_idx - n_samples]
        counts[i] = current_count

    linkage_matrix = np.column_stack(
        [model.children_, model.distances_, counts])
    .astype(float)
```

```

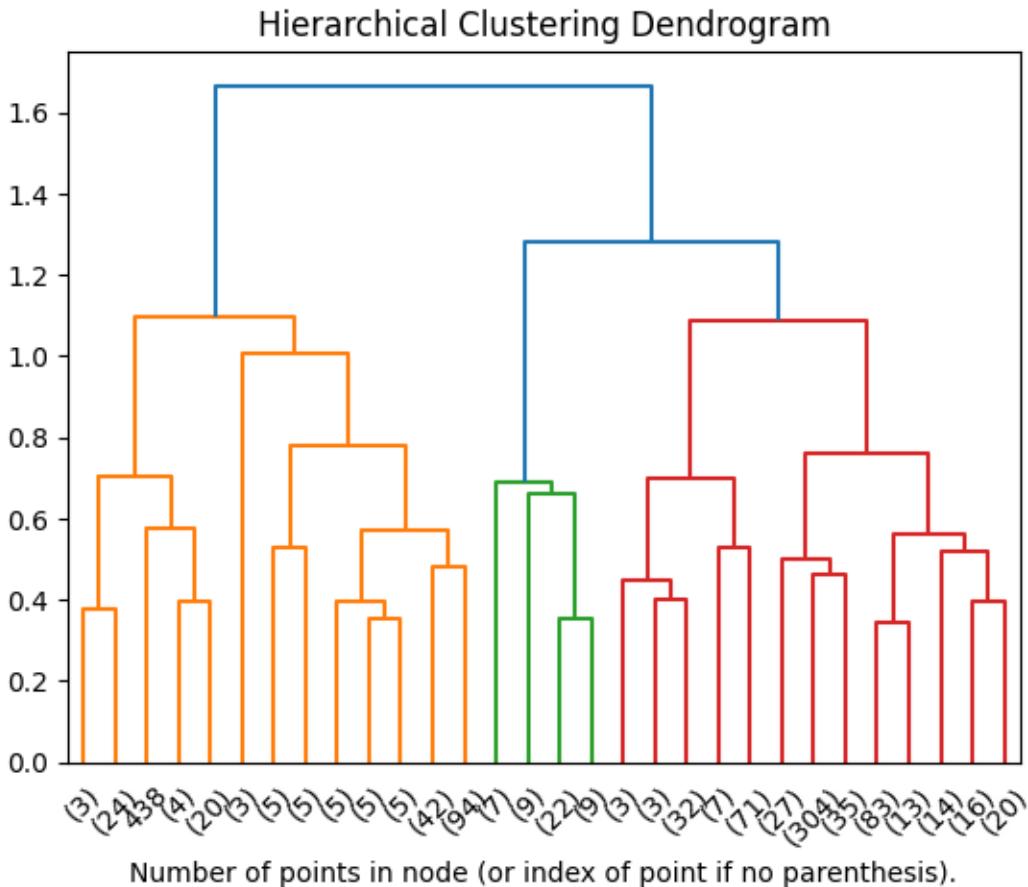
    return linkage_matrix

def plot_dendrogram(model, **kwargs):
    linkage_matrix = get_linkage_matrix(model)
    dendrogram(linkage_matrix, **kwargs)

```

[37]: # setting distance_threshold=0 ensures we compute the full tree.
model = AgglomerativeClustering(distance_threshold=0, n_clusters=None,
metric='euclidean', linkage='complete')
model = model.fit(train_data)

[38]: plt.title("Hierarchical Clustering Dendrogram")
plot_dendrogram(model, truncate_mode="lastp", color_threshold=1.2)
plt.xlabel("Number of points in node (or index of point if no parenthesis).")
plt.show()



[39]: # get the labels according to a specific threshold value cut
Z = get_linkage_matrix(model)

```
labels = fcluster(Z, t=1.2, criterion='distance')
```

[40]: labels

```
[ ]: print('Silhouette', silhouette_score(train_data, labels))
```

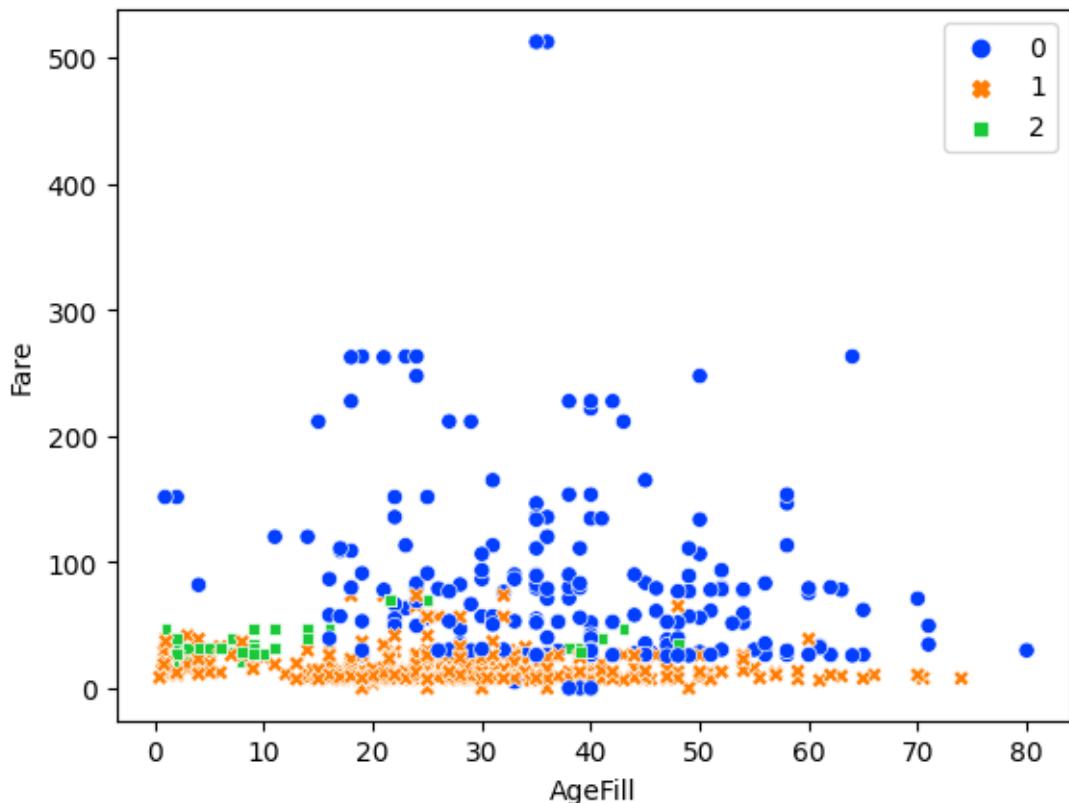
```
Silhouette 0.5026555448852588
```

0.0.5 Choosing the number of clusters

```
[ ]: hier = AgglomerativeClustering(n_clusters=3, metric='euclidean',  
    linkage='complete')  
hier.fit(train_data)
```

```
[ ]: AgglomerativeClustering(linkage='complete', n_clusters=3)
```

```
[ ]: sns.scatterplot(data=df_clusters,  
                     x="AgeFill",  
                     y="Fare",  
                     hue=hier.labels_,  
                     style=hier.labels_,  
                     palette="bright")  
plt.show()
```



connectivity constraint

```
[ ]: # hierarchical clustering  
# Compute the (weighted) graph of k-Neighbors for points in X
```

```

connectivity = kneighbors_graph(train_data, n_neighbors=100, include_self=False)

[ ]: # setting distance_threshold=0 ensures we compute the full tree.
model = AgglomerativeClustering(distance_threshold=0,
                                 n_clusters=None,
                                 metric='euclidean',
                                 linkage='ward',
                                 connectivity=connectivity)

# connecet: Defines for each sample the neighboring
# samples following a given structure of the data.

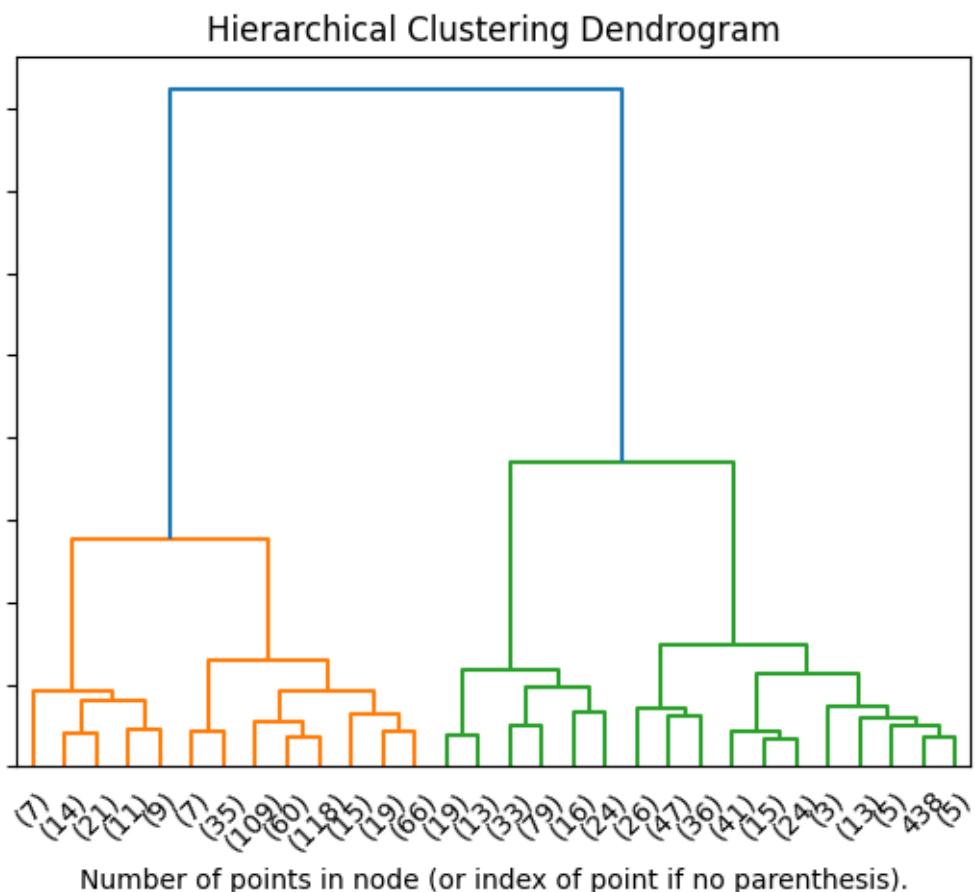
model = model.fit(train_data)

```

```

[ ]: plt.title("Hierarchical Clustering Dendrogram")
plot_dendrogram(model, truncate_mode="lastp")
plt.xlabel("Number of points in node (or index of point if no parenthesis).")
plt.show()

```

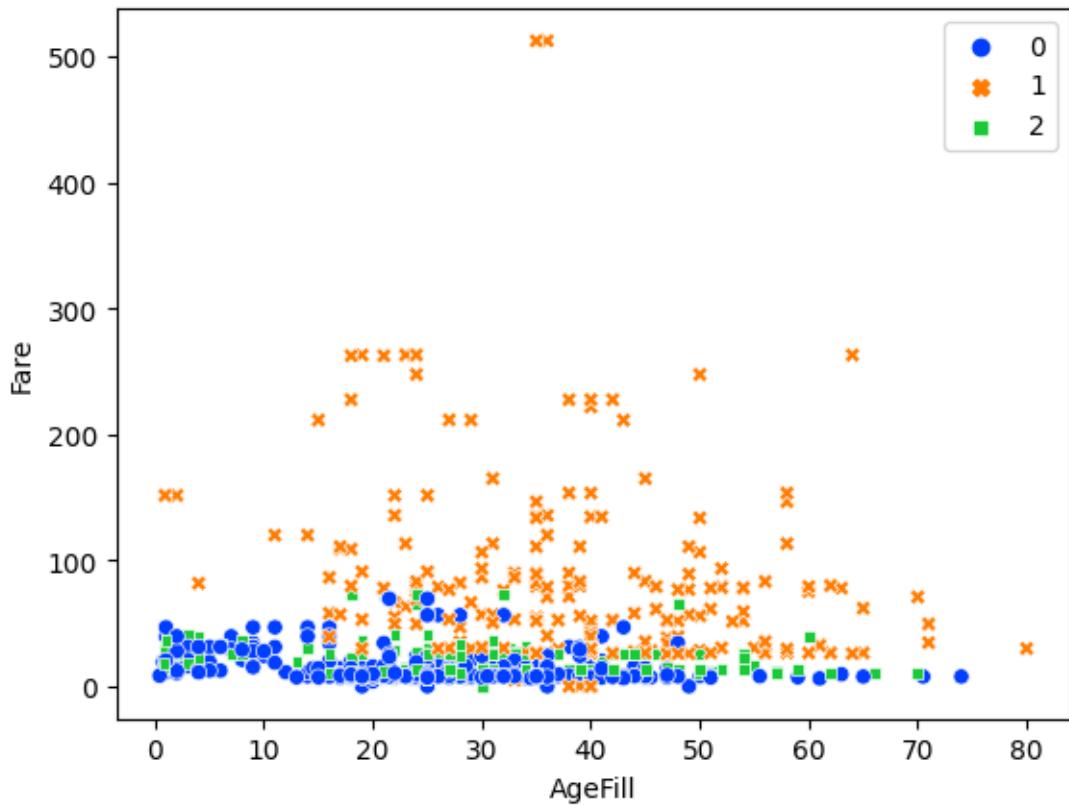


```
[ ]: ward = AgglomerativeClustering(n_clusters=3,
                                      linkage='ward',
                                      metric='euclidean',
                                      connectivity=connectivity)
ward.fit(train_data)

hist, bins = np.histogram(ward.labels_, bins=range(0, len(set(ward.labels_)) + 1))
print('labels', dict(zip(bins, hist)))
print('silhouette', silhouette_score(train_data, ward.labels_))
```

labels {0: 491, 1: 216, 2: 184}
silhouette 0.5676262875725462

```
[ ]: sns.scatterplot(data=df_clusters,
                     x="AgeFill",
                     y="Fare",
                     hue=ward.labels_,
                     style=ward.labels_,
                     palette="bright")
plt.show()
```



```
[ ]: print('average linkage')
average_linkage = AgglomerativeClustering(n_clusters=3, linkage='average', metric='manhattan', connectivity=connectivity)
average_linkage.fit(train_data)

hist, bins = np.histogram(average_linkage.labels_, bins=range(0, len(set(average_linkage.labels_)) + 1))

print('labels', dict(zip(bins, hist)))
print('silhouette', silhouette_score(train_data, average_linkage.labels_))
```

average linkage
 labels {0: 881, 1: 7, 2: 3}
 silhouette 0.37132365914471405

```
[ ]: print('complete linkage')
complete_linkage = AgglomerativeClustering(n_clusters=3, linkage='complete', metric='l1', connectivity=connectivity)
complete_linkage.fit(train_data)

hist, bins = np.histogram(complete_linkage.labels_, bins=range(0, len(set(complete_linkage.labels_)) + 1))

print('labels', dict(zip(bins, hist)))
print('silhouette', silhouette_score(train_data, complete_linkage.labels_))
```

complete linkage
 labels {0: 882, 1: 3, 2: 6}
 silhouette 0.35741232675404144

[]:

Categorical & Mixed distances

```
[54]: cols2drop = ['PassengerId', 'Name', 'Cabin', 'Ticket', 'FamilySize', 'Sex_Val', 'Embarked_Val', 'Age']
df_xm = df.drop(cols2drop, axis=1)
df_xm['Pclass'] = df_xm['Pclass'].map({1: '1st', 2: '2nd', 3: '3rd'})
df_xm.head()
```

	Survived	Pclass	Sex	SibSp	Parch	Fare	Embarked	AgeFill
0	0	3rd	male	1	0	7.2500	S	22.0
1	1	1st	female	1	0	71.2833	C	38.0
2	1	3rd	female	0	0	7.9250	S	26.0
3	1	1st	female	1	0	53.1000	S	35.0
4	0	3rd	male	0	0	8.0500	S	35.0

```
[55]: df_xm2 = pd.get_dummies(df_xm[[c for c in df_xm.columns if c != 'Survived']] ,  
    ↪prefix_sep='=')  
df_xm2
```

```
[55]:      SibSp  Parch     Fare  AgeFill  Pclass=1st  Pclass=2nd  Pclass=3rd  \\\n      0       1      0   7.2500   22.0      False      False      True\n      1       1      0  71.2833   38.0      True      False      False\n      2       0      0   7.9250   26.0      False      False      True\n      3       1      0  53.1000   35.0      True      False      False\n      4       0      0   8.0500   35.0      False      False      True\n      ..     ...    ...    ...    ...    ...    ...    ...    ...\n     886      0      0  13.0000   27.0      False      True      False\n     887      0      0  30.0000   19.0      True      False      False\n     888      1      2  23.4500   21.5      False      False      True\n     889      0      0  30.0000   26.0      True      False      False\n     890      0      0   7.7500   32.0      False      False      True\n\n      Sex=female  Sex=male  Embarked=C  Embarked=Q  Embarked=S\n      0      False      True      False      False      True\n      1      True      False      True      False      False\n      2      True      False      False      False      True\n      3      True      False      False      False      True\n      4      False      True      False      False      True\n      ..     ...    ...    ...    ...    ...    ...    ...\n     886      False      True      False      False      True\n     887      True      False      False      False      True\n     888      True      False      False      False      True\n     889      False      True      True      False      False\n     890      False      True      False      True      False\n\n[891 rows x 12 columns]
```

```
[56]: X = df_xm2[['Pclass=1st', 'Pclass=2nd',           'Pclass=3rd',  
    ↪'Sex=female',           'Sex=male',           'Embarked=C',  
    ↪'Embarked=Q',           'Embarked=S']].values
```

```
[57]: X[:5]
```

```
[57]: array([[False, False,  True,  False,  True,  False,  True],\n            [ True,  False,  False,  True,  False,  True,  False,  False],\n            [False,  False,  True,  True,  False,  False,  True],\n            [ True,  False,  False,  True,  False,  False,  False,  True],\n            [False,  False,  True,  False,  True,  False,  False,  True]])
```

```
[58]: D = pdist(X, 'jaccard')\nD = squareform(D)
```

```
[59]: D
```

```
[59]: array([[0. , 1. , 0.5, ..., 0.5, 0.8, 0.5],
   [1. , 0. , 0.8, ..., 0.8, 0.5, 1. ],
   [0.5, 0.8, 0. , ..., 0. , 1. , 0.8],
   ...,
   [0.5, 0.8, 0. , ..., 0. , 1. , 0.8],
   [0.8, 0.5, 1. , ..., 1. , 0. , 0.8],
   [0.5, 1. , 0.8, ..., 0.8, 0.8, 0. ]])
```

```
[59]: 
```

```
[60]: # Mixed custom distance
```

```
[61]: from scipy.spatial.distance import seuclidean, jaccard
```

```
[ ]: def mixed(a, b):
    index = 4
    d_con = seuclidean(a[:index], b[:index], V=np.ones(index))
    w_con = index/len(a)
    d_cat = jaccard(a[index:], b[index:])
    w_cat = (len(a)-index)/len(a)
    d = w_con * d_con + w_cat * d_cat
    return d
```

```
[ ]: df_xm2.head()
```

```
[ ]:   SibSp  Parch      Fare  AgeFill  Pclass=1st  Pclass=2nd  Pclass=3rd \
0       1      0    7.2500    22.0      False      False      True
1       1      0   71.2833    38.0      True      False      False
2       0      0    7.9250    26.0      False      False      True
3       1      0   53.1000    35.0      True      False      False
4       0      0    8.0500    35.0      False      False      True

      Sex=female  Sex=male Embarked=C Embarked=Q Embarked=S
0      False      True     False     False      True
1      True      False     True     False     False
2      True      False     False     False      True
3      True      False     False     False      True
4      False      True     False     False      True
```

```
[ ]: X = df_xm2.values
```

```
[ ]: X[:5]
```

```
[ ]: array([[1, 0, 7.25, 22.0, False, False, True, False, True, False,
   True],
   [1, 0, 71.2833, 38.0, True, False, False, True, False, True,
```

```
    False, False],
[0, 0, 7.925, 26.0, False, False, True, True, False, False,
 True],
[1, 0, 53.1, 35.0, True, False, False, True, False, False,
 True],
[0, 0, 8.05, 35.0, False, False, True, False, True, False,
 True]], dtype=object)
```

```
[ ]: mixed(X[0], X[10])
```

```
[ ]: 7.118140707983781
```

```
[ ]: D = pdist(X, mixed)
D = squareform(D)
```

```
[ ]: D
```

```
[ ]: array([[ 0.          , 22.66733208,  1.72599765, ... , 5.77688201,
   8.24020256,  3.6874353 ],
 [22.66733208,  0.          , 22.03081168, ... , 17.41288898,
 14.6678715 , 21.94127388],
 [ 1.72599765, 22.03081168,  0.          , ... , 5.43931802,
  8.025       , 2.53418385],
 ...,
 [ 5.77688201, 17.41288898,  5.43931802, ... , 0.          ,
 3.41848425,  6.87315457],
 [ 8.24020256, 14.6678715 ,  8.025       , ... , 3.41848425,
 0.          , 8.21493111],
 [ 3.6874353 , 21.94127388,  2.53418385, ... , 6.87315457,
 8.21493111,  0.        ]])
```

```
[ ]:
```

0.0.6 K-Mode

<https://github.com/nicodv/kmodes>

```
[62]: !pip install kmodes
```

Collecting kmodes

```
  Downloading kmodes-0.12.2-py2.py3-none-any.whl.metadata (8.1 kB)
Requirement already satisfied: numpy>=1.10.4 in /usr/local/lib/python3.12/dist-
packages (from kmodes) (2.0.2)
Requirement already satisfied: scikit-learn>=0.22.0 in
/usr/local/lib/python3.12/dist-packages (from kmodes) (1.6.1)
Requirement already satisfied: scipy>=0.13.3 in /usr/local/lib/python3.12/dist-
packages (from kmodes) (1.16.3)
Requirement already satisfied: joblib>=0.11 in /usr/local/lib/python3.12/dist-
packages (from kmodes) (1.5.2)
```

```
Requirement already satisfied: threadpoolctl>=3.1.0 in
/usr/local/lib/python3.12/dist-packages (from scikit-learn>=0.22.0->kmodes)
(3.6.0)
Downloading kmodes-0.12.2-py2.py3-none-any.whl (20 kB)
Installing collected packages: kmodes
Successfully installed kmodes-0.12.2
```

```
[ ]: from kmodes.kmodes import KModes
[ ]: X = df[['Pclass', 'Sex', 'Embarked']].values
[ ]: X[:5]
[ ]: array([[3, 'male', 'S'],
           [1, 'female', 'C'],
           [3, 'female', 'S'],
           [1, 'female', 'S'],
           [3, 'male', 'S']], dtype=object)
[ ]: km = KModes(n_clusters=4, init='Huang', n_init=5, verbose=0)
      clusters = km.fit_predict(X)
[ ]: km.cluster_centroids_
[ ]: array([('3', 'female', 'S'),
           ('1', 'male', 'C'),
           ('3', 'male', 'S'),
           ('2', 'male', 'S')], dtype='|<U21')
[ ]: km.labels_
[ ]: array([2, 1, 0, 0, 2, 2, 1, 2, 0, 0, 0, 0, 2, 2, 0, 0, 2, 3, 0, 0, 3, 3,
           0, 1, 0, 0, 1, 1, 0, 2, 1, 1, 0, 3, 1, 1, 1, 2, 0, 0, 0, 0, 0, 1, 0,
           0, 2, 2, 0, 1, 0, 2, 2, 1, 0, 1, 1, 0, 1, 0, 2, 1, 0, 1, 2, 1, 1,
           0, 2, 0, 2, 3, 0, 3, 1, 2, 2, 2, 3, 0, 2, 2, 0, 1, 0, 0, 2, 2,
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           2, 1, 0, 2, 2, 2, 0, 2, 2, 2, 0, 0, 1, 2, 1, 2, 0, 2, 1, 2,
           2, 1, 3, 2, 0, 1, 2, 3, 0, 1, 0, 1, 2, 2, 0, 3, 0, 3, 1, 1, 2, 2,
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           2, 3, 2, 2, 1, 2, 3, 2, 0, 0, 2, 3, 0, 3, 0, 3, 0, 3, 3, 0, 0,
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```

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0, 2, 0, 3, 2, 0, 3, 0, 0, 1, 2, 1, 2, 2, 1, 3, 1, 2, 2, 0, 0, 0, 1,
```

[]: