In [1]:

```
import h5py
import numpy as np
import pickle
import random
import plotly.graph_objects as go
import pandas as pd
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt
from sklearn.metrics import silhouette_score, v_measure_score
from sklearn.model_selection import KFold, train_test_split
from sklearn.preprocessing import LabelEncoder

def calculate_percent(sub_df, attrib):
    cnt = sub_df[attrib].count()
    output_sub_df = sub_df.groupby(attrib).count()
    return (output_sub_df / cnt)

# Load Feature Sets
pge_path = 'pge_dim_reduced_feature.h5'
vgg16_path = 'vgg16_dim_reduced_feature.h5'

pge_content = h5py.File(pge_path, mode='r')
vgg16_content = h5py.File(vgg16_path, mode='r')

# PCA feature from 2 feature sets: pge_latent, vgg16_latent
pge_pca_feature = pge_content['pca_feature'][...]
vgg16_pca_feature = vgg16_content['pca_feature'][...]

# UMAP feature from 2 feature sets: pge_latent, vgg16_latent
pge_umap_feature = pge_content['umap_feature'][...]
vgg16_umap_feature = vgg16_content['umap_feature'][...]

# Tissue type as available ground-truth: labels
filename_pge = np.squeeze(pge_content['file_name'])
filename_pge = np.array([str(x) for x in filename_pge])
labels_pge = np.array([x.split('/')[2] for x in filename_pge])

filename_vgg16 = np.squeeze(vgg16_content['file_name'])
filename_vgg16 = np.array([str(x) for x in filename_vgg16])
labels_vgg16 = np.array([x.split('/')[2] for x in filename_vgg16])

random.seed(0)
selected_index_pge = random.sample(list(np.arange(len(pge_pca_feature))), 200)
selected_index_vgg16 = random.sample(list(np.arange(len(vgg16_pca_feature))), 200)

# Selected PCA and UMAP features for PathologyGAN
selected_pca_data_pge = pge_pca_feature[selected_index_pge]
selected_umap_data_pge = pge_umap_feature[selected_index_pge]
selected_labels_pge = labels_pge[selected_index_pge]

# Selected PCA and UMAP features for VGG16
selected_pca_data_vgg16 = vgg16_pca_feature[selected_index_vgg16]
selected_umap_data_vgg16 = vgg16_umap_feature[selected_index_vgg16]
selected_labels_vgg16 = labels_vgg16[selected_index_vgg16]

# K-Means Clustering for PCA Features - PathologyGAN
kmeans_model_pca_pge = KMeans(n_clusters=3, random_state=0)
kmeans_assignment_pca_pge = kmeans_model_pca_pge.fit_predict(selected_pca_data_pge)
kmeans_counts_pca_pge = np.unique(kmeans_assignment_pca_pge, return_counts=True)

# Evaluation Metrics for PCA Features - PathologyGAN
kmeans_silhouette_pca_pge = silhouette_score(selected_pca_data_pge, kmeans_assignme
kmeans_v_measure_pca_pge = v_measure_score(selected_labels_pge, kmeans_assignment_p

# Cluster Analysis for PCA Features - PathologyGAN
resulted_cluster_df_pca_pge = pd.DataFrame({'clusterID': kmeans_assignment_pca_pge,
label_proportion_df_pca_pge = resulted_cluster_df_pca_pge.groupby(['clusterID']).ap
    lambda x: calculate_percent(x, 'type')).rename(
    columns={'clusterID': 'type_occurrence_percentage'}).reset_index()
pivoted_label_proportion_df_pca_pge = pd.pivot_table(label_proportion_df_pca_pge, i
                                                       values='type_occurrence_perce

# K-Means Clustering for UMAP Features - PathologyGAN
kmeans_model_umap_pge = KMeans(n_clusters=3, random_state=0)
kmeans_assignment_umap_pge = kmeans_model_umap_pge.fit_predict(selected_umap_data_p
kmeans_counts_umap_pge = np.unique(kmeans_assignment_umap_pge, return_counts=True)

# Evaluation Metrics for UMAP Features - PathologyGAN
kmeans_silhouette_umap_pge = silhouette_score(selected_umap_data_pge, kmeans_assign
kmeans_v_measure_umap_pge = v_measure_score(selected_labels_pge, kmeans_assignment_

# Cluster Analysis for UMAP Features - PathologyGAN
resulted_cluster_df_umap_pge = pd.DataFrame({'clusterID': kmeans_assignment_umap_pg
label_proportion_df_umap_pge = resulted_cluster_df_umap_pge.groupby(['clusterID']).
    lambda x: calculate_percent(x, 'type')).rename(
    columns={'clusterID': 'type_occurrence_percentage'}).reset_index()
pivoted_label_proportion_df_umap_pge = pd.pivot_table(label_proportion_df_umap_pge,
                                                        values='type_occurrence_perc

# K-Means Clustering for PCA Features - VGG16
kmeans_model_pca_vgg16 = KMeans(n_clusters=3, random_state=0)
kmeans_assignment_pca_vgg16 = kmeans_model_pca_vgg16.fit_predict(selected_pca_data_
kmeans_counts_pca_vgg16 = np.unique(kmeans_assignment_pca_vgg16, return_counts=True

# Evaluation Metrics for PCA Features - VGG16
kmeans_silhouette_pca_vgg16 = silhouette_score(selected_pca_data_vgg16, kmeans_assi
kmeans_v_measure_pca_vgg16 = v_measure_score(selected_labels_vgg16, kmeans_assignme

# Cluster Analysis for PCA Features - VGG16
resulted_cluster_df_pca_vgg16 = pd.DataFrame({'clusterID': kmeans_assignment_pca_vg
label_proportion_df_pca_vgg16 = resulted_cluster_df_pca_vgg16.groupby(['clusterID']
    lambda x: calculate_percent(x, 'type')).rename(
    columns={'clusterID': 'type_occurrence_percentage'}).reset_index()
pivoted_label_proportion_df_pca_vgg16 = pd.pivot_table(label_proportion_df_pca_vgg1
                                                        values='type_occurrence_perc

# K-Means Clustering for UMAP Features - VGG16
kmeans_model_umap_vgg16 = KMeans(n_clusters=3, random_state=0)
kmeans_assignment_umap_vgg16 = kmeans_model_umap_vgg16.fit_predict(selected_umap_da
kmeans_counts_umap_vgg16 = np.unique(kmeans_assignment_umap_vgg16, return_counts=Tr

# Evaluation Metrics for UMAP Features - VGG16
kmeans_silhouette_umap_vgg16 = silhouette_score(selected_umap_data_vgg16, kmeans_as
kmeans_v_measure_umap_vgg16 = v_measure_score(selected_labels_vgg16, kmeans_assignm

# Cluster Analysis for UMAP Features - VGG16
resulted_cluster_df_umap_vgg16 = pd.DataFrame({'clusterID': kmeans_assignment_umap_
label_proportion_df_umap_vgg16 = resulted_cluster_df_umap_vgg16.groupby(['clusterID
    lambda x: calculate_percent(x, 'type')).rename(
    columns={'clusterID': 'type_occurrence_percentage'}).reset_index()
pivoted_label_proportion_df_umap_vgg16 = pd.pivot_table(label_proportion_df_umap_vg
                                                         values='type_occurrence_per

# Plotting Results: Only the first subplot for PCA Features - PathologyGAN
f_pca_pge, axes_pca_pge = plt.subplots(1, 1, figsize=(10, 5))
df_idx_pca_pge = pivoted_label_proportion_df_pca_pge.index
```

```
(pivoted_label_proportion_df_pca_pge * 100).loc[df_idx_pca_pge].plot.bar(stacked=Tr
axes_pca_pge.set_ylabel('Percentage of tissue type')
axes_pca_pge.legend(loc='upper right')
axes_pca_pge.set_title('Cluster configuration by Kmeans for PCA Features - Patholog

plt.show()

# Plotting Results: Only the first subplot for UMAP Features - PathologyGAN
f_umap_pge, axes_umap_pge = plt.subplots(1, 1, figsize=(10, 5))
df_idx_umap_pge = pivoted_label_proportion_df_umap_pge.index
(pivoted_label_proportion_df_umap_pge * 100).loc[df_idx_umap_pge].plot.bar(stacked=
axes_umap_pge.set_ylabel('Percentage of tissue type')
axes_umap_pge.legend(loc='upper right')
axes_umap_pge.set_title('Cluster configuration by Kmeans for UMAP Features - Pathol

plt.show()

# Plotting Results: Only the first subplot for PCA Features - VGG16
f_pca_vgg16, axes_pca_vgg16 = plt.subplots(1, 1, figsize=(10, 5))
df_idx_pca_vgg16 = pivoted_label_proportion_df_pca_vgg16.index
(pivoted_label_proportion_df_pca_vgg16 * 100).loc[df_idx_pca_vgg16].plot.bar(stacke
axes_pca_vgg16.set_ylabel('Percentage of tissue type')
axes_pca_vgg16.legend(loc='upper right')
axes_pca_vgg16.set_title('Cluster configuration by Kmeans for PCA Features - VGG16'

plt.show()

# Plotting Results: Only the first subplot for UMAP Features - VGG16
f_umap_vgg16, axes_umap_vgg16 = plt.subplots(1, 1, figsize=(10, 5))
df_idx_umap_vgg16 = pivoted_label_proportion_df_umap_vgg16.index
(pivoted_label_proportion_df_umap_vgg16 * 100).loc[df_idx_umap_vgg16].plot.bar(stac
axes_umap_vgg16.set_ylabel('Percentage of tissue type')
axes_umap_vgg16.legend(loc='upper right')
axes_umap_vgg16.set_title('Cluster configuration by Kmeans for UMAP Features - VGG1

plt.show()


#To display metrics

# Combine K-Means Assignment Counts for PCA Features
kmeans_assignment_counts_combined = pd.concat([
    pd.DataFrame({'Dataset': ['PathologyGAN']*3, 'Feature Type': ['PCA']*3, 'Cluste
    pd.DataFrame({'Dataset': ['PathologyGAN']*3, 'Feature Type': ['UMAP']*3, 'Clust
    pd.DataFrame({'Dataset': ['VGG16']*3, 'Feature Type': ['PCA']*3, 'Cluster Index
    pd.DataFrame({'Dataset': ['VGG16']*3, 'Feature Type': ['UMAP']*3, 'Cluster Inde
], ignore_index=True)

# Display Combined K-Means Assignment Counts Table
print("\n=== Combined K-Means Assignment Counts ===")
print(kmeans_assignment_counts_combined.set_index(['Dataset', 'Feature Type', 'Clus

# Combine Silhouette and V-Measure Scores
scores_combined = pd.concat([
    pd.DataFrame({'Dataset': ['PathologyGAN']*2, 'Feature Type': ['PCA']*2, 'Metric
    pd.DataFrame({'Dataset': ['PathologyGAN']*2, 'Feature Type': ['UMAP']*2, 'Metri
    pd.DataFrame({'Dataset': ['VGG16']*2, 'Feature Type': ['PCA']*2, 'Metrics': ['S
    pd.DataFrame({'Dataset': ['VGG16']*2, 'Feature Type': ['UMAP']*2, 'Metrics': ['
], ignore_index=True)

# Display Combined Silhouette and V-Measure Scores Table
print("\n=== Combined Silhouette and V-Measure Scores ===")
print(scores_combined.set_index(['Dataset', 'Feature Type', 'Metrics']))
```

```
#Plotting metrics for range of clusters

# Function to calculate silhouette and v-measure scores for a given range of cluste
def calculate_scores_range(data, labels, feature_type, dataset):
    silhouette_scores = []
    v_measure_scores = []

    cluster_range = range(2, 17)  # Change the range if needed

    for num_clusters in cluster_range:
        kmeans_model = KMeans(n_clusters=num_clusters, random_state=0)
        kmeans_assignment = kmeans_model.fit_predict(data)

        silhouette = silhouette_score(data, kmeans_assignment)
        v_measure = v_measure_score(labels, kmeans_assignment)

        silhouette_scores.append(silhouette)
        v_measure_scores.append(v_measure)

    # Find the index of the maximum score for both silhouette and v-measure
    ideal_clusters_silhouette = np.argmax(silhouette_scores) + 2  # Add 2 to accour
    ideal_clusters_v_measure = np.argmax(v_measure_scores) + 2

    # Plot Silhouette and V-Measure Scores
    plt.figure(figsize=(8, 4))
    plt.plot(cluster_range, silhouette_scores, marker='o', label='Silhouette Score'
    plt.plot(cluster_range, v_measure_scores, marker='o', label='V-Measure Score')
    plt.title(f'Silhouette and V-Measure Scores for {feature_type} {dataset}')
    plt.xlabel('Number of Clusters')
    plt.ylabel('Score')
    plt.legend()
    plt.show()

    # Print the ideal number of clusters
    print(f'Ideal number of clusters for {feature_type} {dataset} based on Silhouet
    print(f'Ideal number of clusters for {feature_type} {dataset} based on V-Measur

    return ideal_clusters_silhouette, ideal_clusters_v_measure

# Calculate and plot scores for PCA and UMAP features for both datasets
ideal_clusters_pca_pge = calculate_scores_range(selected_pca_data_pge, selected_lab
ideal_clusters_umap_pge = calculate_scores_range(selected_umap_data_pge, selected_l
ideal_clusters_pca_vgg16 = calculate_scores_range(selected_pca_data_vgg16, selectec
ideal_clusters_umap_vgg16 = calculate_scores_range(selected_umap_data_vgg16, select

# Create a table for ideal clusters
clusters_data = {
    'Dataset': ['PathologyGAN', 'PathologyGAN', 'VGG16', 'VGG16'],
    'Feature Type': ['PCA', 'UMAP', 'PCA', 'UMAP'],
    'Ideal Clusters (Silhouette)': [ideal_clusters_pca_pge[0], ideal_clusters_umap_
    'Ideal Clusters (V-Measure)': [ideal_clusters_pca_pge[1], ideal_clusters_umap_p
}

clusters_table = pd.DataFrame(clusters_data)

# Display the table
print("\n=== Ideal Number of Clusters ===")
print(clusters_table)
```

```
C:\ProgramData\anaconda3\Lib\site-packages\sklearn\cluster\_kmeans.py:1412: Future
Warning: The default value of `n_init` will change from 10 to 'auto' in 1.4. Set t
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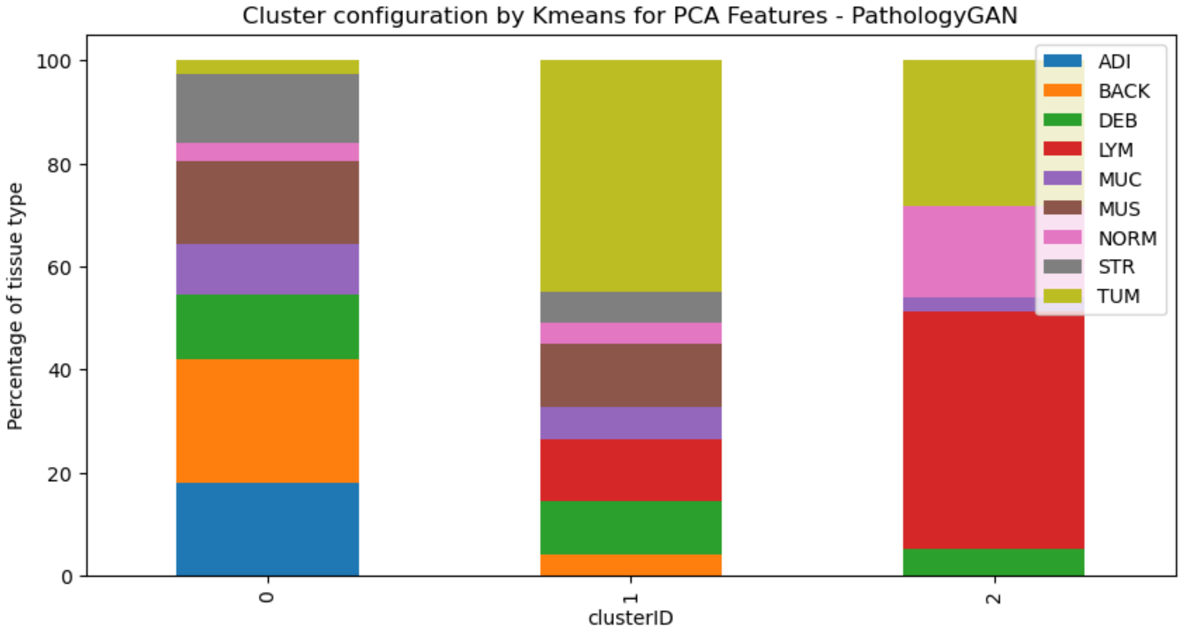
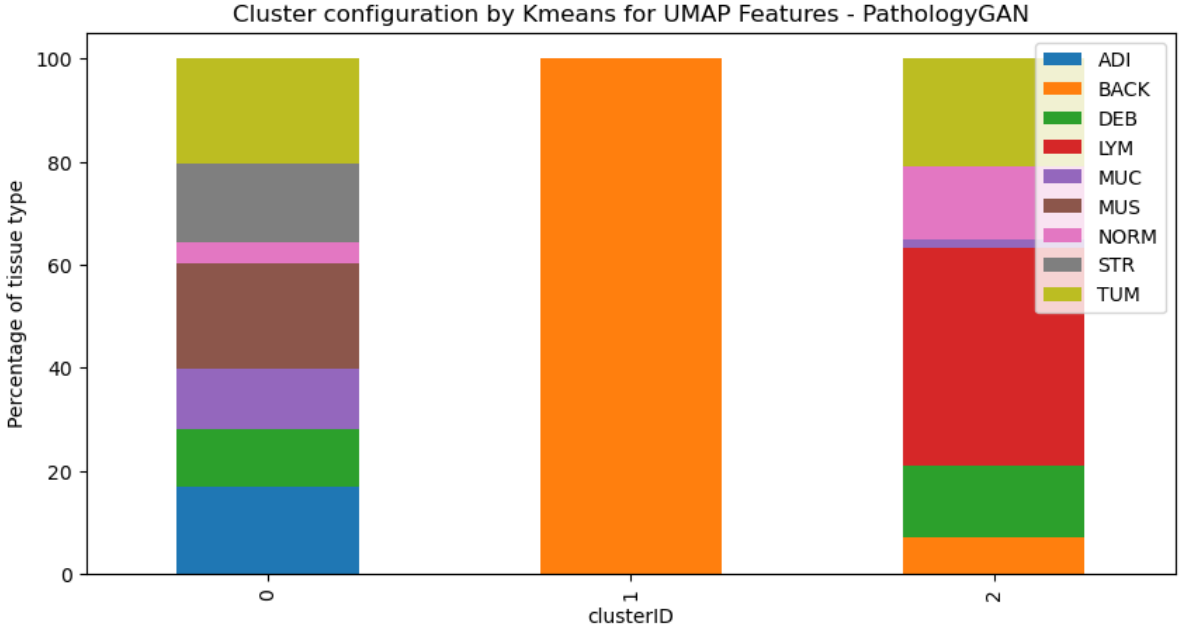
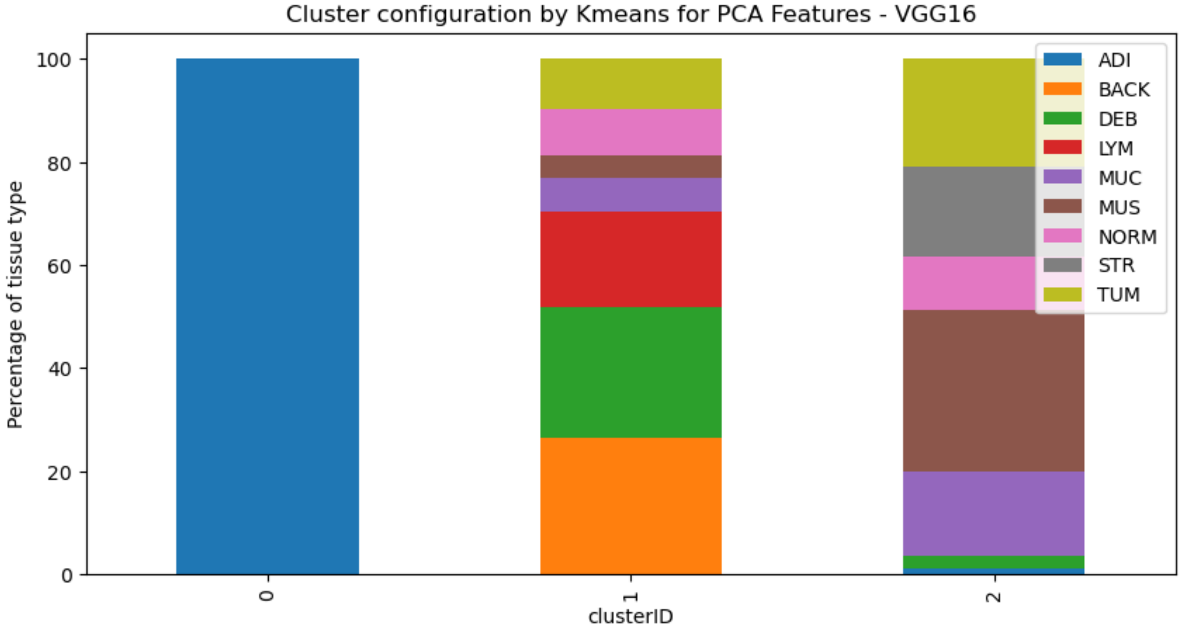
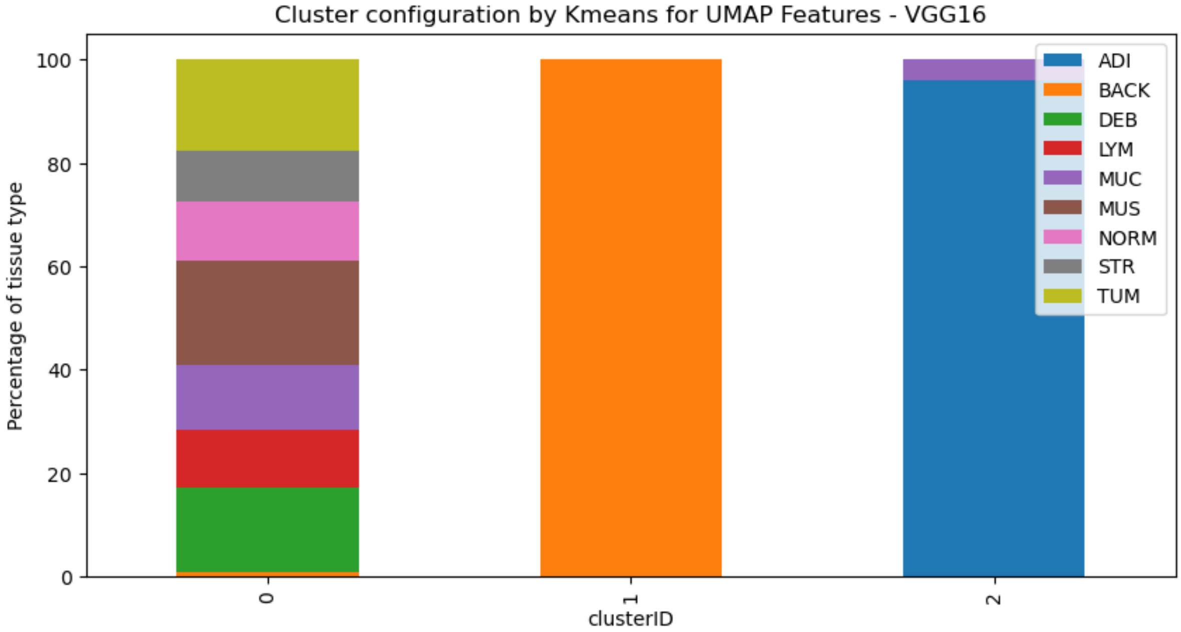



Cluster configuration by Kmeans for UMAP Features - PathologyGAN


Cluster configuration by Kmeans for PCA Features - VGG16


Cluster configuration by Kmeans for UMAP Features - VGG16

```
=== Combined K-Means Assignment Counts ===
                                          Number of members
Dataset      Feature Type Cluster Index
PathologyGAN PCA          0                             112
                          1                              49
                          2                              39
             UMAP         0                             118
                          1                              25
                          2                              57
VGG16        PCA          0                              23
                          1                              91
                          2                              86
             UMAP         0                             152
                          1                              23
                          2                              25

=== Combined Silhouette and V-Measure Scores ===
                                         Scores
Dataset      Feature Type Metrics
PathologyGAN PCA          Silhouette  0.198873
                          V-Measure   0.262987
             UMAP         Silhouette  0.521198
                          V-Measure   0.405433
VGG16        PCA          Silhouette  0.138704
                          V-Measure   0.413101
             UMAP         Silhouette  0.658897
                          V-Measure   0.468403
```

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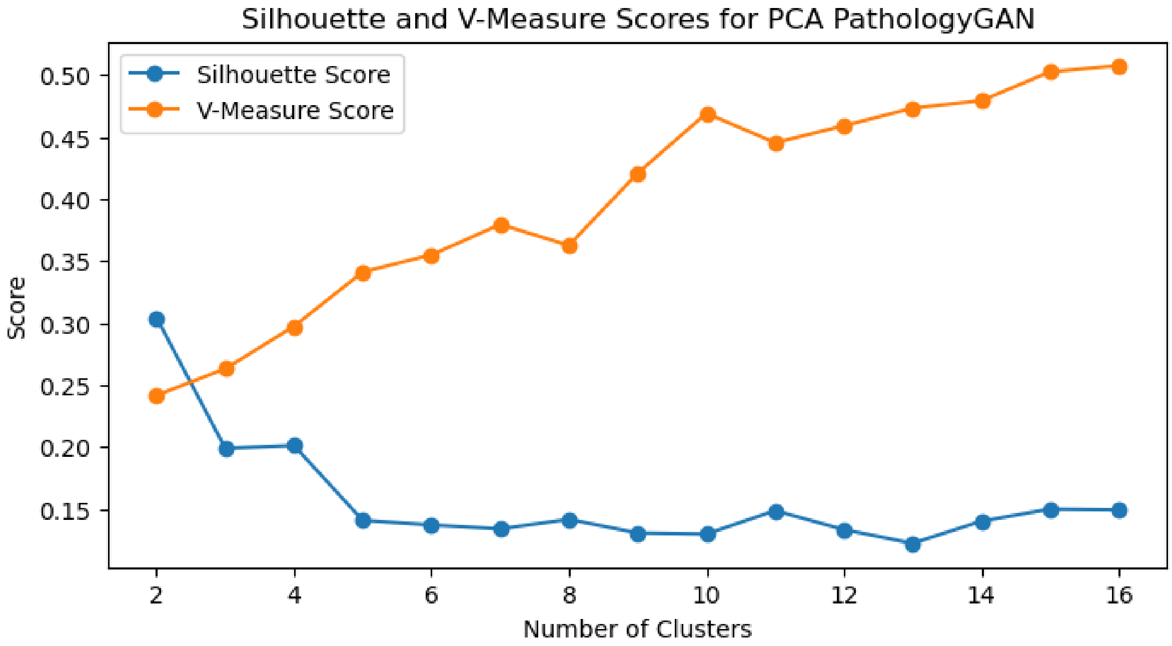

```
Ideal number of clusters for PCA PathologyGAN based on Silhouette Score: 2
Ideal number of clusters for PCA PathologyGAN based on V-Measure Score: 16
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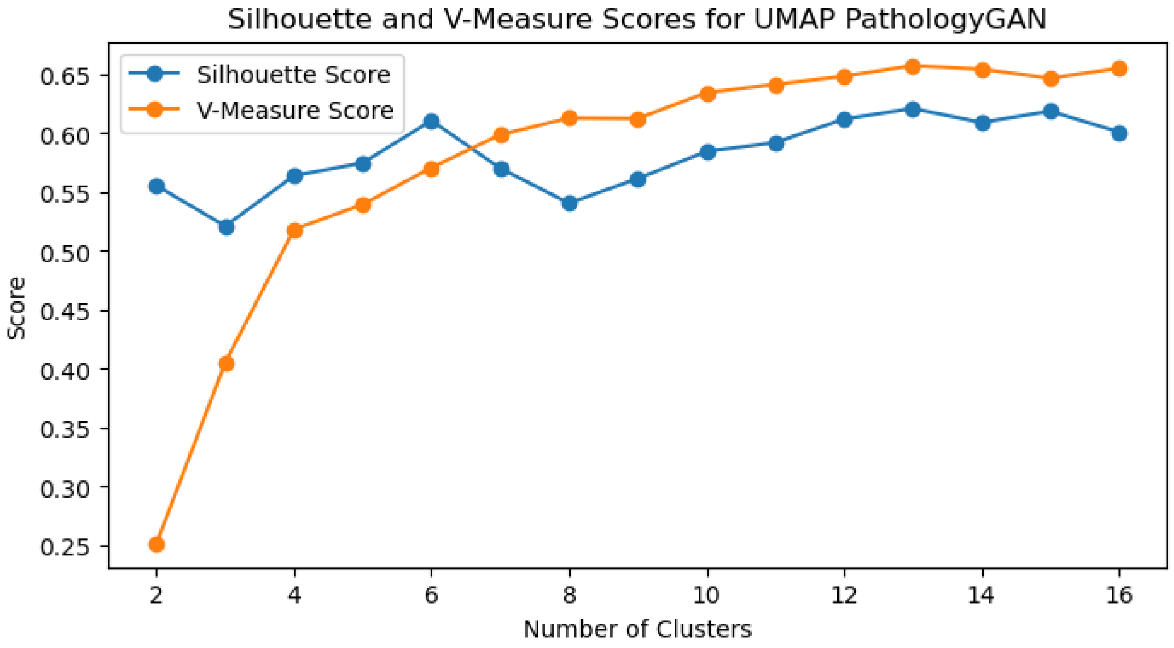

```
Ideal number of clusters for UMAP PathologyGAN based on Silhouette Score: 13
Ideal number of clusters for UMAP PathologyGAN based on V-Measure Score: 13
```

```
C:\ProgramData\anaconda3\Lib\site-packages\sklearn\cluster\_kmeans.py:1412: Future
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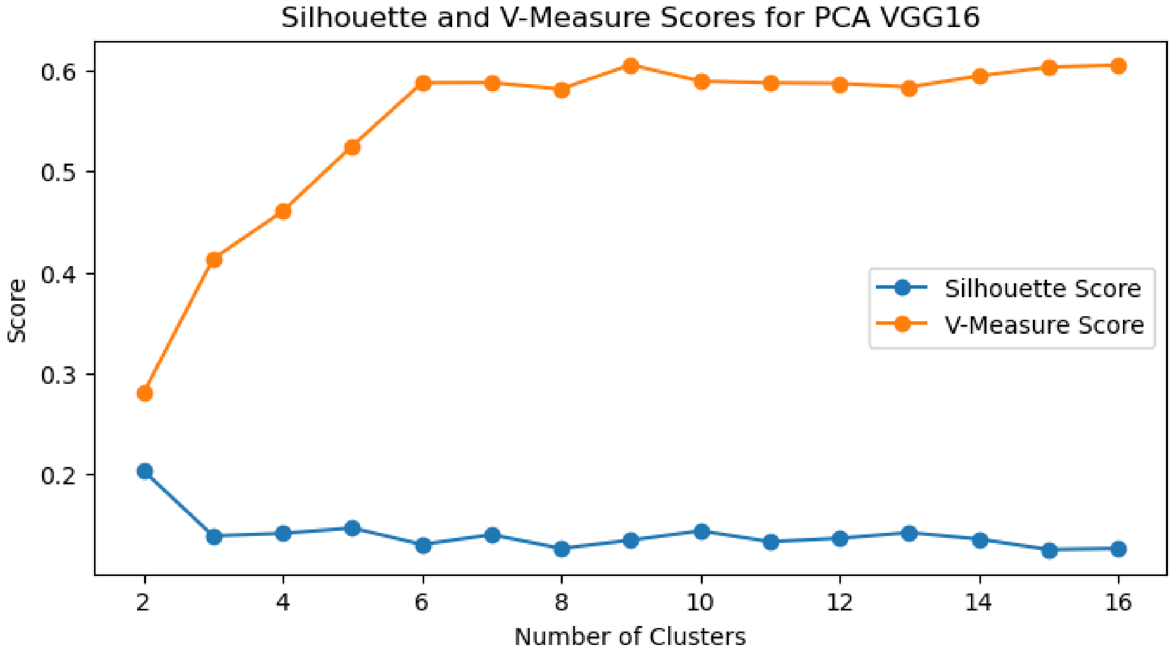

```
Ideal number of clusters for PCA VGG16 based on Silhouette Score: 2
Ideal number of clusters for PCA VGG16 based on V-Measure Score: 9
```

```
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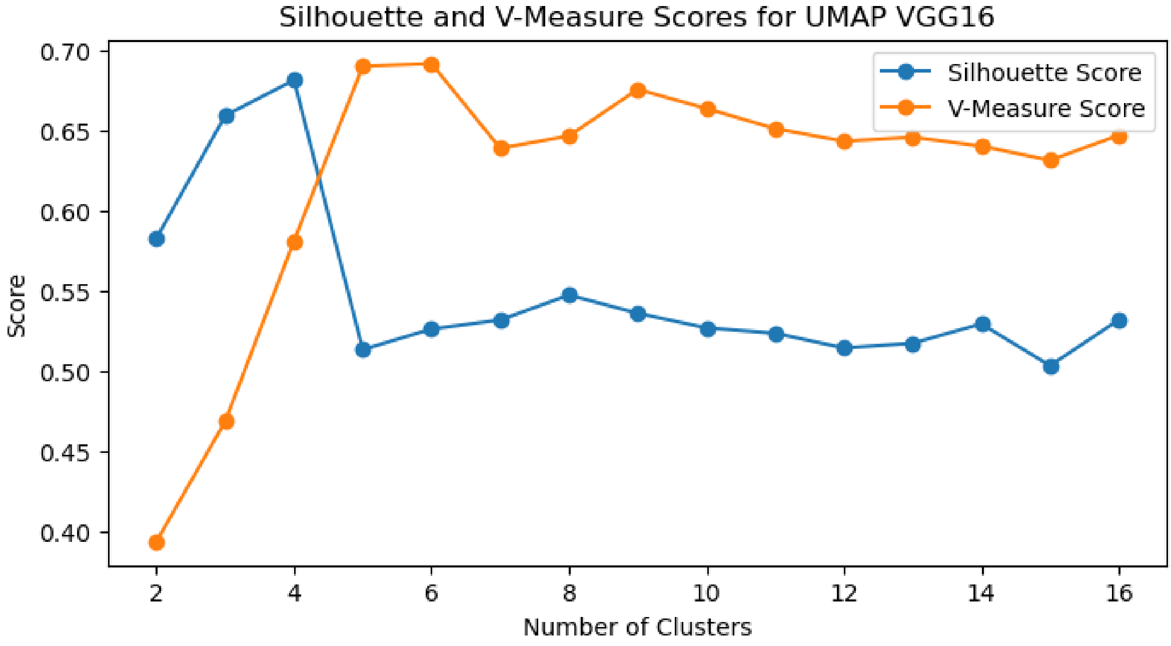

```
Ideal number of clusters for UMAP VGG16 based on Silhouette Score: 4
Ideal number of clusters for UMAP VGG16 based on V-Measure Score: 6

=== Ideal Number of Clusters ===
        Dataset Feature Type  Ideal Clusters (Silhouette)  \
0  PathologyGAN          PCA                            2   
1  PathologyGAN         UMAP                           13   
2         VGG16          PCA                            2   
3         VGG16         UMAP                            4   

   Ideal Clusters (V-Measure)  
0                          16  
1                          13  
2                           9  
3                           6  
```

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In [ ]:
```