Automated Classification of Well Test Responses in Naturally Fractured Reservoirs Using Unsupervised Machine Learning

This notebook aims to follow step-by-step procedure to regenarate the result of a paper entitled Automated Classification of Well Test Responses in Naturally Fractured Reservoirs Using Unsupervised Machine Learning.
The is only for validation part and the final result for synthetic dataset will be in the next report

Import Basic libraries

In [1]:
```
import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns
import scipy
%matplotlib inline
```

In [2]:
```
#ignore warnings in the notebook
import warnings
warnings.filterwarnings("ignore")
```

1.Load data

1.1.Validation Dataset #1

In [3]:
```
FirstPressureDerivativeDataset1= pd.read_excel(r'C:\Users\ekameltarghi\Documents\PH
```

In [4]:
```
pd.DataFrame(FirstPressureDerivativeDataset1.head(5))
```

Out[4]:

	Time (hr)	Dual Porosity	Unnamed: 2	Unnamed: 3	Unnamed: 4	Vertical Fracture	Unnamed: 6	Unnamed: 7	Unnam
0	0.001283	8.850056	8.815821	8.781791	8.723829	2.026622	0.852161	0.432999	0.2182
1	0.001646	8.829196	8.785407	8.741953	8.668075	2.266815	0.959981	0.488866	0.2466
2	0.002111	8.813879	8.757914	8.702499	8.608509	2.537866	1.083465	0.553119	0.2794
3	0.002709	8.790932	8.719484	8.648935	8.529637	2.839838	1.223579	0.626397	0.3168
4	0.003475	8.754042	8.662952	8.573331	8.422370	3.161221	1.376925	0.707202	0.3582

1.2. Validation dataset #2

In [5]:
```
FirstPressureDerivativeDataset2= pd.read_excel(r'C:\Users\ekameltarghi\Documents\PH
```

In [6]:
```
pd.DataFrame(FirstPressureDerivativeDataset2.head(5))
```

Out[6]:

	Time (hr)	Dual Porosity	Unnamed: 2	Unnamed: 3	Unnamed: 4	Vertical Fracture	Unnamed: 6	Unnamed: 7	Unnam
0	0.001283	0.086199	0.577547	2.473335	8.646623	0.037073	0.106668	0.228227	0.432
1	0.001646	0.085264	0.572236	2.446380	8.569692	0.040898	0.119641	0.257178	0.488
2	0.002111	0.084081	0.564209	2.415986	8.483378	0.045065	0.134368	0.290354	0.553
3	0.002709	0.082587	0.555115	2.383544	8.370870	0.049497	0.150899	0.328024	0.626
4	0.003475	0.080712	0.545209	2.336265	8.221545	0.053874	0.168698	0.369293	0.707

In [7]:
```
SecPressureDerivativeDataset2= pd.read_excel(r'C:\Users\ekameltarghi\Documents\PHD
```

In [8]:
```
pd.DataFrame(SecPressureDerivativeDataset2.head(5))
```

Out[8]:

	Time (hr)	Dual Porosity	Unnamed: 2	Unnamed: 3	Unnamed: 4	Vertical Fracture	Unnamed: 6	Unnamed: 7	Unnam
0	0.001283	-0.043768	-0.037086	-0.043989	-0.035877	0.394217	0.460753	0.479434	0.487
1	0.001646	-0.056117	-0.056712	-0.050188	-0.040638	0.389409	0.466037	0.487075	0.495
2	0.002111	-0.071941	-0.065232	-0.054271	-0.053596	0.376592	0.465784	0.489693	0.499
3	0.002709	-0.092210	-0.072279	-0.080428	-0.072258	0.340158	0.447592	0.475717	0.487
4	0.003475	-0.118154	-0.101357	-0.103451	-0.087724	0.304228	0.432637	0.465597	0.478

1.3.DTW matrix from MATLAB

In [9]:
```
DTW_MATLAB= scipy.io.loadmat(r'C:\Users\ekameltarghi\Documents\PHD\scripts\Alfredo
matlabDTW=DTW_MATLAB['dtwForCheck']
```

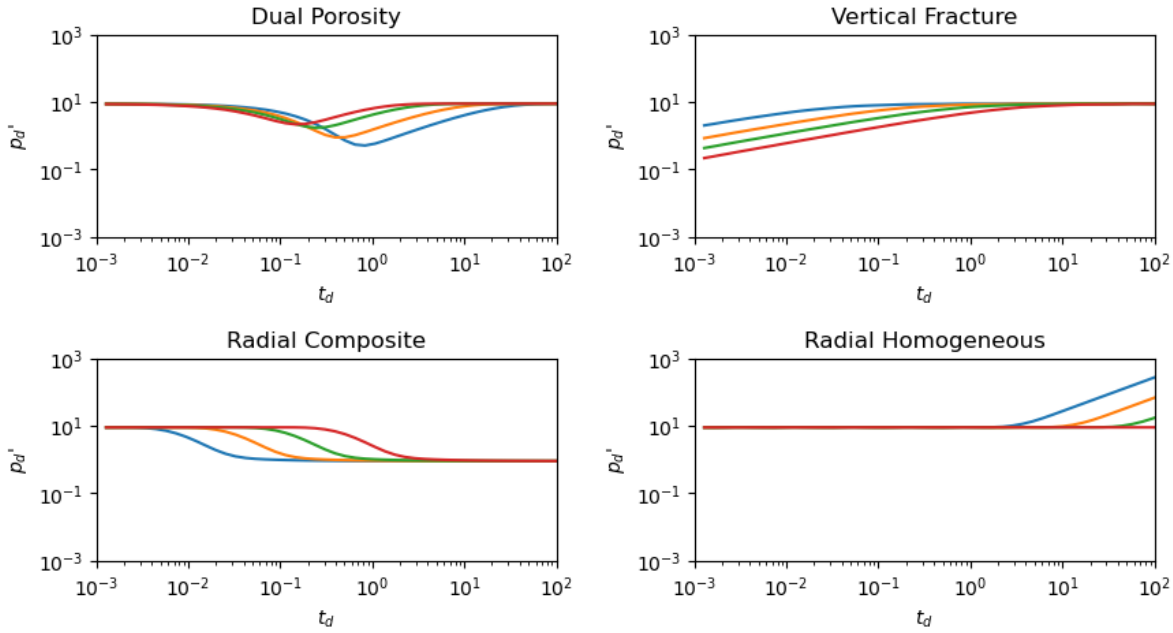
2.DTW, avalable libraries and implementation

PTA data are time-series. so, it is preferable to use dynamic time warping (DTW) instead of Euclidean distance to calculate the similarity or difference between PTA curves. I searched about the best libraries for DTW calculation in python and dtaidistance and fastdtw are the most popular one. but it seems that the implementation in these libraries are different than that of MATLAB. Since all classification algorithm sre completely dependant on goor distance metrics, it is important to make sure we have the same similarity/difference matrix

if we want to replicate the result of the paper:). so in the end of section I provided the function which can exactly replicate the result of DTW calculation in MATLAB.

It should be noted that in this first steps I only used data from validation dataset 1 and the data is visualized as below

In [10]:
```
# Extract the dimensionless pressure data from the DataFrame
pdValuesDataset1 = (FirstPressureDerivativeDataset1.iloc[:, 1:].values).T

# create a subplot for each set
fig, axs = plt.subplots(2, 2, figsize=(10, 5))

# plot each set in seperate figure
for i in range(0,4):
    axs[0,0].plot(FirstPressureDerivativeDataset1.iloc[:, 0],np.where(pdValuesDatas
    axs[0,0].set_title("Dual Porosity")
for i in range(4,8):
    axs[0,1].plot(FirstPressureDerivativeDataset1.iloc[:, 0],np.where(pdValuesDatas
    axs[0,1].set_title("Vertical Fracture")
for i in range(8,12):
    axs[1,0].plot(FirstPressureDerivativeDataset1.iloc[:, 0],np.where(pdValuesDatas
    axs[1,0].set_title("Radial Composite")
for i in range(12,16):
    axs[1,1].plot(FirstPressureDerivativeDataset1.iloc[:, 0],np.where(pdValuesDatas
    axs[1,1].set_title("Radial Homogeneous")

# set x and y limits, scale and lable for all subplots
for i in range(2):
    for j in range(2):
        axs[i, j].set_xscale('log')
        axs[i, j].set_yscale('log')
        axs[i, j].set_xlim(0.001, 100)
        axs[i, j].set_ylim(0.001, 1000)
        axs[i, j].set_xlabel("$t_{d}$")
        axs[i, j].set_ylabel("$p_{d}$'")

#set vertical spacing between plots
fig.subplots_adjust(hspace=0.6, wspace=0.3)

# Show the plot
plt.show()
```



2.1.dtaidistance library

In [11]:
```
#pip install dtaidistance
```

In [12]:
```
from dtaidistance import dtw
# Extract the dimensionless pressure data from the DataFrame
X_sample_1 = (FirstPressureDerivativeDataset1.iloc[:, 1:].values).T

# Compute the DTW distance between each pair of curves
n_samples = X_sample_1.shape[0]

DTW_FirstDerivativeDataset1_dtaidistance = np.zeros((n_samples, n_samples))
DTW_FirstDerivativeDataset1_dtaidistance_log = np.zeros((n_samples, n_samples))
for i in range(n_samples):
    for j in range(n_samples):
        a=X_sample_1[i]
        b=X_sample_1[j]
        #DTW_FirstDerivativeDataset1_dtaidistance[i, j] = dtw.distance(a[a!=0], b[
        DTW_FirstDerivativeDataset1_dtaidistance_log[i, j] = dtw.distance(np.log10
```

2.2.fastDTW

In [13]:
```
#pip install fastdtw
```

In [14]:
```
from fastdtw import fastdtw
# Extract the dimensionless pressure data from the DataFrame
X_sample_1 = (FirstPressureDerivativeDataset1.iloc[:, 1:].values).T

# Compute the DTW distance between each pair of curves
n_samples = X_sample_1.shape[0]

DTW_FirstDerivativeDataset1_fastDTW = np.zeros((n_samples, n_samples))
DTW_FirstDerivativeDataset1_fastDTW_log = np.zeros((n_samples, n_samples))
for i in range(n_samples):
    for j in range(n_samples):
        a=X_sample_1[i]
        b=X_sample_1[j]
```

```
        #DTW_FirstDerivativeDataset1_fastDTW [i, j], _  = fastdtw(a[a!=0], b[b!=0],
        DTW_FirstDerivativeDataset1_fastDTW_log [i, j], _  = fastdtw(np.log10(a[a!=
```

2.3.implementation of MATLAB function for DTW

As it is stated in MathWorks website, the implemetation of DTW in MATLAB is based on this wikiedia webpage

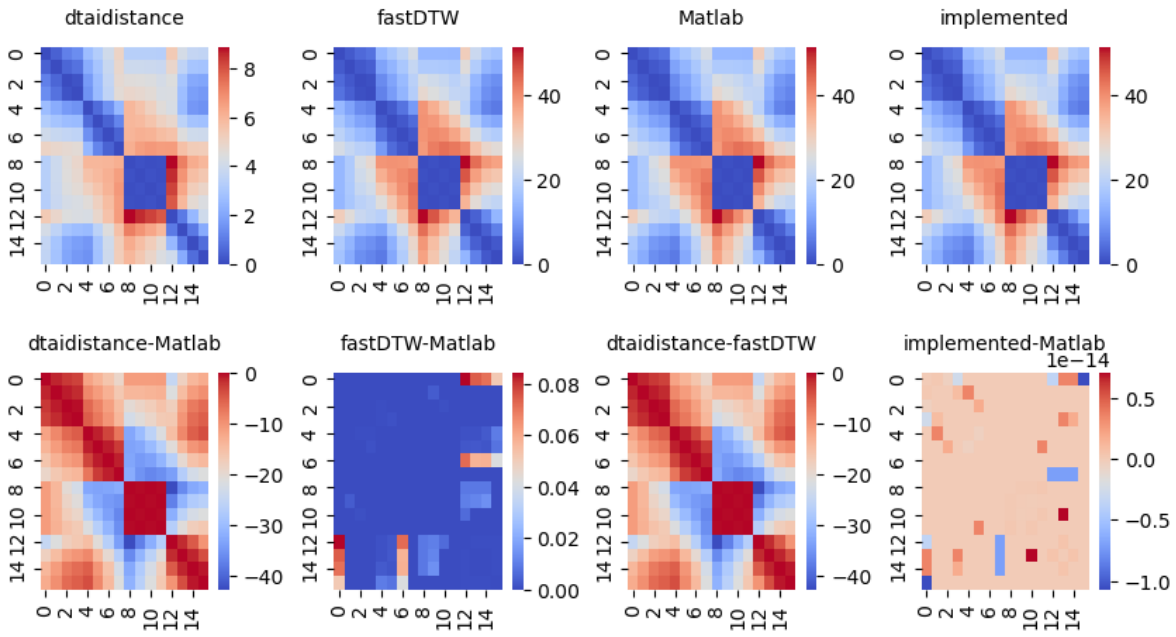
In [15]:
```
def DTWDistance_without_window(x, y):
    n, m = len(x), len(y)
    DTW = np.zeros((n+1, m+1))
    DTW[1:, 0] = np.inf
    DTW[0, 1:] = np.inf

    for i in range(1, n+1):
        for j in range(1, m+1):
            cost = abs(x[i-1] - y[j-1])
            DTW[i, j] = cost + min(DTW[i-1, j],    # insertion
                                   DTW[i, j-1],    # deletion
                                   DTW[i-1, j-1])  # match
    return DTW[n, m]
```

In [16]:
```
def DTWDistance_with_window(x, t, w):
    n = len(x)
    m = len(y)

    w = max(w, abs(n-m))

    DTW = np.full((n+1, m+1), np.inf)
    DTW[0, 0] = 0

    for i in range(1, n+1):
        for j in range(max(1, i-w), min(m+1, i+w)):
            DTW[i, j] = 0

    for i in range(1, n+1):
        for j in range(max(1, i-w), min(m+1, i+w)):
            cost = abs(x[i-1] - y[j-1])
            DTW[i, j] = cost + min(DTW[i-1, j], DTW[i, j-1], DTW[i-1, j-1])

    return DTW[n, m]
```

In [17]:
```
# Extract the dimensionless pressure data from the DataFrame
X_sample_1 = (FirstPressureDerivativeDataset1.iloc[:, 1:].values).T

# Compute the DTW distance between each pair of curves
n_samples = X_sample_1.shape[0]

DTW_FirstDerivativeDataset1_implemented = np.zeros((n_samples, n_samples))
DTW_FirstDerivativeDataset1_implemented_log = np.zeros((n_samples, n_samples))
for i in range(n_samples):
    for j in range(n_samples):
        a=X_sample_1[i]
        b=X_sample_1[j]
        #DTW_FirstDerivativeDataset1_implemented[i, j] = DTWDistance_without_windo
        DTW_FirstDerivativeDataset1_implemented_log[i, j] = DTWDistance_without_wi
```

2.4.plot and compare

In [18]:
```
# create two subplots for the heatmaps
fig, ((ax11, ax12,ax13, ax14), (ax21, ax22, ax23, ax24)) = plt.subplots(ncols=4, n


sns.heatmap(DTW_FirstDerivativeDataset1_dtaidistance_log, cmap='coolwarm', ax=ax11
ax11.set_title('dtaidistance', y=1.05,  fontsize=10)

sns.heatmap(DTW_FirstDerivativeDataset1_fastDTW_log, cmap='coolwarm', ax=ax12)
ax12.set_title('fastDTW', y=1.05,  fontsize=10)

sns.heatmap(matlabDTW, cmap='coolwarm', ax=ax13)
ax13.set_title('Matlab', y=1.05,  fontsize=10)

sns.heatmap(DTW_FirstDerivativeDataset1_implemented_log, cmap='coolwarm', ax=ax14)
ax14.set_title('implemented', y=1.05,  fontsize=10)
####
sns.heatmap(DTW_FirstDerivativeDataset1_dtaidistance_log-matlabDTW, cmap='coolwarm
ax21.set_title('dtaidistance-Matlab', y=1.05,  fontsize=10)

sns.heatmap(DTW_FirstDerivativeDataset1_fastDTW_log-matlabDTW, cmap='coolwarm', ax=
ax22.set_title('fastDTW-Matlab', y=1.05,  fontsize=10)

sns.heatmap(DTW_FirstDerivativeDataset1_dtaidistance_log-DTW_FirstDerivativeDataset
ax23.set_title('dtaidistance-fastDTW', y=1.05,  fontsize=10)

sns.heatmap(DTW_FirstDerivativeDataset1_implemented_log-matlabDTW, cmap='coolwarm'
ax24.set_title('implemented-Matlab', y=1.05,  fontsize=10)

# adjust spacing between subplots
plt.subplots_adjust(wspace=0.4,hspace=0.5)
# display the plot
plt.show()
```



So the implemented version has less than 10E-13 difference with the result of MATLAB and we use this metrics for the rest of this notebook

3.clustering algorithms

The next step is to choose the best implementation of K-medoid. So, I choose 2 number of clusters and checked if the algorithm is capable to produce promising result

3.1.k-medoid clustering algorithm from sckit-learn

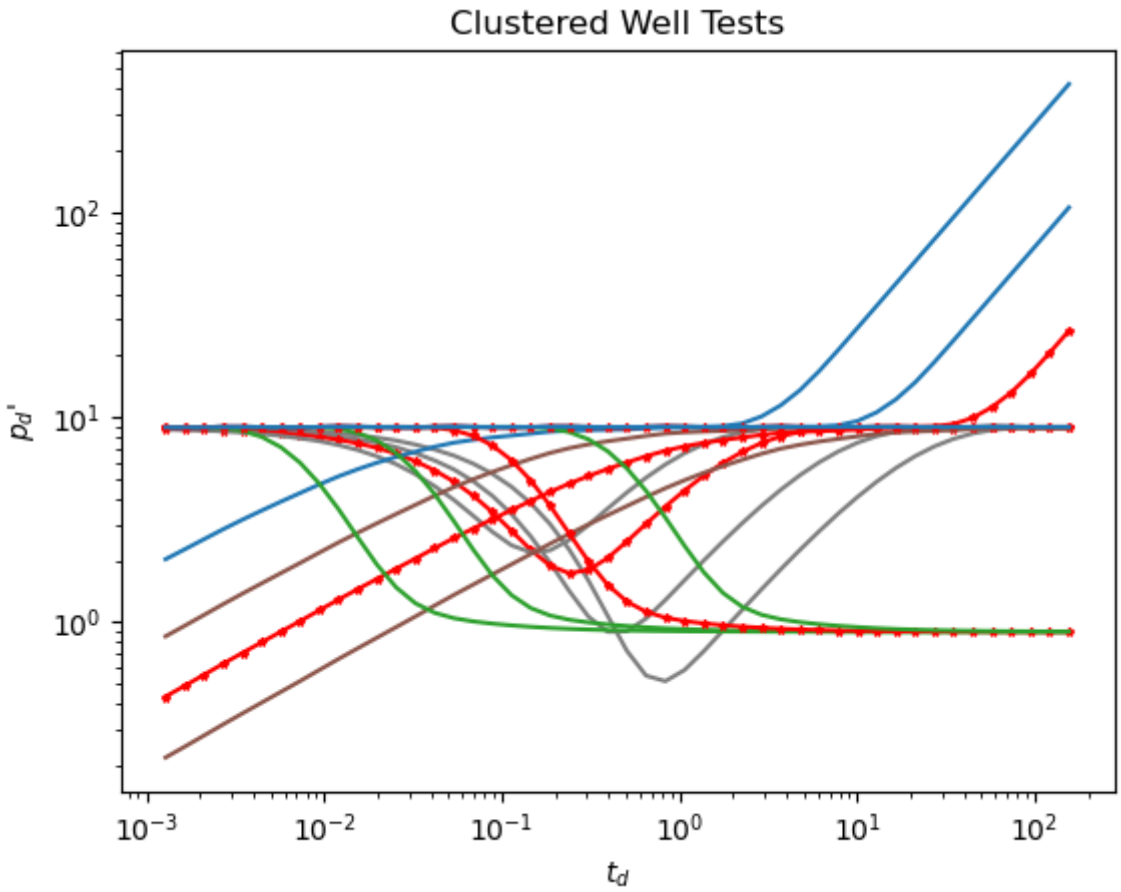
In [19]:
```
from sklearn_extra.cluster import KMedoids
```

In [20]:
```
# Use k-medoids to cluster the well tests
n_clusters=4
max_iter=5
num_initialization=10
best_inertia = float('inf')  # initialize a large value for best inertia
best_kmedoids = None
for i in range(num_initialization):  # number of initializations
    kmedoids = KMedoids(n_clusters, max_iter=max_iter, init='random')
    kmedoids.fit(DTW_FirstDerivativeDataset1_implemented_log)
    if kmedoids.inertia_ < best_inertia:
        best_inertia = kmedoids.inertia_
        best_kmedoids = kmedoids
cluster_assignments_dataset1 = best_kmedoids.labels_
medoids_index_dataset1 = best_kmedoids.medoid_indices_
```

3.1.1 plotting the result

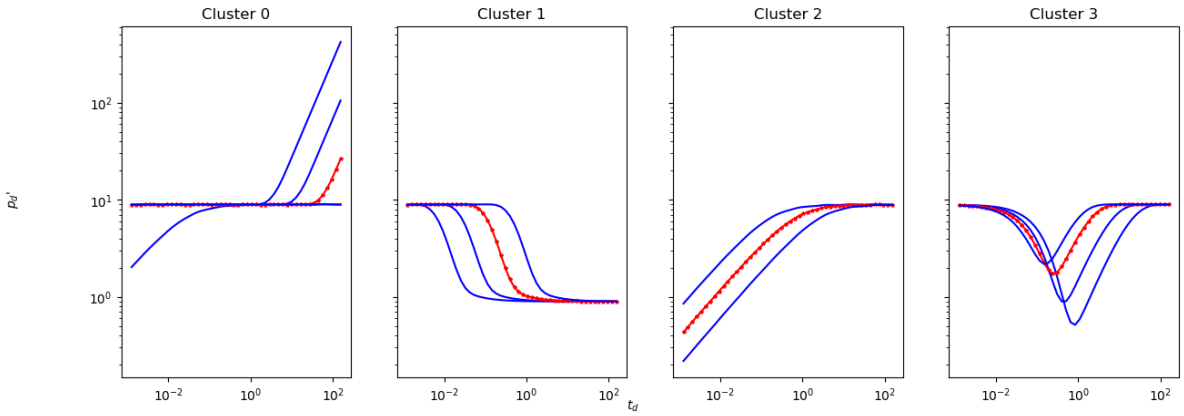
the graph below shows the all curves together which have different color with respect to their cluster medoid

In [21]:
```
# Plot each curve
for i in range(n_samples):
    if i in medoids_index_dataset1 :
        plt.plot(FirstPressureDerivativeDataset1.iloc[:, 0],np.where(X_sample_1[i]
    else:
        plt.plot(FirstPressureDerivativeDataset1.iloc[:, 0],np.where(X_sample_1[i]

# Add a title and labels to the plot
plt.title("Clustered Well Tests")
plt.xlabel("$t_{d}$")
plt.ylabel("$p_{d}$'")
plt.xscale('log')
plt.yscale('log')
# Show the plot
plt.show()
```



Also, we plotted the figures seperated by their clusters

In [22]:
```
unique_clusters = np.unique(cluster_assignments_dataset1)
# create a subplot for each cluster
fig, axs = plt.subplots(1, n_clusters, figsize=(15, 5), sharey=True)

for i, cluster in enumerate(unique_clusters):
    # plot the curves for this cluster
    for j in range(n_samples):
        if cluster_assignments_dataset1[j] == cluster:
            if j in medoids_index_dataset1 :
                axs[i].plot(FirstPressureDerivativeDataset1.iloc[:, 0], np.where(X
            else:
                axs[i].plot(FirstPressureDerivativeDataset1.iloc[:, 0], np.where(X

    axs[i].set_title(f"Cluster {cluster}")
    axs[i].set_xscale('log')
    axs[i].set_yscale('log')

# Add labels to the plot
fig.text(0.5, 0.04, "$t_{d}$", ha='center')
fig.text(0.04, 0.5, "$p_{d}$'", va='center', rotation='vertical')

# Show the plot
plt.show()
```



Since here the only important thing is the performace of grouping(and the lable of the groups does not carry meaningful explanation) we should use Adjusted Rand index. The ARI is a measure of the similarity between two label assignments, adjusted for chance. It takes values between -1 and 1, where values close to 1 indicate that the clustering results are very similar to the actual labels, and values close to -1 indicate that the clustering results are very different from the actual labels.

In [23]:
```
from sklearn.metrics import adjusted_rand_score
```

In [24]:
```
DataframePdDataset1 = pd.DataFrame((FirstPressureDerivativeDataset1.iloc[:, 1:].va
lables=[0,0,0,0,1,1,1,1,2,2,2,2,3,3,3,3]
DataframePdDataset1['lables']=lables
DataframePdDataset1['cluster_assignments']=cluster_assignments_dataset1
ari = adjusted_rand_score(DataframePdDataset1['lables'], DataframePdDataset1['clus
print("Adjusted Rand index: ", ari)
```

```
Adjusted Rand index:  0.8205128205128205
```

After Running the algorithm multiple times, I realized that sometimes it might assign one curve to a wrong cluster (82<ARI=<100).

3.2.Implementation of MATLAB code for clustering

here is the implemented version of MATLAB code for K-medioid clustering which was prvided by authors. It should be noted that I didn't covert this into a function because if we want to do plotting we should update some lines of the code for that

In [25]:
```
# remove rows with zero values
firstDerivativePressure_log = FirstPressureDerivativeDataset1[~(FirstPressureDeriva

# remove rows with NaN values
firstDerivativePressure_log = firstDerivativePressure_log.dropna()
firstDerivativePressure_log= np.log10(firstDerivativePressure_log[firstDerivativeP

K=[4]
#K = [2,4,6,8]  # This script allows to run tests for different number of clusters

# Maximum Number of Iterations
maxIter = 5
# Maximum Number of Initializations
maxInitializations = 10

totalDistanceperClusteringAllClusters = np.zeros((len(K), maxIter))
totalMinimumAssignperClusteringAllClusters = np.zeros((len(K), len(firstDerivativeP
```

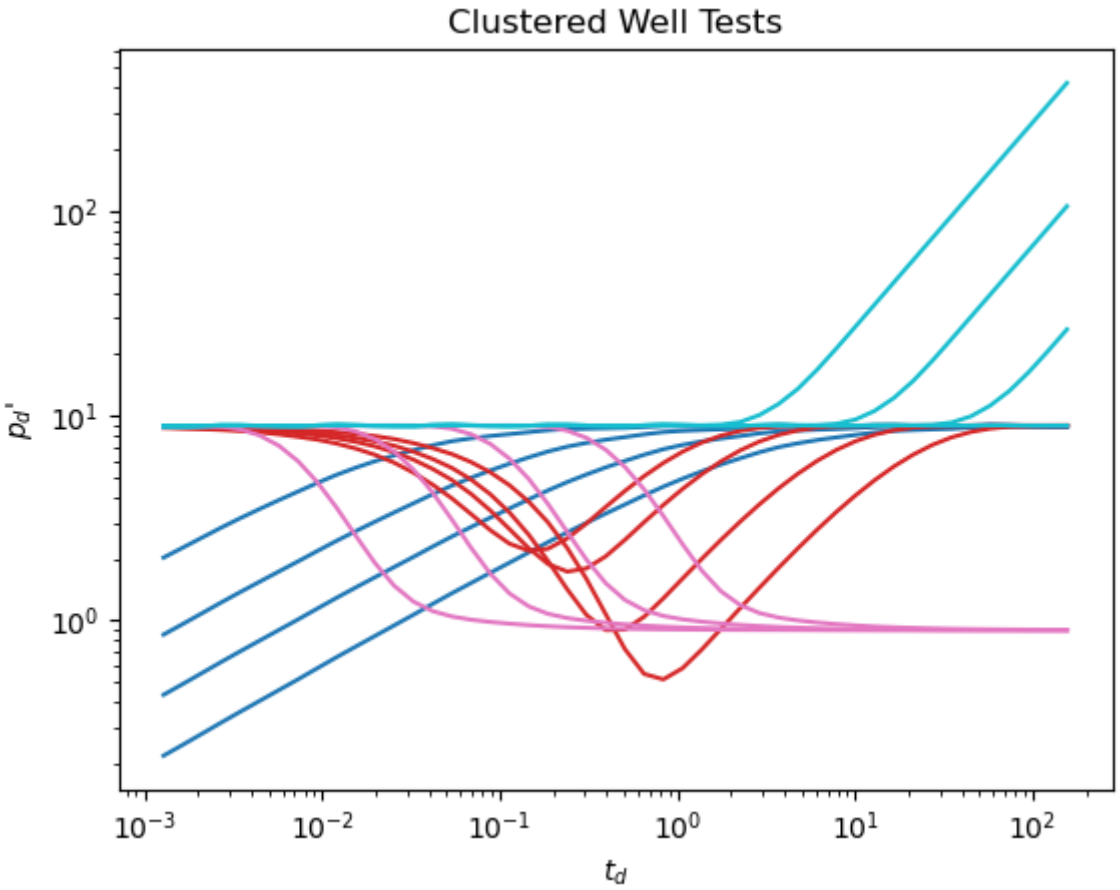
```
distanceMultInitAllClusters= np.zeros((maxInitializations*maxIter, maxIter))
assignMultInitAllClusters= np.zeros((maxInitializations*maxIter,firstDerivativePres
totalMinimumDistanceperClusteringAllClusters=np.zeros((len(K), maxIter))
totalMinimumAssignperClusteringAllClusters=np.zeros((len(K), firstDerivativePressu
for clusters in range(len(K)):
    distanceMultInit= np.zeros((maxInitializations,maxIter))
    assignMultInit= np.zeros((maxInitializations,firstDerivativePressure_log.shape
    for multipleInit in range(maxInitializations):

        # Initialize the centroids to be random samples
        # Randomly reorder the indices of examples
        randidx = np.random.permutation(firstDerivativePressure_log.shape[0])
        # Take the first K examples as centroids
        centroids = firstDerivativePressure_log[randidx[:K[clusters]], :]

        # Cluster Assignment Step
        totalDistance = np.zeros((maxIter,))
        assign = np.zeros((len(firstDerivativePressure_log),))

        for i in range(len(firstDerivativePressure_log)):
            distance = np.zeros((K[clusters],))
            for j in range(K[clusters]):
                a = firstDerivativePressure_log[i, :]
                b = centroids[j, :]
                distance[j]=DTWDistance_without_window(a,b)
            M, assign[i] = distance.min(), distance.argmin()
            # accumulative
            totalDistance[0] += M # measures the total distance from every point t

        for iter in range(1, maxIter):
            # Averaging (point that minimizes the distance to the members of the c
            for n in range(K[clusters]):
                assignTemp = (assign==n)
                clusterMatrix = firstDerivativePressure_log[assignTemp, :]
                intraClusterDist = np.zeros((clusterMatrix.shape[0],))
                for i in range(clusterMatrix.shape[0]):
                    a = clusterMatrix[i, :]
                    tempDist = 0
                    for j in range(clusterMatrix.shape[0]):
                        b = clusterMatrix[j, :]
                        tempDist += DTWDistance_without_window(a, b)
                        intraClusterDist[i] = tempDist
                _, newCentroidRow = intraClusterDist.min(), intraClusterDist.argmi
                centroids[n, :] = clusterMatrix[newCentroidRow, :]


            # Reassigning points to updated centroids
            totalDistance[iter] = 0
            for i in range(len(firstDerivativePressure_log)):
                distance = np.zeros((K[clusters],))
                for j in range(K[clusters]):
                    a = firstDerivativePressure_log[i, :]
                    b = centroids[j, :]
                    distance[j] = DTWDistance_without_window(a, b)
                MMM, assign[i] = distance.min(), distance.argmin()
                totalDistance[iter] += MMM # measures the total distance from every
        distanceMultInit[multipleInit, :] = totalDistance # summarizes the total d
        assignMultInit[multipleInit, :] = assign

        totalDistMinimumColumn = distanceMultInit[:,maxIter-1]
        B = np.argmin(totalDistMinimumColumn)
        totalMinimumDistanceperClustering = distanceMultInit[B,:]
        totalMinimumAssignperClustering = assignMultInit[B,:]
```

```
    distanceMultInitAllClusters[((clusters)*multipleInit):((clusters)*multipleInit
    assignMultInitAllClusters[((clusters)*multipleInit):((clusters)*multipleInit)+

    totalMinimumDistanceperClusteringAllClusters[clusters,:] = totalMinimumDistanc
    totalMinimumAssignperClusteringAllClusters[clusters,:] = totalMinimumAssignper
```

3.2.1 plotting the result

the graph below shows the all curves together which have different color with respect to their category

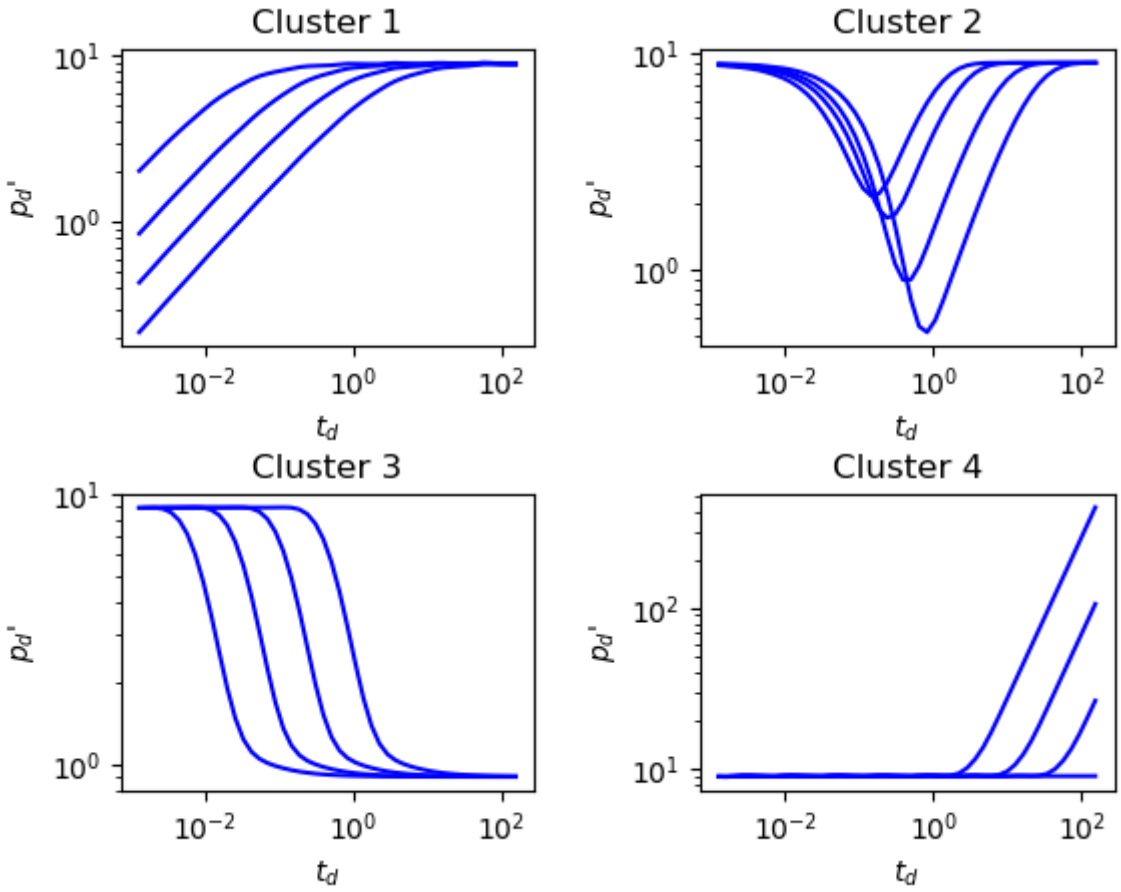
In [26]:
```
# Define color map for clusters
colorMap = plt.cm.tab10(np.linspace(0,1,4))
# Plot curves and add legend
for i in range(4):
    clusterIndices = np.where(totalMinimumAssignperClusteringAllClusters[clusters]
    for j in clusterIndices:
        plt.loglog(FirstPressureDerivativeDataset1[~(FirstPressureDerivativeDataset
# Add a title and labels to the plot
plt.title("Clustered Well Tests")
plt.xlabel("$t_{d}$")
plt.ylabel("$p_{d}$'")
plt.xscale('log')
plt.yscale('log')
```



And this code plots curves which blong to each cluster seperatly

In [27]:
```
#Create subplots for each cluster
for i in range(4):
    plt.subplot(2, 2, i+1)
    clusterIndices = np.where(totalMinimumAssignperClusteringAllClusters[clusters]
    for j in clusterIndices:
```

```
        # Create log-log plot
        plt.loglog(FirstPressureDerivativeDataset1[~(FirstPressureDerivativeDataset
    # Add labels and title
    plt.xlabel("$t_{d}$")
    plt.ylabel("$p_{d}$'")
    plt.title('Cluster ' + str(i+1))
# adjust spacing between subplots
plt.subplots_adjust(wspace=0.4,hspace=0.5)
plt.show()
```



In [28]:
```
DataframePdDataset1 = pd.DataFrame((FirstPressureDerivativeDataset1.iloc[:, 1:].va
lables=[0,0,0,0,1,1,1,1,2,2,2,2,3,3,3,3]
DataframePdDataset1['lables']=lables
DataframePdDataset1['cluster_assignments']=totalMinimumAssignperClusteringAllCluste
ari = adjusted_rand_score(DataframePdDataset1['lables'], DataframePdDataset1['clus
print("Adjusted Rand index: ", ari)
```

```
Adjusted Rand index:  1.0
```

I ran the implemented version multiple time and it gave me ARI=1 in allinstances so I will use this for the rest of the code

4. Replication of the result fot validation

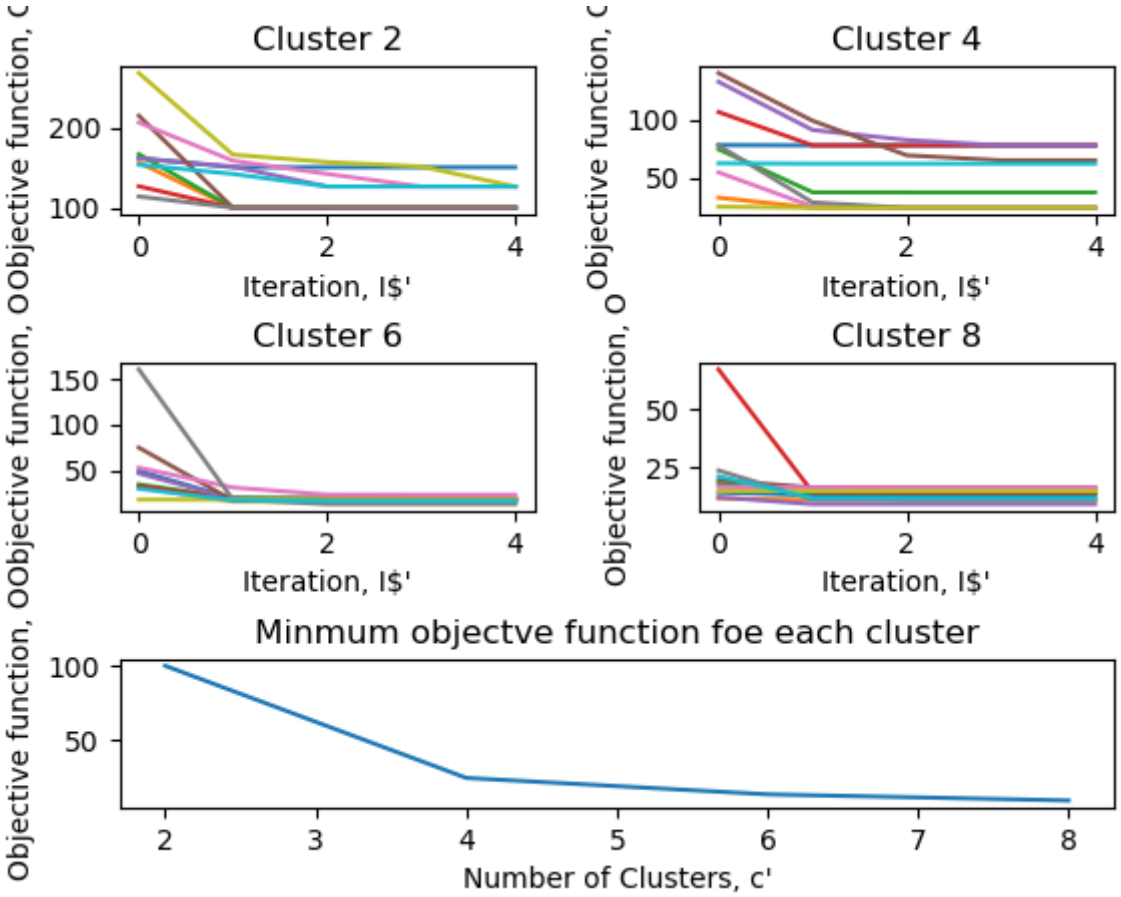
4.1. Dataset number 1

4.1.1. Fig 9.

In [50]:

```
# remove rows with zero values
firstDerivativePressure_log = FirstPressureDerivativeDataset1[~(FirstPressureDeriva

# remove rows with NaN values
firstDerivativePressure_log = firstDerivativePressure_log.dropna()
firstDerivativePressure_log= np.log10(firstDerivativePressure_log[firstDerivativePr

#K=[2,4]
K = [2,4,6,8]  # This script allows to run tests for different number of clusters

# Maximum Number of Iterations
maxIter = 5
# Maximum Number of Initializations
maxInitializations = 10

totalDistanceperClusteringAllClusters = np.zeros((len(K), maxIter))
totalMinimumAssignperClusteringAllClusters = np.zeros((len(K), len(firstDerivativeP
distanceMultInitAllClusters= np.zeros((maxInitializations*maxIter, maxIter))
assignMultInitAllClusters= np.zeros((maxInitializations*maxIter,firstDerivativePres
totalMinimumDistanceperClusteringAllClusters=np.zeros((len(K), maxIter))
totalMinimumAssignperClusteringAllClusters=np.zeros((len(K), firstDerivativePressur
for clusters in range(len(K)):
    distanceMultInit= np.zeros((maxInitializations,maxIter))
    assignMultInit= np.zeros((maxInitializations,firstDerivativePressure_log.shape
    for multipleInit in range(maxInitializations):

        # Initialize the centroids to be random samples
        # Randomly reorder the indices of examples
        randidx = np.random.permutation(firstDerivativePressure_log.shape[0])
        # Take the first K examples as centroids
        centroids = firstDerivativePressure_log[randidx[:K[clusters]], :]

        # Cluster Assignment Step
        totalDistance = np.zeros((maxIter,))
        assign = np.zeros((len(firstDerivativePressure_log),))

        for i in range(len(firstDerivativePressure_log)):
            distance = np.zeros((K[clusters],))
            for j in range(K[clusters]):
                a = firstDerivativePressure_log[i, :]
                b = centroids[j, :]
                distance[j]=DTWDistance_without_window(a,b)
            M, assign[i] = distance.min(), distance.argmin()
            # accumulative
            totalDistance[0] += M # measures the total distance from every point to

        for iter in range(1, maxIter):
            # Averaging (point that minimizes the distance to the members of the cl
            for n in range(K[clusters]):
                assignTemp = (assign==n)
                clusterMatrix = firstDerivativePressure_log[assignTemp, :]
                intraClusterDist = np.zeros((clusterMatrix.shape[0],))
                for i in range(clusterMatrix.shape[0]):
                    a = clusterMatrix[i, :]
                    tempDist = 0
                    for j in range(clusterMatrix.shape[0]):
                        b = clusterMatrix[j, :]
                        tempDist += DTWDistance_without_window(a, b)
                        intraClusterDist[i] = tempDist
                _, newCentroidRow = intraClusterDist.min(), intraClusterDist.argmi
                centroids[n, :] = clusterMatrix[newCentroidRow, :]
```

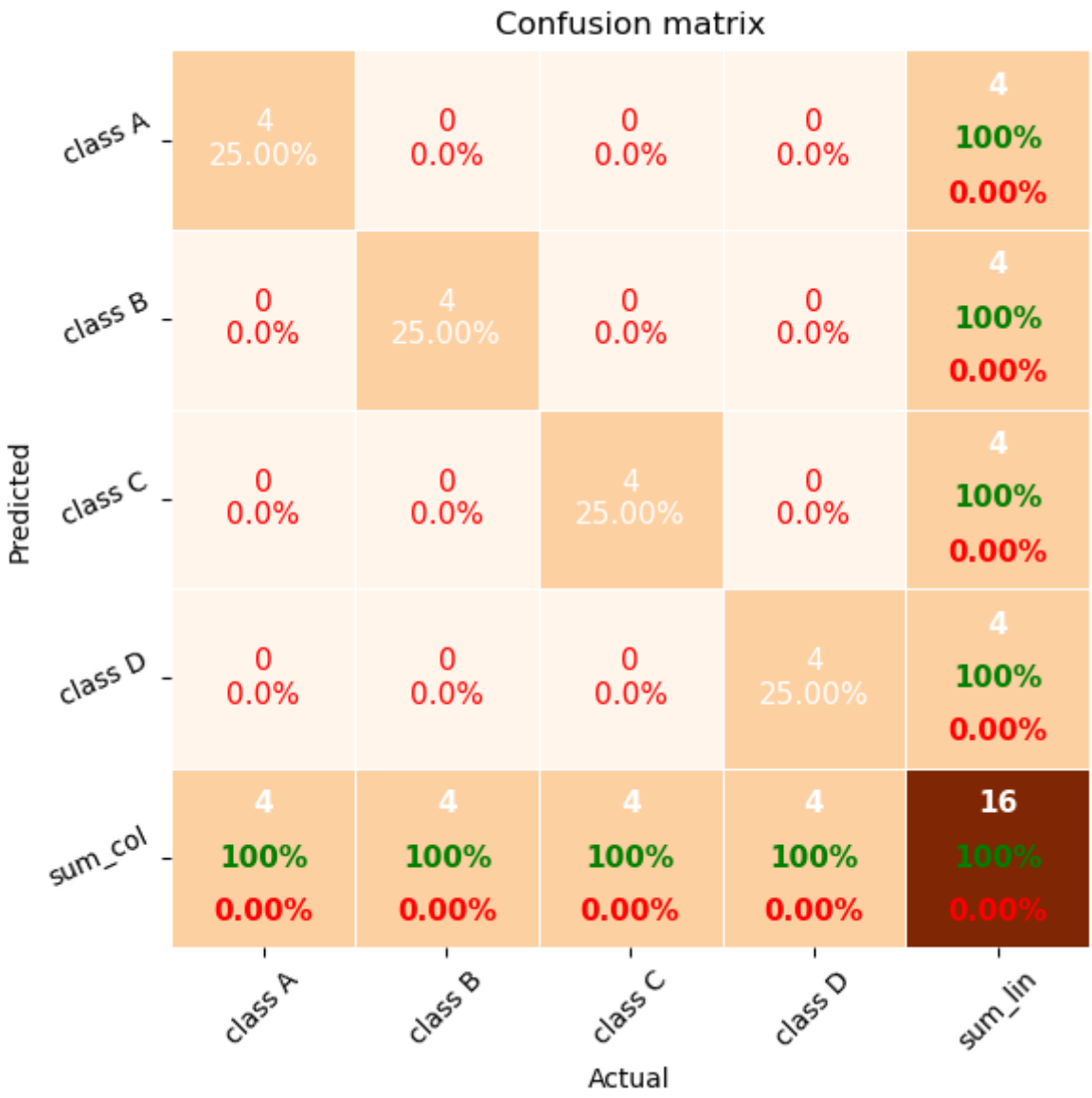
```
            # Reassigning points to updated centroids
            totalDistance[iter] = 0
            for i in range(len(firstDerivativePressure_log)):
                distance = np.zeros((K[clusters],))
                for j in range(K[clusters]):
                    a = firstDerivativePressure_log[i, :]
                    b = centroids[j, :]
                    distance[j] = DTWDistance_without_window(a, b)
                MMM, assign[i] = distance.min(), distance.argmin()
                totalDistance[iter] += MMM # measures the total distance from every
        #plotting Objective function per iteration
        plt.subplot(3, 2, clusters+1)
        totalDistance_forPlot=totalDistance
        plt.plot(range(maxIter),totalDistance_forPlot)
        totalDistance_forPlot=[]
        plt.ylabel("Objective function, O")
        plt.xlabel("Iteration, I$'")
        plt.title('Cluster ' + str(K[clusters]))

        distanceMultInit[multipleInit, :] = totalDistance # summarizes the total d
        assignMultInit[multipleInit, :] = assign

        totalDistMinimumColumn = distanceMultInit[:,maxIter-1]
        B = np.argmin(totalDistMinimumColumn)
        totalMinimumDistanceperClustering = distanceMultInit[B,:]
        totalMinimumAssignperClustering = assignMultInit[B,:]

    distanceMultInitAllClusters[((clusters)*multipleInit):((clusters)*multipleInit
    assignMultInitAllClusters[((clusters)*multipleInit):((clusters)*multipleInit)+

    totalMinimumDistanceperClusteringAllClusters[clusters,:] = totalMinimumDistanc
    totalMinimumAssignperClusteringAllClusters[clusters,:] = totalMinimumAssignperC

totalMinimumDistanceperClusteringAllClusters_forPlot = np.amin(totalMinimumDistanc
mergePlot = plt.subplot2grid((3, 2), (2, 0), colspan=2)
mergePlot.plot(K,totalMinimumDistanceperClusteringAllClusters_forPlot)
plt.ylabel("Objective function, O")
plt.xlabel("Number of Clusters, c'")
plt.title('Minmum objectve function foe each cluster')
plt.subplots_adjust(wspace=0.4,hspace=1)
plt.show()
```



In [45]:
```
from pretty_confusion_matrix import pp_matrix_from_data
from statistics import mode
```

In [49]:
```
DataframePdDataset1 = pd.DataFrame((FirstPressureDerivativeDataset1.iloc[:, 1:].va
predictedClass=totalMinimumAssignperClusteringAllClusters[1]
lables_forPrediction=[mode(predictedClass[0:4]),mode(predictedClass[0:4]),mode(pre
                      mode(predictedClass[4:8]),mode(predictedClass[4:8]),mode(pred
                      mode(predictedClass[8:12]),mode(predictedClass[8:12]),mode(pr
                      mode(predictedClass[12:16]),mode(predictedClass[12:16]),mode(
DataframePdDataset1['lables_forPrediction']=lables_forPrediction
DataframePdDataset1['cluster_assignments']=predictedClass
ari = adjusted_rand_score(DataframePdDataset1['lables_forPrediction'], DataframePdD
print("Adjusted Rand index: ", ari)
pp_matrix_from_data(DataframePdDataset1['lables_forPrediction'], DataframePdDataset
```

```
Adjusted Rand index:  1.0
```



4.2 Dataset number 2

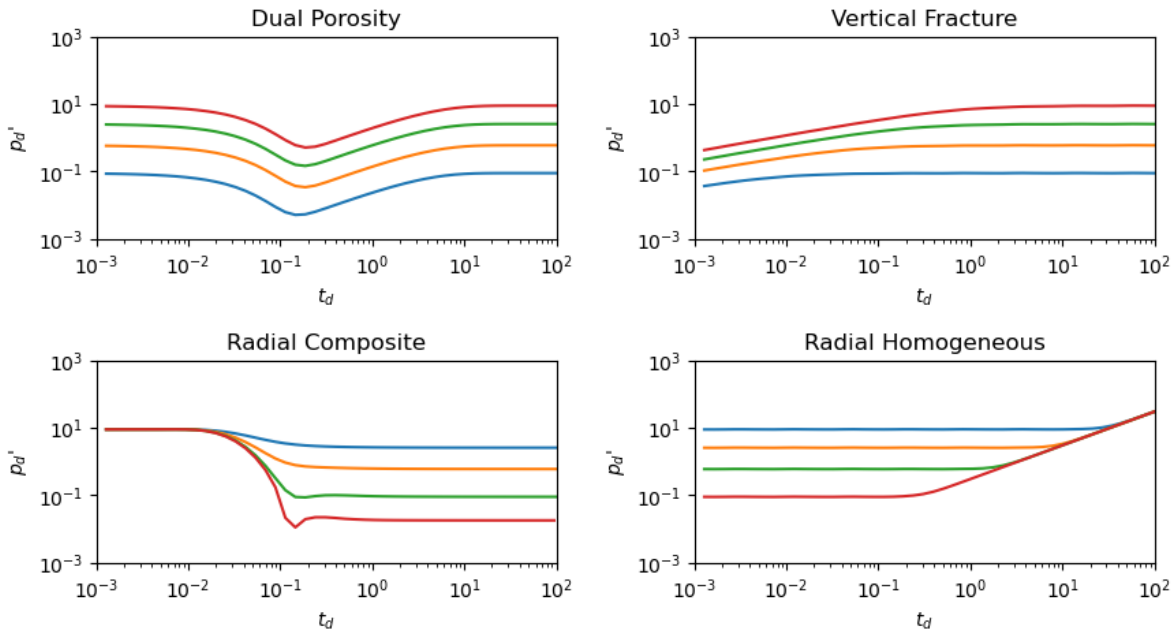
For dataset number 2 we add a displacement of the curves in the vertical direction by varying the reservoir permeability. It is know that DTW can not handle differences in the vertical direction properly so it may raise some difficulties with classification. Let's check it!

4.2.1 Fig 8.

here is the visualization of p'd vs. td curves in dataset number 2

In [32]:
```
# Extract the dimensionless pressure data from the DataFrame
pdValuesDataset2 = (FirstPressureDerivativeDataset2.iloc[:, 1:].values).T

# create a subplot for each set
fig, axs = plt.subplots(2, 2, figsize=(10, 5))

# plot each set in seperate figure
for i in range(0,4):
    axs[0,0].plot(FirstPressureDerivativeDataset2.iloc[:, 0],np.where(pdValuesData
    axs[0,0].set_title("Dual Porosity")
for i in range(4,8):
    axs[0,1].plot(FirstPressureDerivativeDataset2.iloc[:, 0],np.where(pdValuesData
```

```
    axs[0,1].set_title("Vertical Fracture")
for i in range(8,12):
    axs[1,0].plot(FirstPressureDerivativeDataset2.iloc[:, 0],np.where(pdValuesData
    axs[1,0].set_title("Radial Composite")
for i in range(12,16):
    axs[1,1].plot(FirstPressureDerivativeDataset2.iloc[:, 0],np.where(pdValuesData
    axs[1,1].set_title("Radial Homogeneous")

# set x and y limits, scale and lable for all subplots
for i in range(2):
    for j in range(2):
        axs[i, j].set_xscale('log')
        axs[i, j].set_yscale('log')
        axs[i, j].set_xlim(0.001, 100)
        axs[i, j].set_ylim(0.001, 1000)
        axs[i, j].set_xlabel("$t_{d}$")
        axs[i, j].set_ylabel("$p_{d}$'")

#set vertical spacing between plots
fig.subplots_adjust(hspace=0.6, wspace=0.3)

# Show the plot
plt.show()
```



Now we run clustering algorithm in this data set to see if we are able to classify the curves

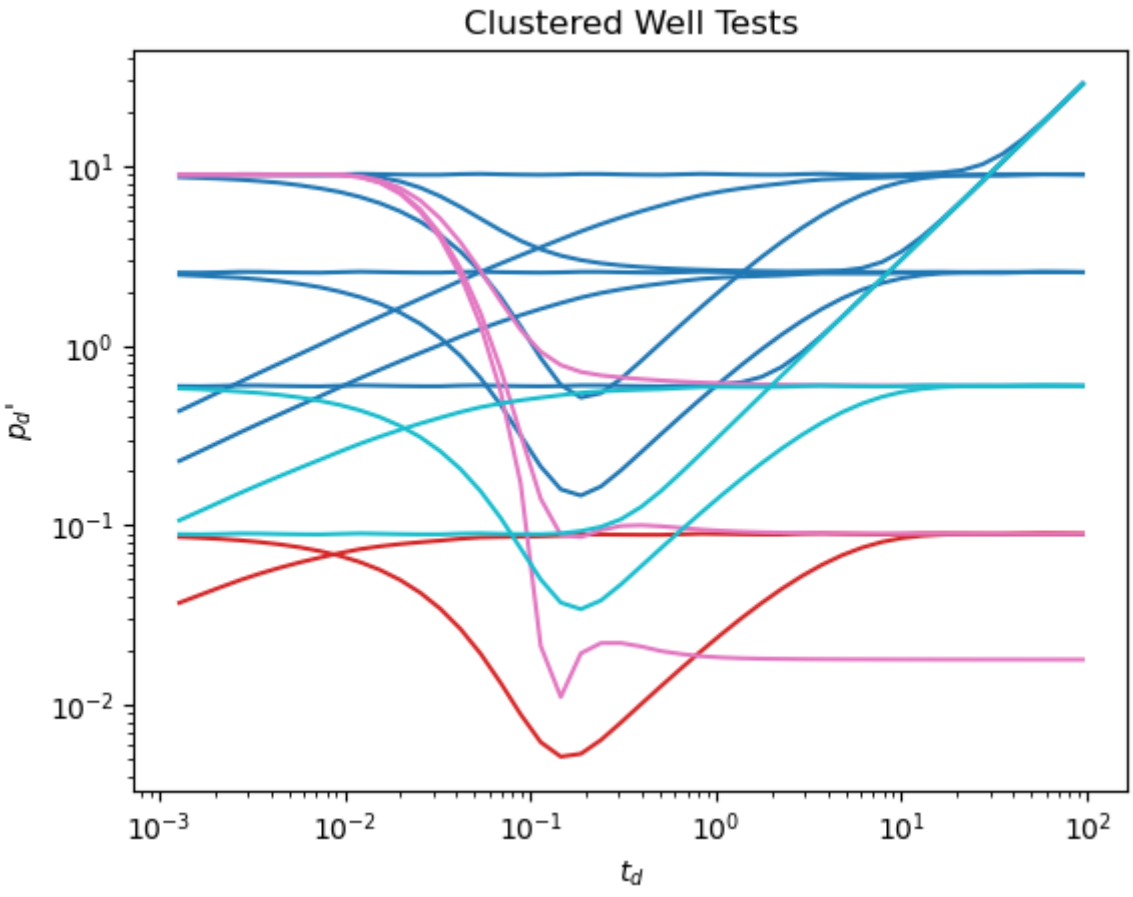
In [33]:
```
# remove rows with zero values
firstDerivativePressure_log = FirstPressureDerivativeDataset2[~(FirstPressureDeriv

# remove rows with NaN values
firstDerivativePressure_log = firstDerivativePressure_log.dropna()
firstDerivativePressure_log= np.log10(firstDerivativePressure_log[firstDerivativeP

K=[4]

# Maximum Number of Iterations
maxIter = 5
# Maximum Number of Initializations
maxInitializations = 10

totalDistanceperClusteringAllClusters = np.zeros((len(K), maxIter))
totalMinimumAssignperClusteringAllClusters = np.zeros((len(K), len(firstDerivativeP
```

```
distanceMultInitAllClusters= np.zeros((maxInitializations*maxIter, maxIter))
assignMultInitAllClusters= np.zeros((maxInitializations*maxIter,firstDerivativePres
totalMinimumDistanceperClusteringAllClusters=np.zeros((len(K), maxIter))
totalMinimumAssignperClusteringAllClusters=np.zeros((len(K), firstDerivativePressu
for clusters in range(len(K)):
    distanceMultInit= np.zeros((maxInitializations,maxIter))
    assignMultInit= np.zeros((maxInitializations,firstDerivativePressure_log.shape
    for multipleInit in range(maxInitializations):

        # Initialize the centroids to be random samples
        # Randomly reorder the indices of examples
        randidx = np.random.permutation(firstDerivativePressure_log.shape[0])
        # Take the first K examples as centroids
        centroids = firstDerivativePressure_log[randidx[:K[clusters]], :]

        # Cluster Assignment Step
        totalDistance = np.zeros((maxIter,))
        assign = np.zeros((len(firstDerivativePressure_log),))

        for i in range(len(firstDerivativePressure_log)):
            distance = np.zeros((K[clusters],))
            for j in range(K[clusters]):
                a = firstDerivativePressure_log[i, :]
                b = centroids[j, :]
                distance[j]=DTWDistance_without_window(a,b)
            M, assign[i] = distance.min(), distance.argmin()
            # accumulative
            totalDistance[0] += M # measures the total distance from every point t

        for iter in range(1, maxIter):
            # Averaging (point that minimizes the distance to the members of the c
            for n in range(K[clusters]):
                assignTemp = (assign==n)
                clusterMatrix = firstDerivativePressure_log[assignTemp, :]
                intraClusterDist = np.zeros((clusterMatrix.shape[0],))
                for i in range(clusterMatrix.shape[0]):
                    a = clusterMatrix[i, :]
                    tempDist = 0
                    for j in range(clusterMatrix.shape[0]):
                        b = clusterMatrix[j, :]
                        tempDist += DTWDistance_without_window(a, b)
                        intraClusterDist[i] = tempDist
                _, newCentroidRow = intraClusterDist.min(), intraClusterDist.argmi
                centroids[n, :] = clusterMatrix[newCentroidRow, :]


            # Reassigning points to updated centroids
            totalDistance[iter] = 0
            for i in range(len(firstDerivativePressure_log)):
                distance = np.zeros((K[clusters],))
                for j in range(K[clusters]):
                    a = firstDerivativePressure_log[i, :]
                    b = centroids[j, :]
                    distance[j] = DTWDistance_without_window(a, b)
                MMM, assign[i] = distance.min(), distance.argmin()
                totalDistance[iter] += MMM # measures the total distance from every
        distanceMultInit[multipleInit, :] = totalDistance # summarizes the total d
        assignMultInit[multipleInit, :] = assign

        totalDistMinimumColumn = distanceMultInit[:,maxIter-1]
        B = np.argmin(totalDistMinimumColumn)
        totalMinimumDistanceperClustering = distanceMultInit[B,:]
        totalMinimumAssignperClustering = assignMultInit[B,:]
```

```
    distanceMultInitAllClusters[((clusters)*multipleInit):((clusters)*multipleInit
    assignMultInitAllClusters[((clusters)*multipleInit):((clusters)*multipleInit)+

    totalMinimumDistanceperClusteringAllClusters[clusters,:] = totalMinimumDistanc
    totalMinimumAssignperClusteringAllClusters[clusters,:] = totalMinimumAssignper
```

the graph below shows the all curves together which have different color with respect to their category

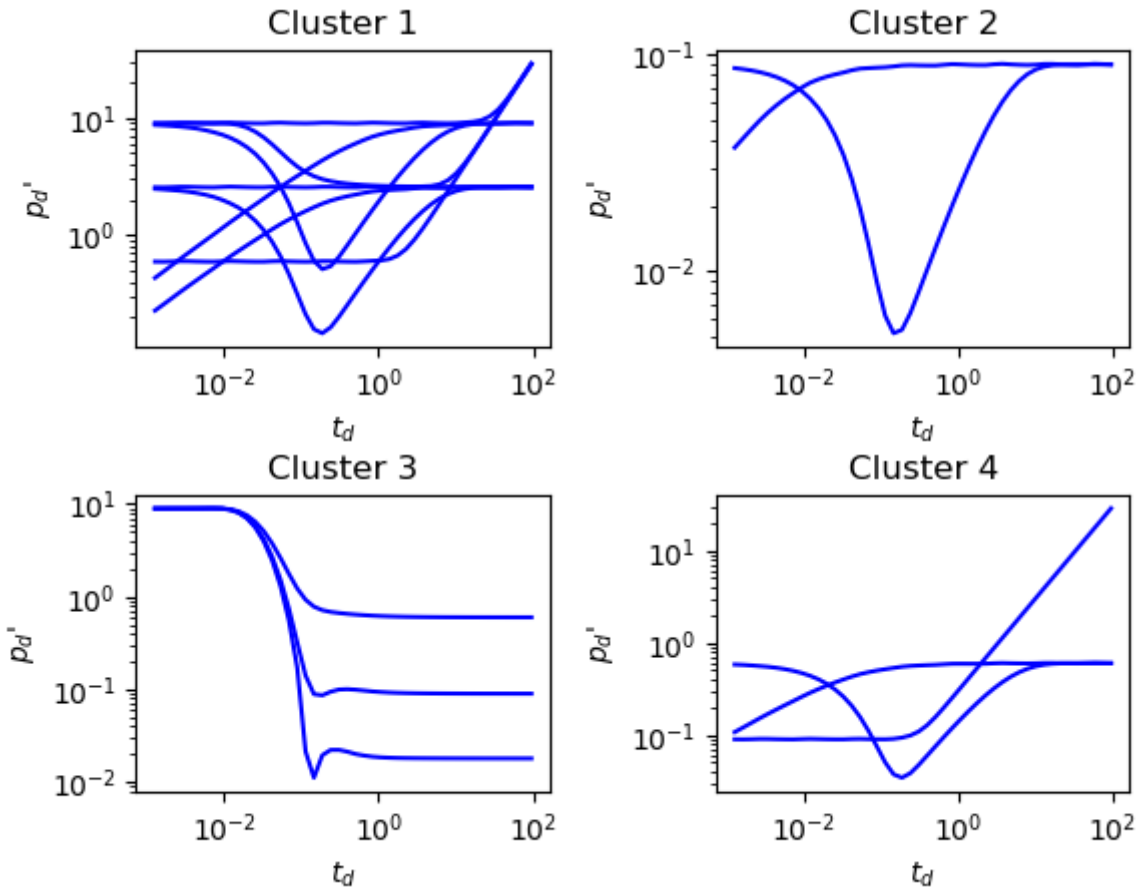
In [34]:
```
# Define color map for clusters
colorMap = plt.cm.tab10(np.linspace(0,1,4))
# Plot curves and add legend
for i in range(4):
    clusterIndices = np.where(totalMinimumAssignperClusteringAllClusters[clusters]
    for j in clusterIndices:
        plt.loglog(FirstPressureDerivativeDataset2[~(FirstPressureDerivativeDataset
# Add a title and labels to the plot
plt.title("Clustered Well Tests")
plt.xlabel("$t_{d}$")
plt.ylabel("$p_{d}$'")
plt.xscale('log')
plt.yscale('log')
```



And this code plots curves which blong to each cluster seperatly

In [35]:
```
#Create subplots for each cluster
for i in range(4):
    plt.subplot(2, 2, i+1)
    clusterIndices = np.where(totalMinimumAssignperClusteringAllClusters[clusters]
    for j in clusterIndices:
        # Create log-log plot
        plt.loglog(FirstPressureDerivativeDataset2[~(FirstPressureDerivativeDataset
    # Add labels and title
```

```
    plt.xlabel("$t_{d}$")
    plt.ylabel("$p_{d}$'")
    plt.title('Cluster ' + str(i+1))
# adjust spacing between subplots
plt.subplots_adjust(wspace=0.4,hspace=0.5)
plt.show()
```



In [36]:
```
DataframePdDataset2 = pd.DataFrame((FirstPressureDerivativeDataset2.iloc[:, 1:].va
predictedClass=totalMinimumAssignperClusteringAllClusters[0]
lables_forPrediction=[mode(predictedClass[0:4]),mode(predictedClass[0:4]),mode(pre
                      mode(predictedClass[4:8]),mode(predictedClass[4:8]),mode(pred
                      mode(predictedClass[8:12]),mode(predictedClass[8:12]),mode(pr
                      mode(predictedClass[12:16]),mode(predictedClass[12:16]),mode(
ari = adjusted_rand_score(lables_forPrediction, predictedClass)
print("Adjusted Rand index: ", ari)
```

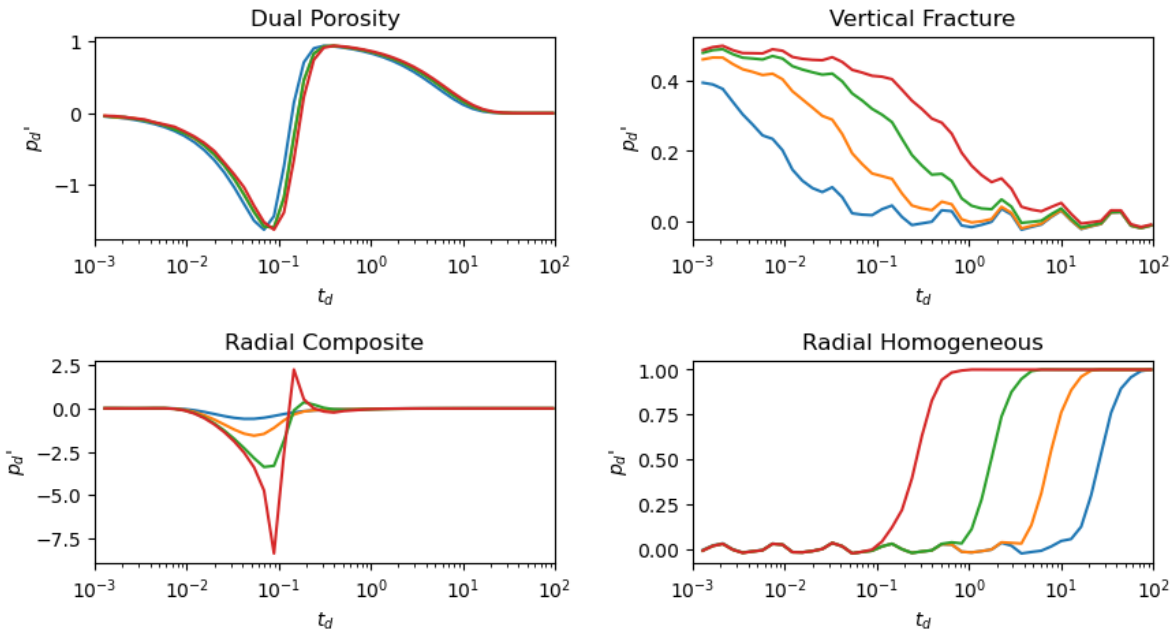
```
Adjusted Rand index:  0.2153846153846154
```

4.3.2. Fig 11.

It seems DTW is not able to distinguish vwerical differences between curves, so we decidd to work on second dreivative of pressure

In [37]:
```
# Extract the dimensionless pressure data from the DataFrame
SecpdValuesDataset2 = (SecPressureDerivativeDataset2.iloc[:, 1:].values).T

# create a subplot for each set
fig, axs = plt.subplots(2, 2, figsize=(10, 5))

# plot each set in seperate figure
for i in range(0,4):
    axs[0,0].plot(SecPressureDerivativeDataset2.iloc[:, 0],np.where(SecpdValuesDat
    axs[0,0].set_title("Dual Porosity")
```

```
for i in range(4,8):
    axs[0,1].plot(SecPressureDerivativeDataset2.iloc[:, 0],np.where(SecpdValuesData
    axs[0,1].set_title("Vertical Fracture")
for i in range(8,12):
    axs[1,0].plot(SecPressureDerivativeDataset2.iloc[:, 0],np.where(SecpdValuesData
    axs[1,0].set_title("Radial Composite")
for i in range(12,16):
    axs[1,1].plot(SecPressureDerivativeDataset2.iloc[:, 0],np.where(SecpdValuesData
    axs[1,1].set_title("Radial Homogeneous")

# set x and y limits, scale and lable for all subplots
for i in range(2):
    for j in range(2):
        axs[i, j].set_xscale('log')
        axs[i, j].set_xlim(0.001, 100)
        axs[i, j].set_xlabel("$t_{d}$")
        axs[i, j].set_ylabel("$p_{d}$'")

#set vertical spacing between plots
fig.subplots_adjust(hspace=0.6, wspace=0.3)

# Show the plot
plt.show()
```



Now we run clustering algorithm in this data set to see if we are able to classify the curves

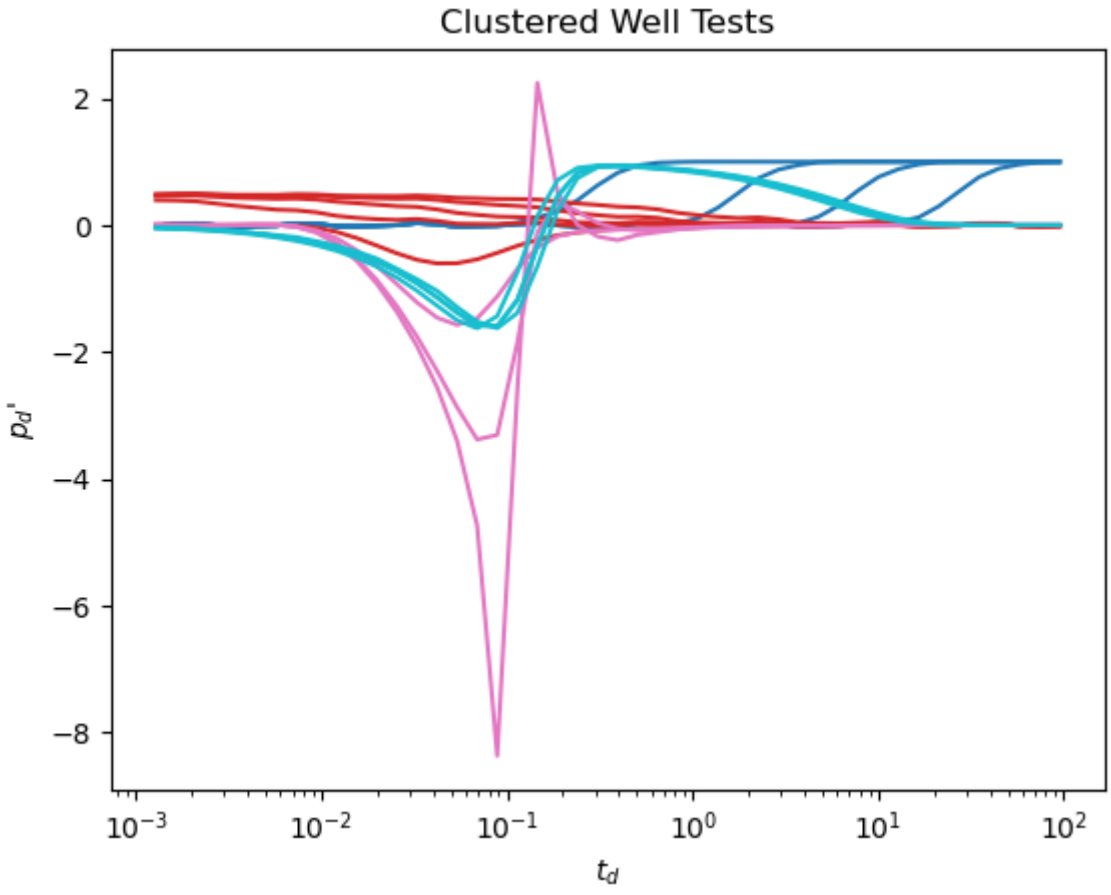
In [51]:
```
# remove rows with zero values
secDerivativePressure_log = SecPressureDerivativeDataset2[~(SecPressureDerivativeDa
#print(secDerivativePressure_log)
# remove rows with NaN values
secDerivativePressure_log = secDerivativePressure_log.dropna()

secDerivativePressure_log= secDerivativePressure_log[secDerivativePressure_log!=0]

K=[4]

# Maximum Number of Iterations
maxIter = 5
# Maximum Number of Initializations
maxInitializations = 10

totalDistanceperClusteringAllClusters = np.zeros((len(K), maxIter))
```

```
totalMinimumAssignperClusteringAllClusters = np.zeros((len(K), len(secDerivativePr
distanceMultInitAllClusters= np.zeros((maxInitializations*maxIter, maxIter))
assignMultInitAllClusters= np.zeros((maxInitializations*maxIter,secDerivativePressu
totalMinimumDistanceperClusteringAllClusters=np.zeros((len(K), maxIter))
totalMinimumAssignperClusteringAllClusters=np.zeros((len(K), secDerivativePressure_
for clusters in range(len(K)):
    distanceMultInit= np.zeros((maxInitializations,maxIter))
    assignMultInit= np.zeros((maxInitializations,secDerivativePressure_log.shape[0
    for multipleInit in range(maxInitializations):

        # Initialize the centroids to be random samples
        # Randomly reorder the indices of examples
        randidx = np.random.permutation(secDerivativePressure_log.shape[0])
        # Take the first K examples as centroids
        centroids = secDerivativePressure_log[randidx[:K[clusters]], :]

        # Cluster Assignment Step
        totalDistance = np.zeros((maxIter,))
        assign = np.zeros((len(secDerivativePressure_log),))

        for i in range(len(secDerivativePressure_log)):
            distance = np.zeros((K[clusters],))
            for j in range(K[clusters]):
                a = secDerivativePressure_log[i, :]
                b = centroids[j, :]
                distance[j]=DTWDistance_without_window(a,b)
            M, assign[i] = distance.min(), distance.argmin()
            # accumulative
            totalDistance[0] += M # measures the total distance from every point t

        for iter in range(1, maxIter):
            # Averaging (point that minimizes the distance to the members of the c
            for n in range(K[clusters]):
                assignTemp = (assign==n)
                clusterMatrix = secDerivativePressure_log[assignTemp, :]
                intraClusterDist = np.zeros((clusterMatrix.shape[0],))
                for i in range(clusterMatrix.shape[0]):
                    a = clusterMatrix[i, :]
                    tempDist = 0
                    for j in range(clusterMatrix.shape[0]):
                        b = clusterMatrix[j, :]
                        tempDist += DTWDistance_without_window(a, b)
                        intraClusterDist[i] = tempDist
                        #print(intraClusterDist)
                _, newCentroidRow = intraClusterDist.min(), intraClusterDist.argmi
                centroids[n, :] = clusterMatrix[newCentroidRow, :]


            # Reassigning points to updated centroids
            totalDistance[iter] = 0
            for i in range(len(secDerivativePressure_log)):
                distance = np.zeros((K[clusters],))
                for j in range(K[clusters]):
                    a = secDerivativePressure_log[i, :]
                    b = centroids[j, :]
                    distance[j] = DTWDistance_without_window(a, b)
                MMM, assign[i] = distance.min(), distance.argmin()
                totalDistance[iter] += MMM # measures the total distance from every
        distanceMultInit[multipleInit, :] = totalDistance # summarizes the total d
        assignMultInit[multipleInit, :] = assign

        totalDistMinimumColumn = distanceMultInit[:,maxIter-1]
        B = np.argmin(totalDistMinimumColumn)
        totalMinimumDistanceperClustering = distanceMultInit[B,:]
```

```
        totalMinimumAssignperClustering = assignMultInit[B,:]

    distanceMultInitAllClusters[((clusters)*multipleInit):((clusters)*multipleInit
    assignMultInitAllClusters[((clusters)*multipleInit):((clusters)*multipleInit)+

    totalMinimumDistanceperClusteringAllClusters[clusters,:] = totalMinimumDistanc
    totalMinimumAssignperClusteringAllClusters[clusters,:] = totalMinimumAssignper
```

the graph below shows the all curves together which have different color with respect to their category

In [52]:
```
# Define color map for clusters
colorMap = plt.cm.tab10(np.linspace(0,1,4))
# Plot curves and add legend
for i in range(4):
    clusterIndices = np.where(totalMinimumAssignperClusteringAllClusters[clusters]
    for j in clusterIndices:
        plt.plot(SecPressureDerivativeDataset2[~(SecPressureDerivativeDataset2 == (
# Add a title and labels to the plot
plt.title("Clustered Well Tests")
plt.xlabel("$t_{d}$")
plt.ylabel("$p_{d}$'")
plt.xscale('log')
#plt.yscale('log')
```



And this code plots curves which blong to each cluster seperatly

In [53]:
```
#Create subplots for each cluster
for i in range(4):
    plt.subplot(2, 2, i+1)
    clusterIndices = np.where(totalMinimumAssignperClusteringAllClusters[clusters]
    for j in clusterIndices:
        # Create log-log plot
```

```
        plt.plot(SecPressureDerivativeDataset2[~(SecPressureDerivativeDataset2 == (
    # Add labels and title
    plt.xlabel("$t_{d}$")
    plt.ylabel("$p_{d}$''")
    plt.xscale('log')
    plt.title('Cluster ' + str(i+1))
# adjust spacing between subplots
plt.subplots_adjust(wspace=0.4,hspace=0.5)
plt.show()
```

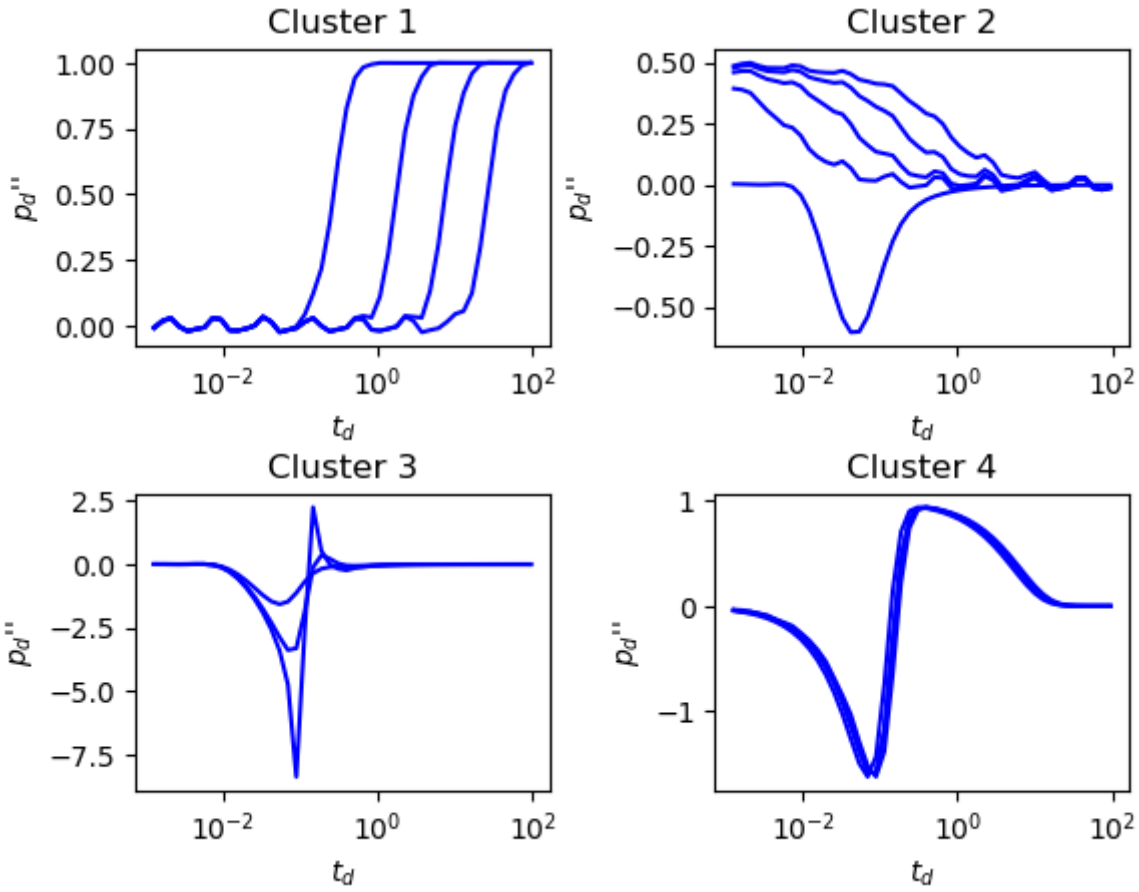
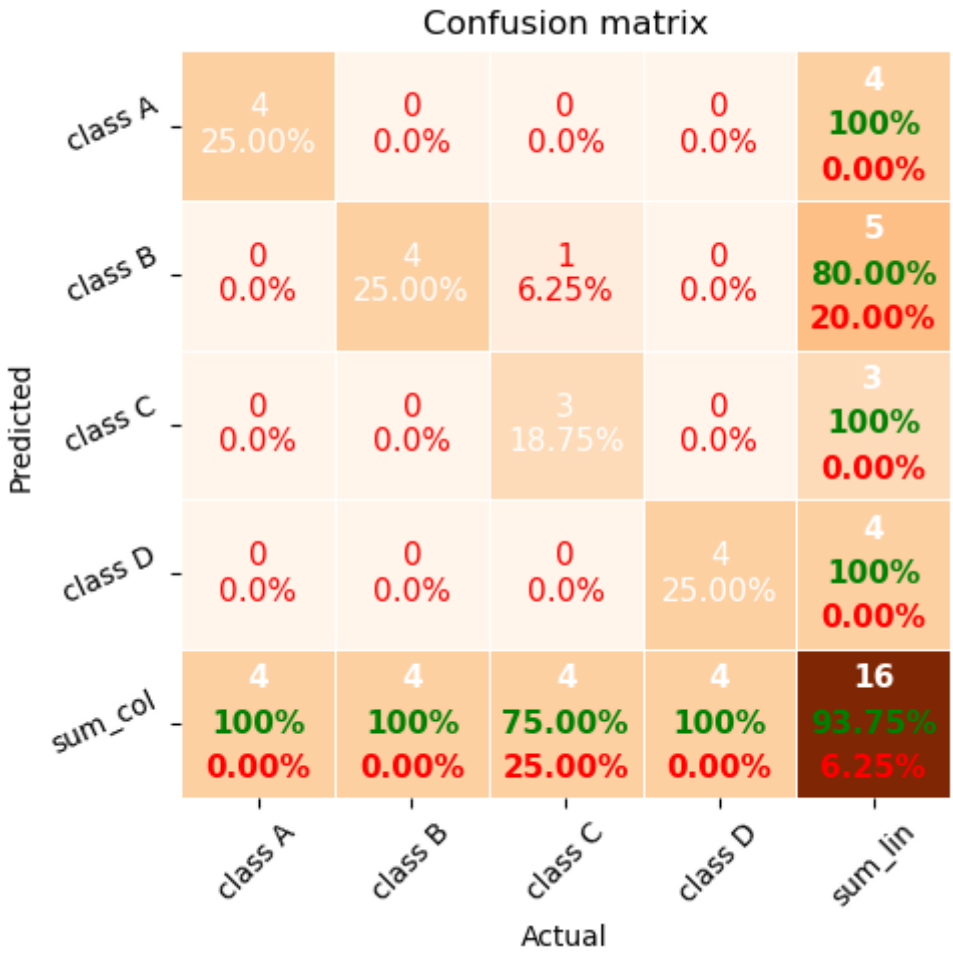


Fig. 12

In [43]:
```
DataframePdDataset1 = pd.DataFrame((SecPressureDerivativeDataset2.iloc[:, 1:].valu
predictedClass=totalMinimumAssignperClusteringAllClusters[0]
lables_forPrediction=[mode(predictedClass[0:4]),mode(predictedClass[0:4]),mode(pre
                      mode(predictedClass[4:8]),mode(predictedClass[4:8]),mode(pred
                      mode(predictedClass[8:12]),mode(predictedClass[8:12]),mode(pr
                      mode(predictedClass[12:16]),mode(predictedClass[12:16]),mode(
DataframePdDataset1['lables_forPrediction']=lables_forPrediction
DataframePdDataset1['cluster_assignments']=predictedClass
ari = adjusted_rand_score(DataframePdDataset1['lables_forPrediction'], DataframePdD
print("Adjusted Rand index: ", ari)
pp_matrix_from_data(DataframePdDataset1['lables_forPrediction'], DataframePdDataset
```

```
Adjusted Rand index:  0.8205128205128205
```



So second derivative of pressure is better indicator for classification of PTA in fractured reserviors