ID5004: AI in Predictive Maintenance, Reliability, and Warranty Assignment: Multivariate Statistics and Fault Detection

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2. For the given dataset,
   (a) Find the trace of Λ.
   (b) Find the basic statistics (mean and standard deviation) for the all the types of seeds.
   (c) Split the data into training and test data (80:20) and calculate the T^2 statistic.
   (d) Perform PCA and visualize the explained variance ratio for the training set.
   (e) Find the T^2 statistic threshold for the training data with 90% confidence interval using PCA representation
      - Assuming that the T^2 statistic follows a χ^2 distribution
      - Using the sample covariance
   (f) Report whether there are faults in the test data and outliers in the training set.

Importing Library

In [1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import matplotlib.patches as Patches
from matplotlib.patches import Ellipse
from mpl_toolkits.mplot3d import Axes3D
import seaborn as sns

from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler, MinMaxScaler
from sklearn import preprocessing
from sklearn.decomposition import PCA

from scipy.stats import f
from scipy.stats import chi2
```

In [2]:
```
# Use seaborn style aesthetics
sns.set_style('darkgrid')
```

Common variable

In [3]:
```
scaler = StandardScaler()
dataset_whole = pd.read_csv('seeds.csv')
unique_type = np.unique(dataset_whole['Type'])
variance_consideration = 0.95
```

```
alpha_90 = 0.1    # 90% confidence level (10% significance level)
alpha_95 = 0.05   # 95% confidence level (5% significance level)
alpha_99 = 0.01   # 99% confidence level (1% significance level)
seed = 30
```

Common Functionality

In [4]:
```
def dataProcessing(dataset, scaler):
    """
    Preprocesses the dataset by dropping the 'Type' column, scaling the data, and return
    the original and scaled datasets.

    Args:
        dataset (DataFrame): The input dataset.
        scaler (object): The scaler object for data scaling.

    Returns:
        dataset (DataFrame): The preprocessed original dataset.
        dataset_scale (ndarray): The scaled dataset.
    """
    # Drop the 'Type' column from the dataset
    dataset = dataset.drop('Type', axis=1)

    # Display descriptive statistics of the whole dataset
    display(dataset_whole.describe())

    # Display information about the dataset
    display(dataset_whole.info())

    # Fit the scaler on the dataset and transform the dataset
    #scaler.fit(dataset)
    dataset_scale = preprocessing.scale(dataset)

    # Print the scaled dataset
    print(dataset_scale)

    return dataset, dataset_scale

def eigendecomposition(dataset, meanshifting):
    """
    Performs eigendecomposition on the dataset, optionally applying mean shifting.

    Args:
        dataset (ndarray): The input dataset.
        meanshifting (bool): Whether to apply mean shifting.

    Returns:
        covarince_mat (ndarray): The covariance matrix.
        eigenvalues (ndarray): The eigenvalues.
        eigenvectors (ndarray): The eigenvectors.
    """
    # Apply mean shifting if meanshifting is True
    if meanshifting:
        dataset_meaned = (dataset - np.mean(dataset, axis=0))
    else:
        dataset_meaned = dataset

    # Calculate the length of the dataset
    length = len(dataset_meaned)

    # Calculate the covariance matrix
    covarince_mat = (1/(length-1)) * (dataset_meaned.T @ dataset_meaned)

    # Display the covariance matrix
```

```python
    display(covarince_mat)

    # Perform eigendecomposition on the covariance matrix
    eigenvalues, eigenvectors = np.linalg.eig(covarince_mat)

    # Print the shape of the covariance matrix, eigenvalues, and eigenvectors
    print("Covariance matrix shape:", covarince_mat.shape)
    print("Eigen Vector shape:", eigenvectors.shape)
    print("Eigen Value shape:", eigenvalues.shape)
    print("Eigen Vector:", eigenvectors)
    print("Eigen Value:", eigenvalues)

    return covarince_mat, eigenvalues, eigenvectors

def datasplitting(dataset, dataset_whole):
    """
    Splits the dataset into training and test sets.

    Args:
        dataset (DataFrame): The input dataset.
        dataset_whole (DataFrame): The complete dataset.

    Returns:
        X_train (DataFrame): The training features.
        X_test (DataFrame): The test features.
        y_train (Series): The training labels.
        y_test (Series): The test labels.
    """
    # Split the dataset into training and test sets
    X_train, X_test, y_train, y_test = train_test_split(dataset, dataset_whole['Type'],

    return X_train, X_test, y_train, y_test

def tsquaredStat(eigenvalues, eigenvectors, data, dataset_type):
    """
    Calculates the T-squared statistic for each data point.

    Args:
        eigenvalues (ndarray): The eigenvalues.
        eigenvectors (ndarray): The eigenvectors.
        data (DataFrame): The input data.
        dataset_type (str): The type of dataset.

    Returns:
        Lambda (ndarray): The diagonal matrix of eigenvalues.
        t_squared_values (list): The list of T-squared values.
        sum_t_squared_val (float): The sum of T-squared values.
    """
    # Sort the eigenvalues and eigenvectors in descending order
    eigenvalue_indices = np.argsort(eigenvalues)[::-1]
    eigenvalues_sorted = eigenvalues[eigenvalue_indices]
    eigenvectors_sorted = eigenvectors[:, eigenvalue_indices]
    Lambda = np.diag(eigenvalues_sorted)
    Lambda_inv = np.diag(1 / np.diag(Lambda)) #np.linalg.inv(Lambda)
    t_squared_values = []
    data_array = np.array(data)
    sum_t_squared_val = 0
    for i in range(len(data_array)):
        t_squared = 0
        data_loop = data_array[i, :].reshape(-1,1)
        t_squared = data_loop.T @ eigenvectors_sorted @ Lambda_inv @ eigenvectors_sorted
        sum_t_squared_val += t_squared
        t_squared_values.append(t_squared[0][0])


    Z = ((np.linalg.inv(np.sqrt(Lambda))).dot(eigenvectors_sorted.T)).dot(data.T)
```

```python
    T_squared = np.diag(Z.T@Z)
    print('T Squared Values in a without PCA: \n', T_squared)

    # Print the dataset type
    print(f'{dataset_type} :')

    # Print the T-squared values
    print('T Squared Values with PCA: \n', t_squared_values)

    # Print the sum of T-squared values
    print('Sum of T Squared Values : ', sum_t_squared_val[0][0])

    return Lambda, t_squared_values, sum_t_squared_val[0][0]

def pc_required(explained_variances):
    '''
    Determine the explained variation in comparison to a predetermined threshold value,
    and then provide the number of principle components to be chosen.
    '''
    # Find the number of principal components that explain the desired variance threshol
    return np.argmax(np.cumsum(explained_variances) >= variance_consideration) + 1

def perform_PCA(input_data):
    """
    Performs Principal Component Analysis (PCA) on the input data.

    Args:
        input_data (ndarray): The input data.

    Returns:
        considerable_PC (int): The number of considerable principle components.
        input_data_transformed (ndarray): The transformed input data.
    """
    # Create a PCA object
    pca = PCA()

    # Fit the PCA model to the input data
    pca.fit(input_data)

    # Transform the input data using the PCA model
    input_data_transformed = pca.transform(input_data)

    # Obtain the explained variance ratio for each principal component
    explained_variance_ratio = pca.explained_variance_ratio_

    # Calculate the cumulative explained variance
    cumulative_variance = np.cumsum(explained_variance_ratio)

    # Get the total number of principal components
    num_components = len(explained_variance_ratio)

    # Determine the number of considerable principle components based on a threshold
    considerable_PC = pc_required(explained_variance_ratio)

    # Print the number of total components and the number of considerable principle comp
    print(f'Number of total component : {num_components}')
    print('Considerable Principle Component : ', considerable_PC)

    # Create a scree plot to visualize the explained variance
    plt.figure(figsize=(8, 6))
    plt.plot(np.arange(1, num_components + 1), cumulative_variance, marker='o', linestyl
    plt.xlabel('Number of Principal Components')
    plt.ylabel('Cumulative Explained Variance')
    plt.title('Scree Plot')
    plt.grid(True)
    plt.xticks(np.arange(1, num_components + 1))
```

```python
    plt.yticks(np.arange(0, 1.1, 0.1))
    plt.axhline(y=0.95, color='r', linestyle='--', label='95% Explained Variance')
    plt.legend()
    plt.tight_layout()
    plt.show()

    # Print the explained variance ratio for each principal component
    print("Explained Variance Ratio:")
    for i, ratio in enumerate(explained_variance_ratio):
        print(f"Principal Component {i+1}: {ratio:.4f}")

    # Print the cumulative explained variance for each principal component
    print("\nCumulative Explained Variance:")
    for i, var in enumerate(cumulative_variance):
        print(f"Principal Components {i+1}: {var:.4f}")

    return considerable_PC, input_data_transformed, explained_variance_ratio

def statisticalAnalysis(inputdata, considerable_PC, transformed_data, alpha):
    """
    Performs statistical analysis on the transformed data.

    Args:
        inputdata (ndarray): The input data.
        considerable_PC (int): The number of considerable principle components.
        transformed_data (ndarray): The transformed data.
        alpha (float): The significance level.

    Returns:
        None
    """
    # Part 1
    print('Part 1 : Assuming that the T2 statistic follows a χ2 distribution')
    # Calculate the T2 statistic threshold as per input alpha
    total_num_features = transformed_data.shape[1]
    print("Total Number of Features:", total_num_features)
    print('Considerable Principle Component : ', considerable_PC)

    # Degrees of freedom for the chi-square distribution
    dof = considerable_PC # number of Considerable Principle Component
    print('Degree of Freedom', dof)

    # Calculate the T2 statistic threshold using the chi-square distribution
    threshold = chi2.ppf(1 - alpha, df=dof)
    print("T2 Statistic Threshold:", threshold)


    # Part 2
    print('Part 2 : Using sample covariance')
    # Calculating T2 statistic threshold when sample covariance is used
    dfn = considerable_PC  # Degrees of freedom numerator
    dfd = inputdata.shape[0] - considerable_PC  # Degrees of freedom denominator

    # Calculate the critical value of F-distribution
    critical_value = f.ppf(1 - alpha, dfn, dfd)
    print("Critical value F_alpha(a, n-a):", critical_value)

    # Calculating T^2 statistic threshold
    n = inputdata.shape[0] - considerable_PC
    a = considerable_PC
    T_2_alpha = ((a * (n - 1) * (n + 1)) / (n * (n - a))) * critical_value
    print("T2 Statistic Threshold:", T_2_alpha)

def outlier_threshold(alpha, input_data, considerablePC):
    """
    This function calculates the threshold for identifying outliers based on Hotelling's
```

```
    distribution and the F-distribution. This is used in multivariate outlier detection.

    Args:

    alpha : float
        The significance level for the F-distribution. This is used to control the Type
        rate, i.e., the probability of falsely identifying an observation as an outlier.

    input_data : array-like
        A 2-dimensional numpy array or pandas DataFrame containing the multivariate data
        row represents an observation and each column represents a variable.

    considerablePC : int
        The number of principal components to be considered for outlier detection. This
        less than or equal to the number of variables (columns) in the input data.

    Returns:

    float
        The threshold for identifying outliers. Observations with a T-square value great
        this threshold are identified as outliers.
    """
    n = input_data.shape[0]
    a = considerablePC
    f_alpha = f.ppf(1 - alpha, a, n - a - 1)
    threshold_outlier= ((n - 1) ** 2 * (a / (n - a - 1)) * f_alpha) / (n * (1 + (a / (n
    return threshold_outlier

def fault_threshold_method(alpha, input_data, considerablePC):
    """
    This function calculates the threshold for identifying fault based on Hotelling's T-
    distribution and the F-distribution. This is used in multivariate fault detection.

    Args:

    alpha : float
        The significance level for the F-distribution. This is used to control the Type
        rate, i.e., the probability of falsely identifying an observation as an fault.

    input_data : array-like
        A 2-dimensional numpy array or pandas DataFrame containing the multivariate data
        row represents an observation and each column represents a variable.

    considerablePC : int
        The number of principal components to be considered for outlier detection. This
        less than or equal to the number of variables (columns) in the input data.

    Returns:

    float
        The threshold for identifying faults. Observations with a T-square value greater
        this threshold are identified as faults.
    """
    n = input_data.shape[0]
    a = considerablePC
    f_alpha = f.ppf(1 - alpha, a, n - a)
    fault_threshold_val = ((a*(n-1)*(n+1))/(n*(n-a)))*f_alpha
    return fault_threshold_val


def generate_ellipsoid(center, radii, rotation, num_points=100):
    """
    Generate points on an ellipsoid surface given the center, radii, and rotation matrix

    Parameters:
        center (numpy.ndarray): The center point of the ellipsoid.
```

```
        radii (numpy.ndarray): The radii of the ellipsoid in the x, y, and z directions.
        rotation (numpy.ndarray): The rotation matrix for orienting the ellipsoid.
        num_points (int): The number of points to generate on the ellipsoid surface. Def

    Returns:
        numpy.ndarray: Array of shape (num_points, num_points, 3) containing the points

    """

    # Generate angles u and v for parameterizing the ellipsoid surface
    u = np.linspace(0, 2 * np.pi, num_points)
    v = np.linspace(0, np.pi, num_points)

    # Calculate the x, y, and z coordinates for each point on the ellipsoid surface
    x = radii[0] * np.outer(np.cos(u), np.sin(v))
    y = radii[1] * np.outer(np.sin(u), np.sin(v))
    z = radii[2] * np.outer(np.ones_like(u), np.cos(v))

    # Stack the x, y, and z coordinates to form the ellipsoid points array
    ellipsoid = np.stack((x, y, z), axis=-1)

    # Apply rotation and translation to each point on the ellipsoid surface
    for i in range(num_points):
        for j in range(num_points):
            ellipsoid[i, j] = np.dot(rotation, ellipsoid[i, j]) + center

    # Return the array of points on the ellipsoid surface
    return ellipsoid


def OutlierAndFaultAnalysis(dataset_whole, seed_type, alpha):
    """
    Perform outlier analysis and fault analysis on the Seeds dataset for a specific seed

    Args:
        dataset_whole (DataFrame): The entire Seeds dataset containing all samples and f
        seed_type (int): The seed type for which to perform outlier and fault analysis.

    Returns:
        None (Displays various plots and printed results.)
    """

    # Segregating data
    x_dataset = dataset_whole.drop('Type', axis=1)
    y_dataset = dataset_whole['Type']
    type_dataset = dataset_whole[dataset_whole['Type'] == seed_type]
    x_type_dataset = type_dataset.drop('Type', axis=1)
    y_type_dataset = type_dataset['Type']

    # Splitting the data
    X_train_type, X_test_type, y_train_type, y_test_type = train_test_split(x_type_datas

    # Scaling the data
    X_train_type_scaled = preprocessing.scale(X_train_type)

    # Plot 1 - Original and Scaled Train Data Histograms
    fig, axes = plt.subplots(1, 2, figsize=(10, 4))
    axes[0].hist(np.array(X_train_type).flatten(), bins=20, color='blue', alpha=0.5)
    axes[0].set_title('Original Train Data')
    axes[1].hist(np.array(X_train_type_scaled).flatten(), bins=20, color='red', alpha=0.
    axes[1].set_title('Autoscaled Train Data')
    plt.tight_layout()
    plt.show()

    # Outlier Analysis - PCA
    pca = PCA()
```

```
pca.fit(X_train_type_scaled)
X_train_type_scaled_transformed = pca.transform(X_train_type_scaled)
explained_variance_ratio = pca.explained_variance_ratio_
cumulative_variance = np.cumsum(explained_variance_ratio)
num_components = len(explained_variance_ratio)
considerable_PC = pc_required(explained_variance_ratio)
print(f'Number of total component : {num_components}')
print('Considerable Principle Component : ', considerable_PC)

# Scree Plot
plt.figure(figsize=(8, 6))
plt.plot(np.arange(1, num_components + 1), cumulative_variance, marker='o', linestyl
plt.xlabel('Number of Principal Components')
plt.ylabel('Cumulative Explained Variance')
plt.title('Scree Plot')
plt.grid(True)
plt.xticks(np.arange(1, num_components + 1))
plt.yticks(np.arange(0, 1.1, 0.1))
plt.axhline(y=0.95, color='r', linestyle='--', label='95% Explained Variance')
plt.legend()
plt.tight_layout()
plt.show()

# Print the explained variance ratio for each principal component
print("Explained Variance Ratio:")
for i, ratio in enumerate(explained_variance_ratio):
    print(f"Principal Component {i+1}: {ratio:.4f}")

# Print the cumulative explained variance for each principal component
print("\nCumulative Explained Variance:")
for i, var in enumerate(cumulative_variance):
    print(f"Principal Components {i+1}: {var:.4f}")


# Eigen Value Decomposition
meanshifting = True
if meanshifting:
    dataset_meaned = (X_train_type_scaled - np.mean(X_train_type_scaled, axis=0))
else:
    dataset_meaned = X_train_type_scaled
# Calculate the length of the dataset
length = len(dataset_meaned)
# Calculate the covariance matrix
covarince_mat = (1/(length-1)) * (dataset_meaned.T @ dataset_meaned)
# Display the covariance matrix
display(covarince_mat)
# Perform eigendecomposition on the covariance matrix
eigenvalues, eigenvectors = np.linalg.eig(covarince_mat)
# Print the shape of the covariance matrix, eigenvalues, and eigenvectors
print("Covariance matrix shape:", covarince_mat.shape)
print("Eigen Vector shape:", eigenvectors.shape)
print("Eigen Value shape:", eigenvalues.shape)
print("Eigen Vector:", eigenvectors)
print("Eigen Value:", eigenvalues)

#Sorting and ordering
eigenvalue_indices = np.argsort(eigenvalues)[::-1]
eigenvalues_sorted = eigenvalues[eigenvalue_indices]
eigenvectors_sorted = eigenvectors[:, eigenvalue_indices]
Lambda = np.diag(eigenvalues_sorted)
Lambda_inv = np.diag(1 / np.diag(Lambda)) #np.linalg.inv(Lambda)
print(f'Lambda : {Lambda} & Lambda Incerse : {Lambda_inv}')

#TSquared Statistics Calculation
TSquaredStatistics=[]
for loop_i in range(len(X_train_type_scaled)):
```

```
    TSquaredStatistics.append(X_train_type_scaled[loop_i].T@eigenvectors_sorted[:,:c
TSquaredStatistics=np.array(TSquaredStatistics)
print(f'T_squared statistic : {TSquaredStatistics}')

#Outlier Threshold
type_outlier_threshold = outlier_threshold(alpha_90, X_train_type_scaled, considerab
print(f'Outlier Threhold : {type_outlier_threshold}')

#Plot 1
pca = PCA(n_components=considerable_PC)
x_dataset_pca = pca.fit_transform(x_dataset)
y_labels = y_dataset
custom_palette = sns.color_palette('viridis', len(np.unique(y_labels)))
type_indices = np.where(y_labels == seed_type)[0]
type_data = x_dataset_pca[type_indices, :]
threshold = chi2.ppf(1 - alpha, df=considerable_PC)
sns.scatterplot(x=x_dataset_pca[:, 0], y=x_dataset_pca[:, 1], palette=custom_palette
# Adding the T2 threshold ellipse for seed type data
ellipse = Ellipse(xy=np.mean(type_data, axis=0), width=2 * np.sqrt(threshold) * np.s
                  height=2 * np.sqrt(type_outlier_threshold) * np.sqrt(pca.explained
                  label=f'{seed_type} $T^2$ Threshold')

# Adding the ellipse to the plot
plt.gca().add_patch(ellipse)
plt.xlabel('PC1', fontsize=14)
plt.ylabel('PC2', fontsize=14)
plt.title(f'PCA of Seeds Dataset for {seed_type}', fontsize=16)
plt.legend(fontsize=12, loc='upper left')
plt.grid(True)
plt.show()

# Plot 2 - Outlier Boundary for Seeds Dataset in 3D
PCs = eigenvectors_sorted[:, :considerable_PC].T @ X_train_type_scaled.T
fig = plt.figure(figsize=(10, 6))
ax = fig.add_subplot(111, projection='3d')
scatter = ax.scatter(xs=PCs[0, :].T, ys=PCs[1, :].T, zs=PCs[2, :].T, c=np.array(y_tr
                     cmap='Set1', s=50, edgecolor='white', alpha=0.7)
ax.set_box_aspect([1, 1, 1])
center = np.mean(np.array([PCs[0, :].T, PCs[1, :].T, PCs[2, :].T]), axis=1)
radii = 2 * np.sqrt(type_outlier_threshold) * np.sqrt(explained_variance_ratio)
rotation = np.eye(3)
ellipsoid_points = generate_ellipsoid(center, radii, rotation)
ax.plot_surface(ellipsoid_points[..., 0], ellipsoid_points[..., 1], ellipsoid_points
                edgecolor='green', linewidth=1, alpha=0.2, color='lightgray')
ax.scatter(center[0], center[1], center[2], marker='*', color='yellow', s=100, edgec
ax.set_xlabel('PC1', fontsize=12)
ax.set_ylabel('PC2', fontsize=12)
ax.set_zlabel('PC3', fontsize=12)
ax.set_title(f'Outlier Boundary for Seeds Dataset in 3D of type {seed_type}', fontsi
cbar = fig.colorbar(scatter)
cbar.set_label('Class', fontsize=12)
ax.spines['top'].set_visible(False)
ax.spines['right'].set_visible(False)
plt.show()

# Fault Analysis
X_test_type_scaled = preprocessing.scale(X_test_type)
fig, axes = plt.subplots(1, 2, figsize=(10, 4))
axes[0].hist(np.array(X_test_type).flatten(), bins=20, color='blue', alpha=0.5)
axes[0].set_title('Original Test Data')
axes[1].hist(np.array(X_test_type_scaled).flatten(), bins=20, color='red', alpha=0.5
axes[1].set_title('Autoscaled Test Data')
plt.tight_layout()
plt.show()

# Fault Threshold Calculation
```

```
    type_fault_threshold = fault_threshold_method(alpha_90, X_test_type_scaled, consider
    print(f'Fault Threhold : {type_fault_threshold}')

    TSquaredStatistics_Fault=[]
    for loop_fault in range(len(X_test_type_scaled)):
        TSquaredStatistics_Fault.append(X_test_type_scaled[loop_fault].T@eigenvectors_so
    TSquaredStatistics_Fault=np.array(TSquaredStatistics_Fault)
    print(f"T_squared statistic", TSquaredStatistics_Fault,"\n\n")

    # Plot 3
    PCs = np.array(eigenvectors_sorted[:, :considerable_PC].T @ X_test_type_scaled.T)
    fig = plt.figure(figsize=(10, 6))
    ax = fig.add_subplot(111, projection='3d')
    scatter = ax.scatter(xs=PCs[0, :].T, ys=PCs[1, :].T, zs=PCs[2, :].T, c=np.array(y_te
                         cmap='Set1', s=50, edgecolor='white', alpha=0.7)
    ax.set_box_aspect([1, 1, 1])
    center = np.mean(np.array([PCs[0, :].T, PCs[1, :].T, PCs[2, :].T]), axis=1)
    radii = 2 * np.sqrt(type_fault_threshold) * np.sqrt(explained_variance_ratio)
    rotation = np.eye(3)
    ellipsoid_points = generate_ellipsoid(center, radii, rotation)
    ax.plot_surface(ellipsoid_points[..., 0], ellipsoid_points[..., 1], ellipsoid_points
                    edgecolor='green', linewidth=1, alpha=0.2, color='lightgray')
    ax.scatter(center[0], center[1], center[2], marker='*', color='yellow', s=100, edgec
    ax.set_xlabel('PC1', fontsize=12)
    ax.set_ylabel('PC2', fontsize=12)
    ax.set_zlabel('PC3', fontsize=12)
    ax.set_title(f'Fault Boundary for Seeds Dataset in 3D of type {seed_type}', fontsize
    cbar = fig.colorbar(scatter)
    cbar.set_label('Class', fontsize=12)
    ax.spines['top'].set_visible(False)
    ax.spines['right'].set_visible(False)
    plt.show()
```

Data Loading & Processing

In [5]:
```
dataset, dataset_scale = dataProcessing(dataset_whole, scaler)
```

	Area	Perimeter	Compactness	Kernel.Length	Kernel.Width	Asymmetry.Coeff	Kernel.Groove	
count	199.000000	199.000000	199.000000	199.000000	199.000000	199.000000	199.000000	199.0
mean	14.918744	14.595829	0.870811	5.643151	3.265533	3.699217	5.420653	1.9
std	2.919976	1.310445	0.023320	0.443593	0.378322	1.471102	0.492718	0.8
min	10.590000	12.410000	0.808100	4.899000	2.630000	0.765100	4.519000	1.0
25%	12.330000	13.470000	0.857100	5.267000	2.954500	2.570000	5.046000	1.0
50%	14.430000	14.370000	0.873400	5.541000	3.245000	3.631000	5.228000	2.0
75%	17.455000	15.805000	0.886800	6.002000	3.564500	4.799000	5.879000	3.0
max	21.180000	17.250000	0.918300	6.675000	4.033000	8.315000	6.550000	3.0

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 199 entries, 0 to 198
Data columns (total 8 columns):
 #   Column           Non-Null Count  Dtype
---  ------           --------------  -----
 0   Area             199 non-null    float64
 1   Perimeter        199 non-null    float64
 2   Compactness      199 non-null    float64
 3   Kernel.Length    199 non-null    float64
```

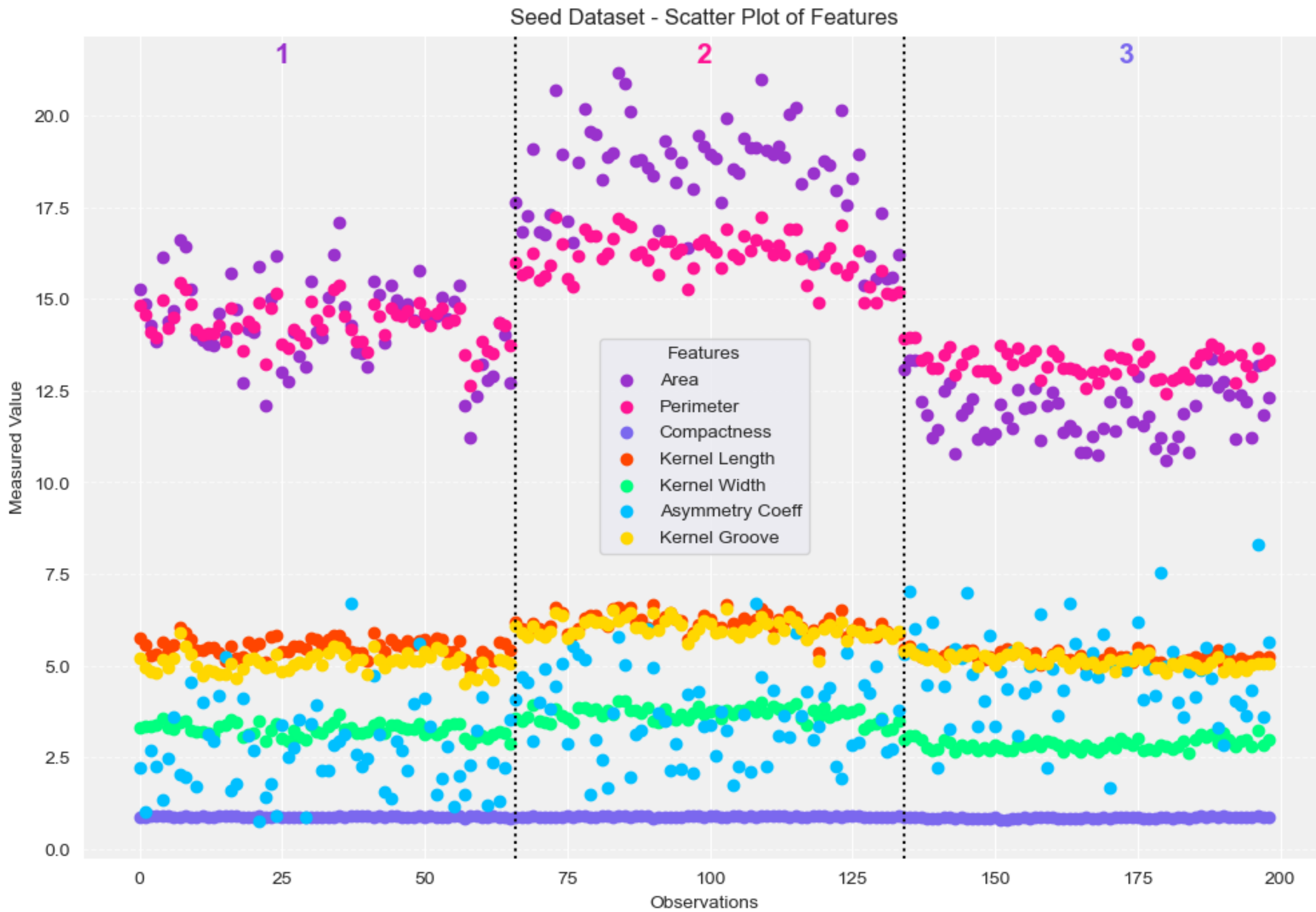
```
 4   Kernel.Width     199 non-null    float64
 5   Asymmetry.Coeff  199 non-null    float64
 6   Kernel.Groove    199 non-null    float64
 7   Type             199 non-null    int64
dtypes: float64(7), int64(1)
memory usage: 12.6 KB
None
[[ 0.11716431  0.18679667  0.0081443  ...  0.12313474 -1.00737062
  -0.40826475]
 [-0.01330197 -0.01975993  0.44234139 ...  0.17878306 -1.82718718
  -0.9454197 ]
 [-0.21586804 -0.38697165  1.46979786 ...  0.18938275 -0.68162472
  -1.21196249]
 ...
 [-0.59010028 -0.71593216  0.75186803 ... -0.08885888  3.14554887
  -0.74195192]
 [-1.05703224 -1.06019315 -0.80436312 ... -1.13822732 -0.06897709
  -0.76636805]
 [-0.89909937 -0.96073998 -0.10362921 ... -0.77253832  1.32055406
  -0.72770917]]
```

Visualization of the dataset

In [6]:

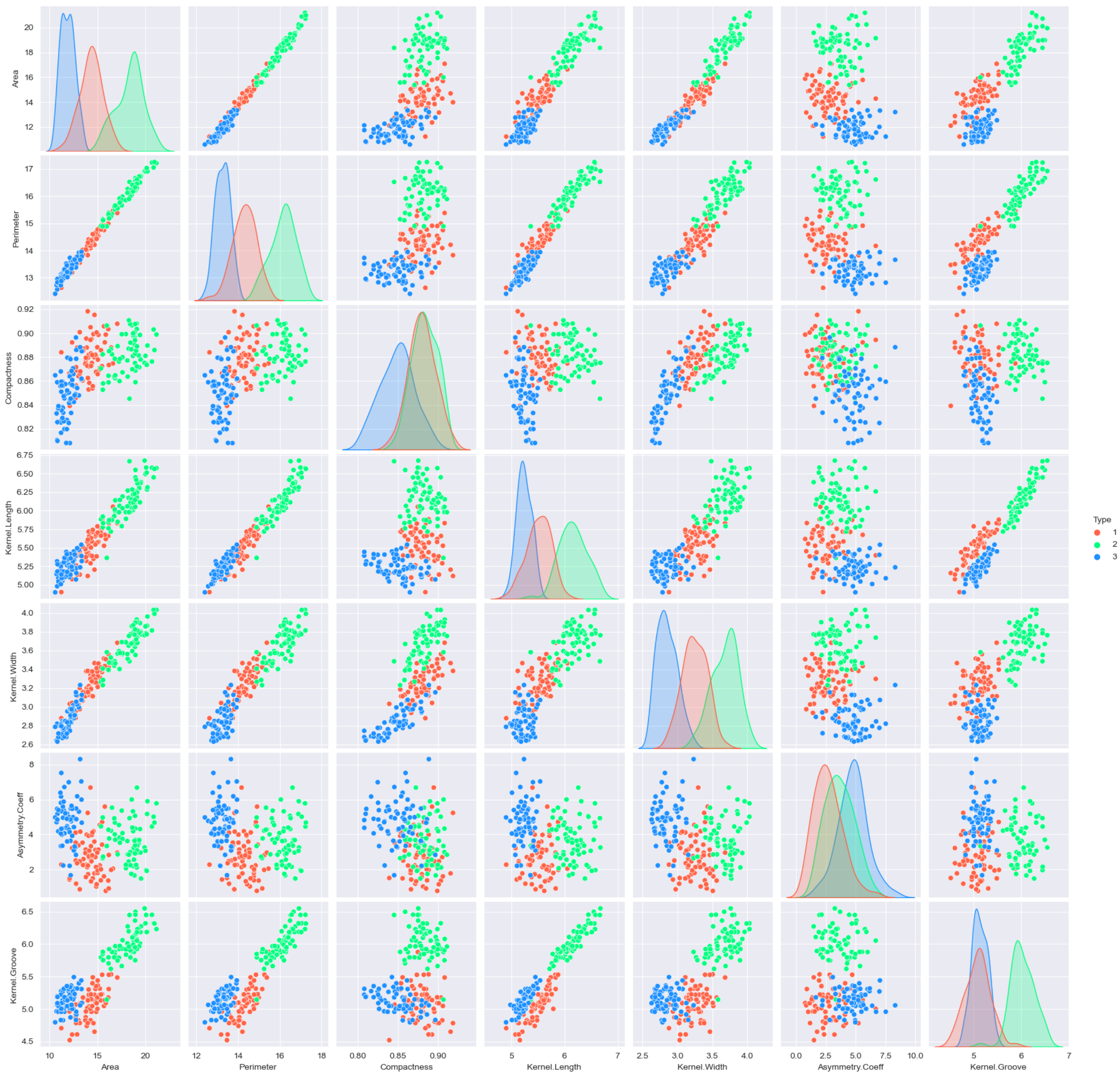
```python
# Define the features and their labels
features = {
    'Area': 'Area',
    'Perimeter': 'Perimeter',
    'Compactness': 'Compactness',
    'Kernel.Length': 'Kernel Length',
    'Kernel.Width': 'Kernel Width',
    'Asymmetry.Coeff': 'Asymmetry Coeff',
    'Kernel.Groove': 'Kernel Groove',
}

# Create a single plot for all features
plt.figure(figsize=(12, 8))

# Set custom colors for the scatter plots
colors = ['#9932CC', '#FF1493', '#7B68EE', '#FF4500', '#00FF7F', '#00BFFF', '#FFD700']

# Iterate through the features and plot scatter plots with custom colors and markers
for i, (feature, label) in enumerate(features.items()):
    plt.scatter(dataset_whole.index, dataset_whole[feature], label=label, color=colors[i

# Add legends and labels
plt.legend(title='Features', loc = 'center')
plt.xlabel('Observations')
plt.ylabel('Measured Value')
plt.title('Seed Dataset - Scatter Plot of Features')

# Draw dotted lines to separate classes
for index in [66, 134]:
    plt.axvline(index, color='black', linestyle='dotted')

# Add class labels
class_labels = ['1', '2', '3']
for i, label in enumerate(class_labels):
    plt.text(25 + i * 74, 22, label, ha='center', va='top', color=colors[i], fontweight=

# Customize grid lines
plt.grid(axis='y', linestyle='--', alpha=0.7)

# Customize background color
plt.gca().set_facecolor('#f0f0f0')
```

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



In [7]:

```python
custom_palette = ['#FF6347', '#00FF7F', '#1E90FF']
sns.pairplot(dataset_whole, hue='Type', palette=custom_palette)
plt.show()
```



a) Find the trace of Λ.

In [8]:
```
covarince_mat_scale, eigenvalues_scale, eigenvectors_scale = eigendecomposition(dataset_
```

```
array([[ 1.00505051,  0.99945967,  0.61296771,  0.95592951,  0.97588352,
        -0.22394581,  0.86708441],
       [ 0.99945967,  1.00505051,  0.5345268 ,  0.97785806,  0.95027092,
        -0.21210008,  0.89403606],
       [ 0.61296771,  0.5345268 ,  1.00505051,  0.3759002 ,  0.7660163 ,
        -0.33106381,  0.22816301],
       [ 0.95592951,  0.97785806,  0.3759002 ,  1.00505051,  0.8670369 ,
        -0.17056152,  0.9368318 ],
       [ 0.97588352,  0.95027092,  0.7660163 ,  0.8670369 ,  1.00505051,
        -0.25440081,  0.75200687],
       [-0.22394581, -0.21210008, -0.33106381, -0.17056152, -0.25440081,
         1.00505051, -0.00336631],
       [ 0.86708441,  0.89403606,  0.22816301,  0.9368318 ,  0.75200687,
        -0.00336631,  1.00505051]])
Covariance matrix shape: (7, 7)
Eigen Vector shape: (7, 7)
Eigen Value shape: (7,)
```

```
Eigen Vector: [[ 0.44444526  0.0268951  -0.02541939  0.19763627  0.19751625 -0.73412145
  -0.42905925]
 [ 0.44156742  0.08298812  0.06019769  0.30034829  0.16637062  0.67153918
  -0.47503082]
 [ 0.27791499 -0.52535969 -0.63238211 -0.34000075 -0.32627308  0.07310414
  -0.13947927]
 [ 0.42412605  0.200075    0.21443932  0.25098045 -0.76832639 -0.0463691
   0.28042137]
 [ 0.43293659 -0.11572453 -0.2151238   0.20373132  0.46870015  0.03700686
   0.70024261]
 [-0.1157433   0.72122562 -0.67513087  0.09326364 -0.04045161  0.00383945
  -0.01691821]
 [ 0.38669933  0.37788656  0.21853787 -0.80120818  0.12333864  0.0349609
   0.03920887]]
Eigen Value: [5.05691778e+00 1.20519035e+00 6.79631565e-01 6.85475795e-02
 1.89074688e-02 8.16380060e-04 5.34241202e-03]
```

In [9]:

```
trace_scale = np.trace(np.diag(eigenvalues_scale))
print("Trace of Λ with scalling:", trace_scale)
```

```
Trace of Λ with scalling: 7.035353535353538
```

Conclusion of a)

We have clauclated trace of Λ derived from the scaled data using eigen value decomposition. In a scalled data trace is appear as approximately 7.035.

b) Find the basic statistics (mean and standard deviation) for the all the types of seeds.

In [10]:

```
unique_type
```

Out[10]:

```
array([1, 2, 3], dtype=int64)
```

Five summary table for individual seeds type

In [11]:

```
# Group the data by seed type
grouped_data = dataset_whole.groupby('Type')
print(grouped_data)
df_groupdata_stats = grouped_data.describe()
display(grouped_data.describe())
df_groupdata_stats.to_csv('groupwiseStat.csv', sep=',', index=False, encoding='utf-8')
```

```
<pandas.core.groupby.generic.DataFrameGroupBy object at 0x000002381C2BE820>
```

	Area								Perimeter		...	Asymmetry.Coeff		
	count	mean	std	min	25%	50%	75%	max	count	mean	...	75%	max	co
Type														
1	66.0	14.354394	1.178117	11.23	13.75	14.36	15.0450	17.08	66.0	14.306818	...	3.36175	6.685	(
2	68.0	18.370147	1.413670	15.38	17.35	18.72	19.1425	21.18	68.0	16.156912	...	4.45375	6.682	(
3	65.0	11.881077	0.720822	10.59	11.27	11.84	12.3800	13.37	65.0	13.256154	...	5.46200	8.315	(

3 rows × 56 columns

Mean of the dataset

In [12]:

```
#Mean information separately
```

```
print(f'Mean of the given data based on type :')
grouped_data.mean()
```

```
Mean of the given data based on type :
```

Out[12]:

Type	Area	Perimeter	Compactness	Kernel.Length	Kernel.Width	Asymmetry.Coeff	Kernel.Groove
1	14.354394	14.306818	0.879892	5.513000	3.247485	2.690670	5.087197
2	18.370147	16.156912	0.882965	6.157838	3.678647	3.657250	6.026515
3	11.881077	13.256154	0.848874	5.236862	2.851677	4.767185	5.125415

Standard deviation of the dataset

In [13]:

```
#standard deviation information separately
print(f'Standard Deviation of the given data based on type :')
grouped_data.std()
```

```
Standard Deviation of the given data based on type :
```

Out[13]:

Type	Area	Perimeter	Compactness	Kernel.Length	Kernel.Width	Asymmetry.Coeff	Kernel.Groove
1	1.178117	0.559209	0.016349	0.228527	0.173251	1.198981	0.259822
2	1.413670	0.599224	0.015371	0.259336	0.185824	1.195293	0.246663
3	0.720822	0.347975	0.020807	0.136917	0.143343	1.237093	0.160033

Conclusion of b)

Basic statistical analysis has been done on the entire data. Initially we have calculated the 5 point summary table for each type in the main dataset and next as per the request we have separately display the mean and standard deviation for each type of the seed.

c) Split the data into training and test data (80:20) and calculate the T2 statistic.

Formulation using PCA $T^2 = x^T V \Lambda^{-1} V^T x$

Formulation without PCA $z = \Lambda^{-1/2} V^T x$, $T^2 = z^T z$

In [14]:

```
X_train_scale, X_test_scale, y_train_scale, y_test_scale = datasplitting(dataset_scale,
```

In [15]:

```
print("Scaled Training data shape:", X_train_scale.shape)
print("Scaled Test data shape:", X_test_scale.shape)
```

```
Scaled Training data shape: (159, 7)
Scaled Test data shape: (40, 7)
```

Analysis on train dataset

In [16]:

```
print('Analysis on Train dataset : ')
covarince_mat_scale, eigenvalues_scale, eigenvectors_scale = eigendecomposition(X_train_
Lambda_train_scale, t_squared_values_train_scale, sum_t_squared_values_train_scale = tsq
```

```
Analysis on Train dataset :
array([[ 0.96998048,  0.96334701,  0.59931379,  0.92219736,  0.95218448,
        -0.19894364,  0.82316815],
```

```
       [ 0.96334701,  0.96850848,  0.51743217,  0.94448966,  0.92483881,
        -0.18570187,  0.85134023],
       [ 0.59931379,  0.51743217,  1.01555981,  0.3575976 ,  0.76355007,
        -0.33623986,  0.19297432],
       [ 0.92219736,  0.94448966,  0.3575976 ,  0.97394067,  0.84478869,
        -0.14487271,  0.89443549],
       [ 0.95218448,  0.92483881,  0.76355007,  0.84478869,  0.99130419,
        -0.23276407,  0.71876968],
       [-0.19894364, -0.18570187, -0.33623986, -0.14487271, -0.23276407,
         1.01922112,  0.0104037 ],
       [ 0.82316815,  0.85134023,  0.19297432,  0.89443549,  0.71876968,
         0.0104037 ,  0.95110651]])
Covariance matrix shape: (7, 7)
Eigen Vector shape: (7, 7)
Eigen Value shape: (7,)
Eigen Vector: [[ 0.4446199   0.0302841  -0.02601202  0.17782854  0.25661405 -0.72410249
  -0.42299081]
 [ 0.44110619  0.08797006  0.06025852  0.29272503  0.23821032  0.68145179
  -0.43272032]
 [ 0.2826643  -0.53341971 -0.62037301 -0.31025567 -0.34112073  0.08034061
  -0.17783444]
 [ 0.42370744  0.2026861   0.21185989  0.31944064 -0.7647388  -0.05492641
   0.211237  ]
 [ 0.43846746 -0.11065527 -0.21472648  0.13818673  0.41658418  0.01813921
   0.74594052]
 [-0.11016562  0.71878068 -0.68113547  0.07559293 -0.03357756  0.00527387
  -0.02006947]
 [ 0.37936947  0.36991302  0.23641493 -0.81214426  0.03932502  0.03834948
   0.02749006]]
Eigen Value: [4.87621224e+00 1.23797670e+00 6.89879269e-01 6.26560732e-02
 1.72535017e-02 8.33788927e-04 4.80969208e-03]
T Squared Values in a without PCA:
 [ 8.13882491  1.23670108 21.09492629  8.92054082  5.02947442 11.69291696
  4.60229843  6.64995453  7.24398194  5.55438987  4.07351861 16.9512111
  7.97039663  4.15212712  7.43444324  4.60938172  5.17924836  7.10570842
  1.52922268  4.16306111  2.95254655  2.68375153  9.99706042  9.26548297
  6.16446687  5.47830679 15.30351367  9.20873942  1.65382808  4.96869507
  6.75424073  4.55098013  2.75125083 15.61621288  9.54481     3.78318964
  9.83372446  6.0775467   6.08664904 23.58196005 10.38649918  3.92903017
  6.71343892  9.21704212 13.53557082  5.54888799  3.33882041  3.78349372
  4.42697837  8.57572218  8.52188964  8.26346     3.72788055 12.00572676
  2.69241881  2.58458613  9.93306193  4.51108036  5.15324549 11.29601839
 10.87344399  3.27759015  2.34344232  5.68784796 11.82173965  3.30033672
 12.65691465 13.88556494  4.60444625  8.17826818  5.87486244  6.95820998
  5.35126898  9.19555378  6.30918259 13.94091329  5.00750794 11.18451816
  5.95950136  5.47556436  5.6336645   4.66475512 12.48263204  4.52732595
  3.50397833 10.36767905  8.14360916  4.27068059  4.76214348 10.90646275
  9.44617242  6.97060868  7.60052302  2.86550461 10.09848442  7.55128126
  4.84735381  4.8390176   8.67157769  3.27423967  5.6159516   4.8840861
  2.39583654  3.8936841   4.33571725  5.40854165  5.90433233 10.43719359
  4.09989932  2.4382669   4.42462878 11.73743608  3.51674416  7.1024437
  7.81720723  4.86045652  4.638807    3.83816478  3.72724993  4.57797516
 13.77395788  5.28595618  6.81406693  3.00965935  7.13053808  4.36034498
  8.73940005  2.47981027 12.4489993  11.24031369  1.59086883  4.57602463
  2.36746041  3.92459912  5.63978891  3.77932796  4.41686507  2.72187544
 11.56896208  9.29155384  1.92695751  6.65850519 17.92385646  4.83574279
  4.60118113 17.37722591  6.45800181  5.74936011  8.42181345  4.25626672
  7.58467286  4.68281604  5.01229667 16.71657718  8.43512161  2.08202953
  2.05682231 15.15786671 11.91283974]
Scale Train Dataset :
T Squared Values with PCA:
 [8.13882491384439, 1.2367010821001228, 21.094926288066432, 8.920540822092203, 5.0294744
18188186, 11.692916958298257, 4.6022984285373925, 6.649954533841717, 7.243981943230949,
5.554389868202854, 4.073518614275013, 16.95121109745561, 7.970396629349359, 4.1521271166
98981, 7.434443237589036, 4.609381721534699, 5.179248357976144, 7.105708415997523, 1.529
2226751955793, 4.163061106752796, 2.952546547722268, 2.6837515306321102, 9.9970604215996
```

```
97, 9.26548296630822, 6.164466871272035, 5.4783067886129455, 15.303513666583214, 9.20873
9416326313, 1.6538280847451197, 4.968695066363118, 6.754240729395844, 4.550980133764817,
2.75125083240547, 15.616212876222086, 9.544810002443207, 3.783189639630023, 9.8337244573
1061, 6.077546699244152, 6.086649044450844, 23.5819600492265, 10.386499182790546, 3.929
0301711897477, 6.713438919352948, 9.217042117211928, 13.53557082475716, 5.54888798756436
3, 3.338820412694245, 3.7834937248495915, 4.426978372826483, 8.57572217592259, 8.5218896
41274202, 8.263460000927454, 3.727880551423873, 12.005726762443082, 2.692418809076801,
2.5845861329617925, 9.933061927806953, 4.511080362644873, 5.153245486335267, 11.29601839
2317134, 10.8734439928444, 3.277590151837914, 2.3434423206229273, 5.687847960345104, 11.
821739646642975, 3.300336718214655, 12.656914653763797, 13.885564941325843, 4.6044462527
47834, 8.178268177490589, 5.874862435548876, 6.95820998160852, 5.351268979974606, 9.195
553778306635, 6.3091825892065785, 13.940913287512373, 5.007507936629312, 11.184518160090
956, 5.959501363850383, 5.475564357120878, 5.633664501715668, 4.664755117040384, 12.4826
32042240745, 4.527325953654611, 3.503978333273607, 10.367679049798662, 8.14360915790966
7, 4.270680586356384, 4.762143475015012, 10.906462745995285, 9.446172423755272, 6.970608
6842030395, 7.600523020914651, 2.865504609363125, 10.098484417156843, 7.551281258905821,
4.8473538087763846, 4.839017598995613, 8.671577689549183, 3.274239667162341, 5.615951595
681793, 4.8840860960905745, 2.3958365382032474, 3.8936840974011253, 4.335717253380257,
5.408541649283386, 5.904332334285032, 10.437193591604599, 4.099899322140906, 2.438266901
243238, 4.424628781293438, 11.737436081117608, 3.516744163971893, 7.102443700391088, 7.8
17207231415863, 4.860456524232341, 4.638806999443669, 3.8381647849798575, 3.727249934565
508, 4.577975155325884, 13.77395787834563, 5.2859561821326455, 6.814066927477706, 3.0096
5934952963, 7.1305380770331155, 4.360344979206007, 8.739400045377412, 2.47981027491413,
12.448999301669675, 11.240313692009993, 1.5908688323540643, 4.576024631506845, 2.3674604
09907139, 3.924599123162026, 5.639788909966537, 3.779327963521915, 4.416865074966853, 2.
721875436001497, 11.568962078943404, 9.291553837971062, 1.9269575061180628, 6.6585051934
93582, 17.923856461225387, 4.835742794466712, 4.601181130982387, 17.377225914843557, 6.4
58001809255805, 5.749360108358253, 8.421813449176227, 4.256266724751586, 7.5846728586835
36, 4.682816041082498, 5.012296669762042, 16.716577183194296, 8.435121607782477, 2.08202
9533580849, 2.056822307931184, 15.157866711403955, 11.912839735027012]
Sum of T Squared Values :  1107.7134573204887
```

Analysis on test dataset

As per general process to calculate the T-squared value using PCA:

- Perform PCA on the training data to obtain the eigenvectors and eigenvalues.
- Calculate the T-squared statistic for each observation in the test data using the eigenvectors and eigenvalues obtained from PCA.

In [17]:

```python
Lambda_test_scale, t_squared_values_test_scale, sum_t_squared_values_test_scale = tsquar
```

```
T Squared Values in a without PCA:
 [17.97155017  6.80592556  5.50127547  5.65725954  8.0396095   5.77217545
  4.03445262  3.00241146 12.54252833  7.28318068 13.18650766  7.50862326
  6.23381861  7.29001726 10.64162135  5.91240681  6.922252    4.73017239
 18.87708884  3.48900462  9.51545672  1.25711585  9.67187523  5.48889851
  4.70654293  3.84898714  4.94566494  7.53919448  2.80443316 14.37988432
  8.43320372 58.59438464  2.75988509  6.66049781 13.20741235  5.46526952
  7.69906123  5.23101903  6.84047085  7.85321699]
Scale Test Dataset :
T Squared Values with PCA:
 [17.971550165014854, 6.805925558256483, 5.501275471155701, 5.657259544247429, 8.0396095
03680417, 5.772175453332268, 4.034452621218396, 3.0024114593468343, 12.542528330103499,
7.2831806768427, 13.186507664826166, 7.508623255239154, 6.233818606354115, 7.29001725783
9727, 10.641621352936081, 5.912406812535059, 6.922252002986429, 4.730172393957201, 18.87
7088836442873, 3.489004622573003, 9.515456722511141, 1.2571158509818683, 9.6718752293720
16, 5.488898507864132, 4.706542931358148, 3.8489871432005067, 4.945664935745864, 7.53919
4483770487, 2.8044331625250845, 14.379884319037942, 8.433203723169978, 58.5943846385128
9, 2.7598850909318733, 6.660497809256992, 13.207412354166735, 5.465269516901283, 7.69906
1234123771, 5.231019032217535, 6.840470852079385, 7.8532169909451]
Sum of T Squared Values :  348.3043561175611
```

Conclusion of c)

We have analyze the T squared statistics on the scaled data after splitting them into train and test set. In first cell we have given the report for train dataset and in next cell same report has been given for test dataset.

We have calculated the T Squared statistics using below two possible way,

- **Using PCA** : Using PCA method we have find out the eigen value and vector of the covariance matrix of the dataset and then perfom T Squared calculating using $T^2 = x^T V \Lambda^{-1} V^T x$.
- **Without using PCA** : In this method without PCA we are using $z = \Lambda^{-1/2} V^T x$, $T^2 = z^T z$ formulation to calculate the same.

Using both the formulation we are getting same value as the T Squared statistics.

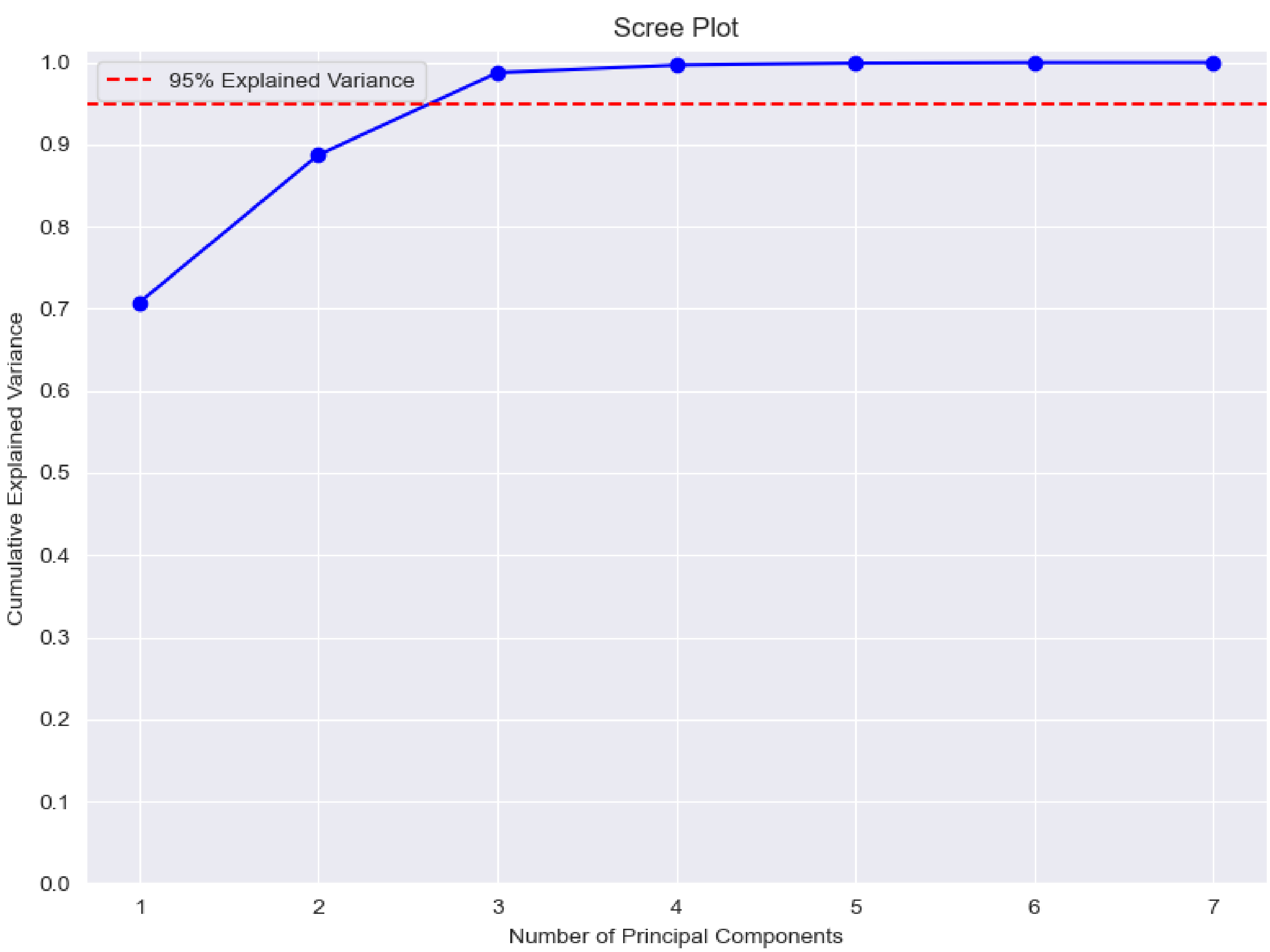
Moreover on test dataset we are following below in general consideration,

- Calculate the T-squared statistic for each observation in the test data using the eigenvectors and eigenvalues obtained from PCA of Train data

d) Perform PCA and visualize the explained variance ratio for the training set.

In [18]:
```
perform_PCA(X_train_scale)
```

```
Number of total component : 7
Considerable Principle Component :  3
```




```
Explained Variance Ratio:
Principal Component 1: 0.7078
```

```
Principal Component 2: 0.1797
Principal Component 3: 0.1001
Principal Component 4: 0.0091
Principal Component 5: 0.0025
Principal Component 6: 0.0007
Principal Component 7: 0.0001

Cumulative Explained Variance:
Principal Components 1: 0.7078
Principal Components 2: 0.8874
Principal Components 3: 0.9876
Principal Components 4: 0.9967
Principal Components 5: 0.9992
Principal Components 6: 0.9999
Principal Components 7: 1.0000
```

Out[18]:

```
(3,
 array([[ 2.91227405,  0.78722967,  0.42897615, ..., -0.02472031,
         -0.05352962,  0.00722962],
        [-1.20394502,  0.07443273,  0.25963188, ..., -0.06520818,
         -0.00970153, -0.01526807],
        [ 2.89880671, -2.54645106, -1.09249702, ..., -0.43710109,
          0.02350067, -0.02691593],
        ...,
        [-1.97989981, -0.48594054,  0.2770536 , ..., -0.01557391,
         -0.02190397, -0.00569306],
        [-3.18433125, -1.82110649, -1.02961763, ...,  0.12881505,
          0.16043915,  0.04483931],
        [-0.60008419, -0.46027835,  2.30203398, ..., -0.11540018,
         -0.06251794, -0.02797115]]),
 array([7.07762017e-01, 1.79687192e-01, 1.00133119e-01, 9.09426960e-03,
        2.50427433e-03, 6.98106891e-04, 1.21021010e-04]))
```

Conclusion of d)

We are performing the PCA on a train dataset and based on the eigen values we have caluclated the explained variance for each principle component and plotted. While finalizing the minimum considerable principle components need to keep for further reconstruction we have considered to maintain 95% explained variance as a threshold. Considering the same we have got minimum 3 principle components should be reserve for further resconstruction.

e) Find the T2 statistic threshold for the training data with 90% confidence interval using PCA representation

- Assuming that the T2 statistic follows a χ2 distribution
- Using the sample covariance

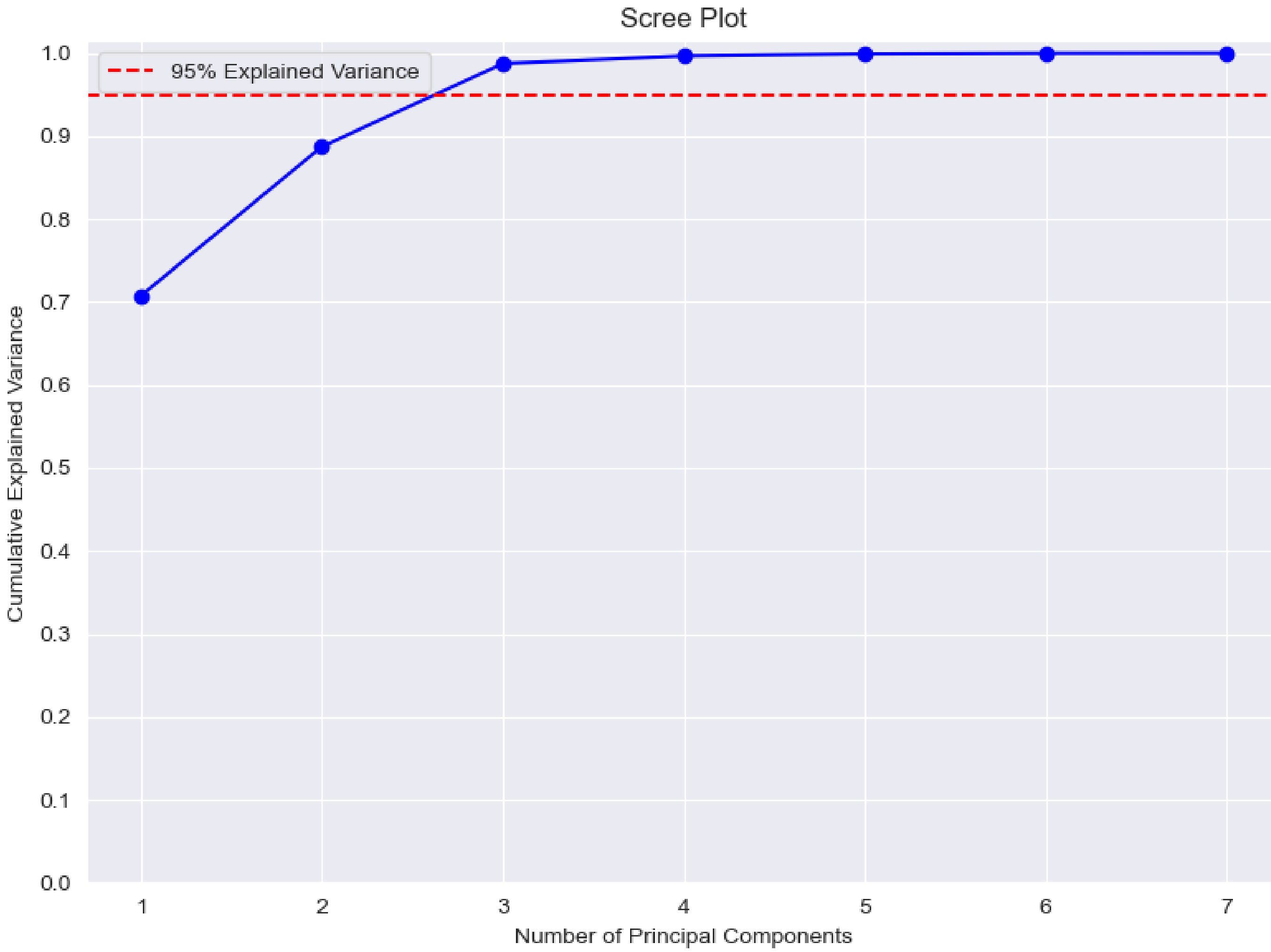
Formulation

T Squared threshold when actual covariance matrix is estimated from sample covariance : $\frac{a(n-1)(n+1)F_\alpha}{n(n-a)}$

In [19]:

```
considerable_PC_scale, transformed_data_scale, variance_explained_ratio_scale = perform_
```

```
Number of total component : 7
Considerable Principle Component :  3
```




```
Explained Variance Ratio:
Principal Component 1: 0.7078
Principal Component 2: 0.1797
Principal Component 3: 0.1001
Principal Component 4: 0.0091
Principal Component 5: 0.0025
Principal Component 6: 0.0007
Principal Component 7: 0.0001

Cumulative Explained Variance:
Principal Components 1: 0.7078
Principal Components 2: 0.8874
Principal Components 3: 0.9876
Principal Components 4: 0.9967
Principal Components 5: 0.9992
Principal Components 6: 0.9999
Principal Components 7: 1.0000
```

In [20]:
```
print('Conclusion :')
print('Result with scale data : ')
statisticalAnalysis(X_train_scale, considerable_PC_scale, transformed_data_scale, alpha_
```

```
Conclusion :
Result with scale data :
Part 1 : Assuming that the T2 statistic follows a χ2 distribution
Total Number of Features: 7
Considerable Principle Component :  3
Degree of Freedom 3
T2 Statistic Threshold: 6.251388631170325
Part 2 : Using sample covariance
Critical value F_alpha(a, n-a): 2.1192236622197966
T2 Statistic Threshold: 6.482064834102407
```

Conclusion of e)

We have performed the analysis on scaled train data of the given dataset. The problem statement has two assumption to made.

- Assuming that the T2 statistic follows a χ2 distribution
- Using sample covariance

As per the assumption and considering that there are only 3 considerable principle components we have achieved the threshold as below,

- **Assuming that the T2 statistic follows a χ2 distribution**
  - T2 Statistic Threshold: 6.251388631170325
- **Using sample covariance**
  - T2 Statistic Threshold: 6.482064834102407

f) Report whether there are faults in the test data and outliers in the training set.

Outlier Detection : -

Formulation:

Outliers in the training set can be detected using the T^2 statistic for a selected confidence level = $\frac{(n-1)^2(a/(n-a-1))F_\alpha(a,n-a-1)}{n(1+(a/(n-a-1)))}$

We have calculated the T Squared statistics using below two possible way,

- **Using PCA** : Using PCA method we have find out the eigen value and vector of the covariance matrix of the dataset and then perfom T Squared calculating using $T^2 = x^T V \Lambda^{-1} V^T x$.
- **Without using PCA** : In this method without PCA we are using $z = \Lambda^{-1/2} V^T x$, $T^2 = z^T z$ formulation to calculate the same.

Fault Identification : -

Formulation:

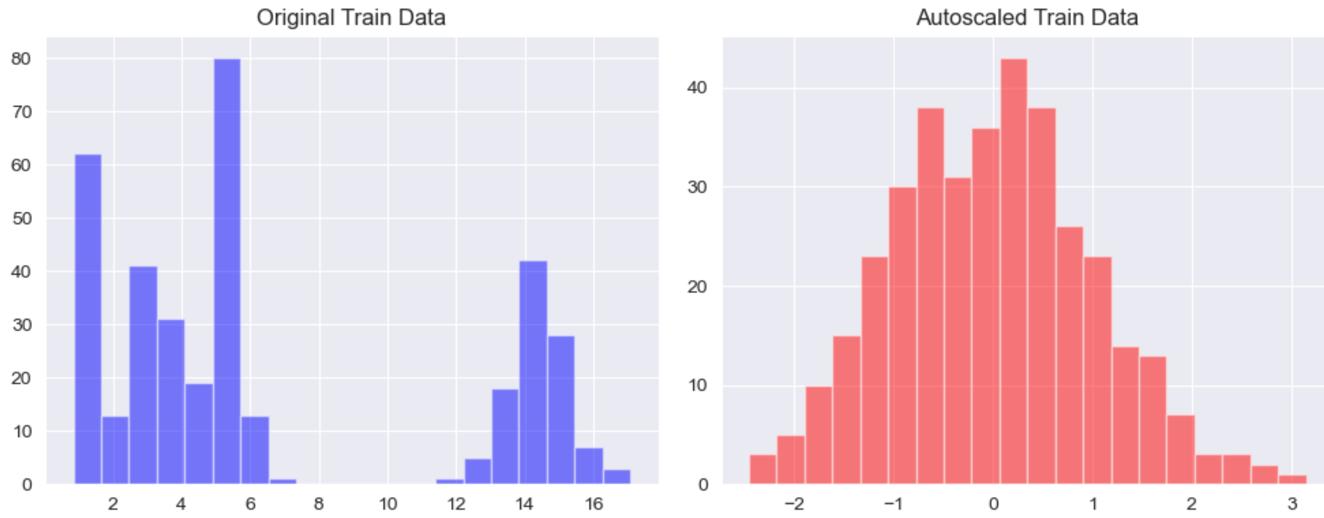
Faults in the test set can be detected using the T^2 statistic for a selected confidence level = $\frac{a(n-1)(n+1)F_\alpha}{n(n-a)}$z

We have calculated the T Squared statistics using below two possible way,

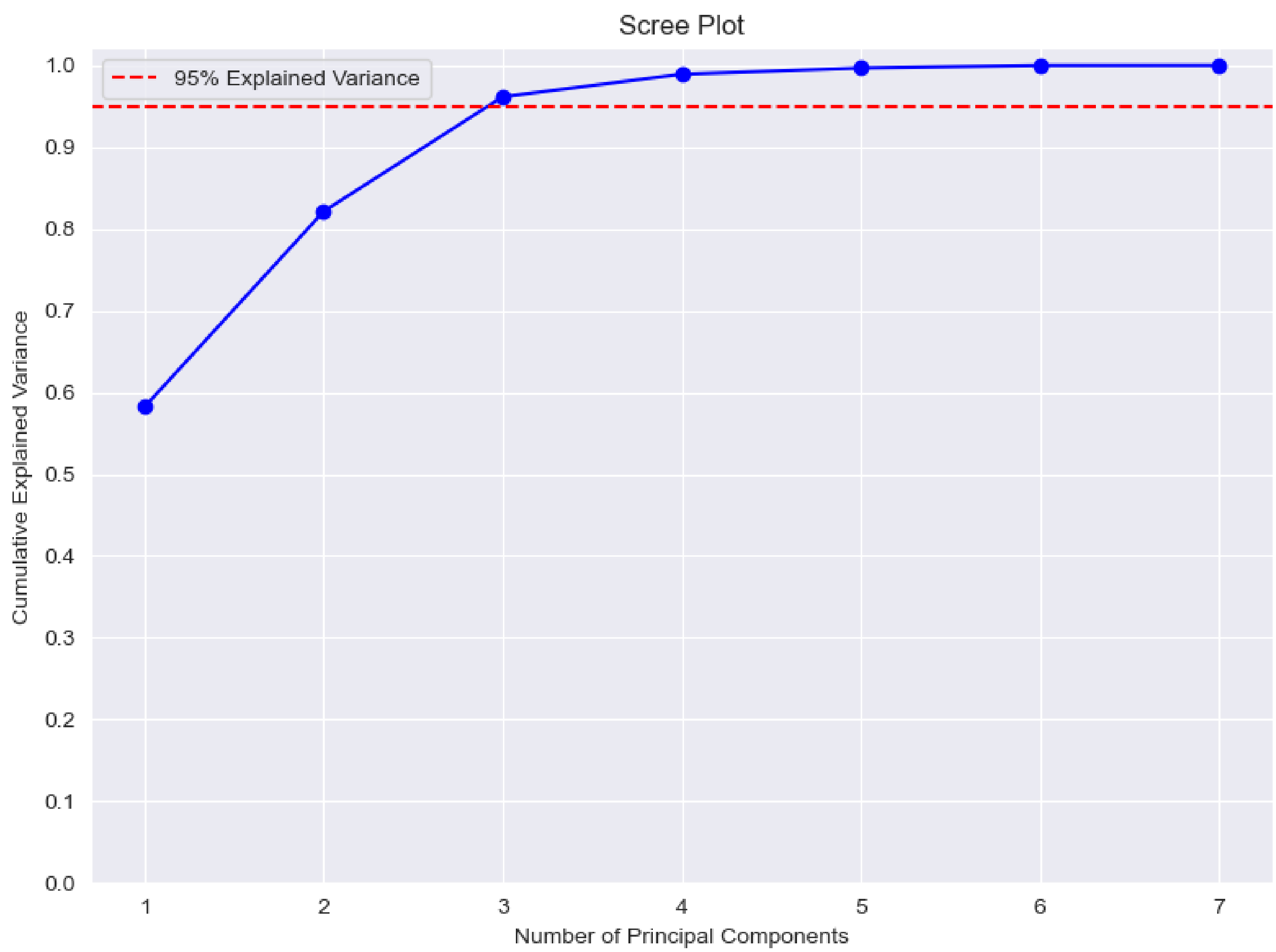
- **Using PCA** : Using PCA method we have find out the eigen value and vector of the covariance matrix of the dataset and then perfom T Squared calculating using $T^2 = x^T V \Lambda^{-1} V^T x$.
- **Without using PCA** : In this method without PCA we are using $z = \Lambda^{-1/2} V^T x$, $T^2 = z^T z$ formulation to calculate the same.

For Type 1 - Fault & Outlier Analysis

In [21]:
```
OutlierAndFaultAnalysis(dataset_whole, unique_type[0], alpha_90)
```



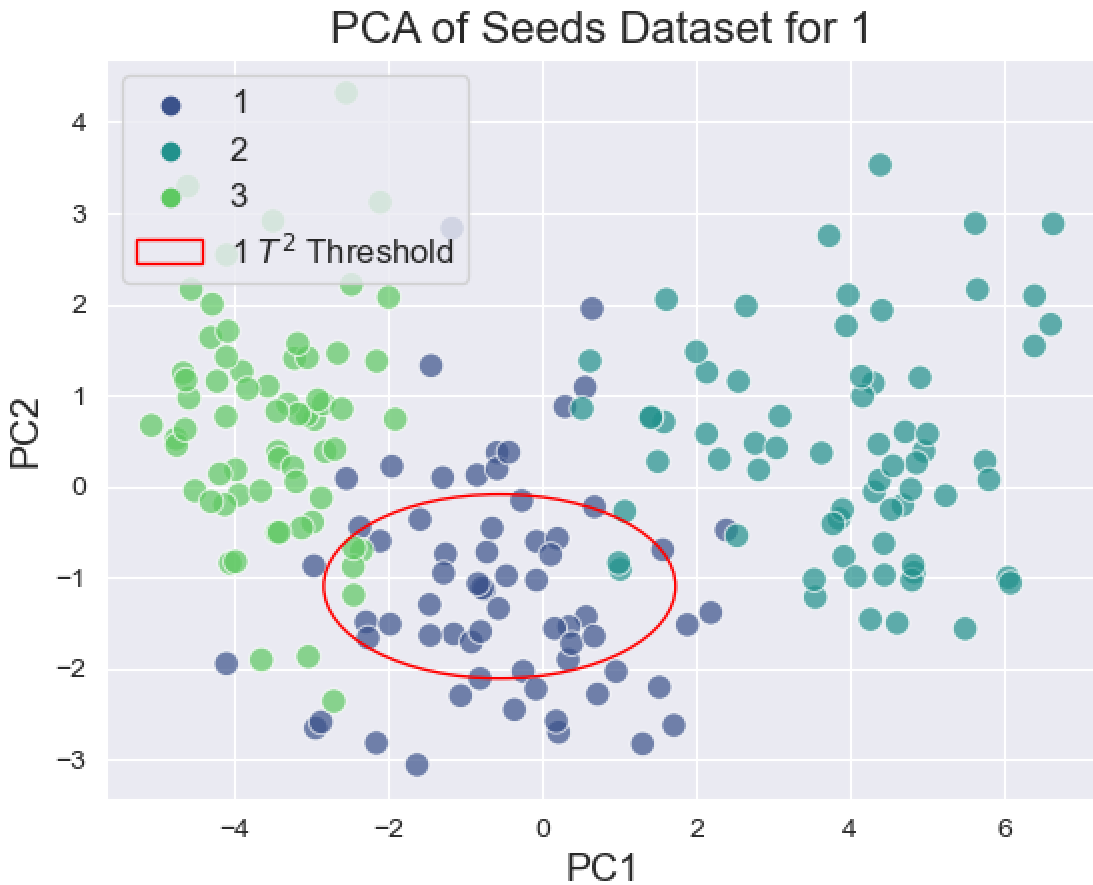

```
Number of total component : 7
Considerable Principle Component :  3
```

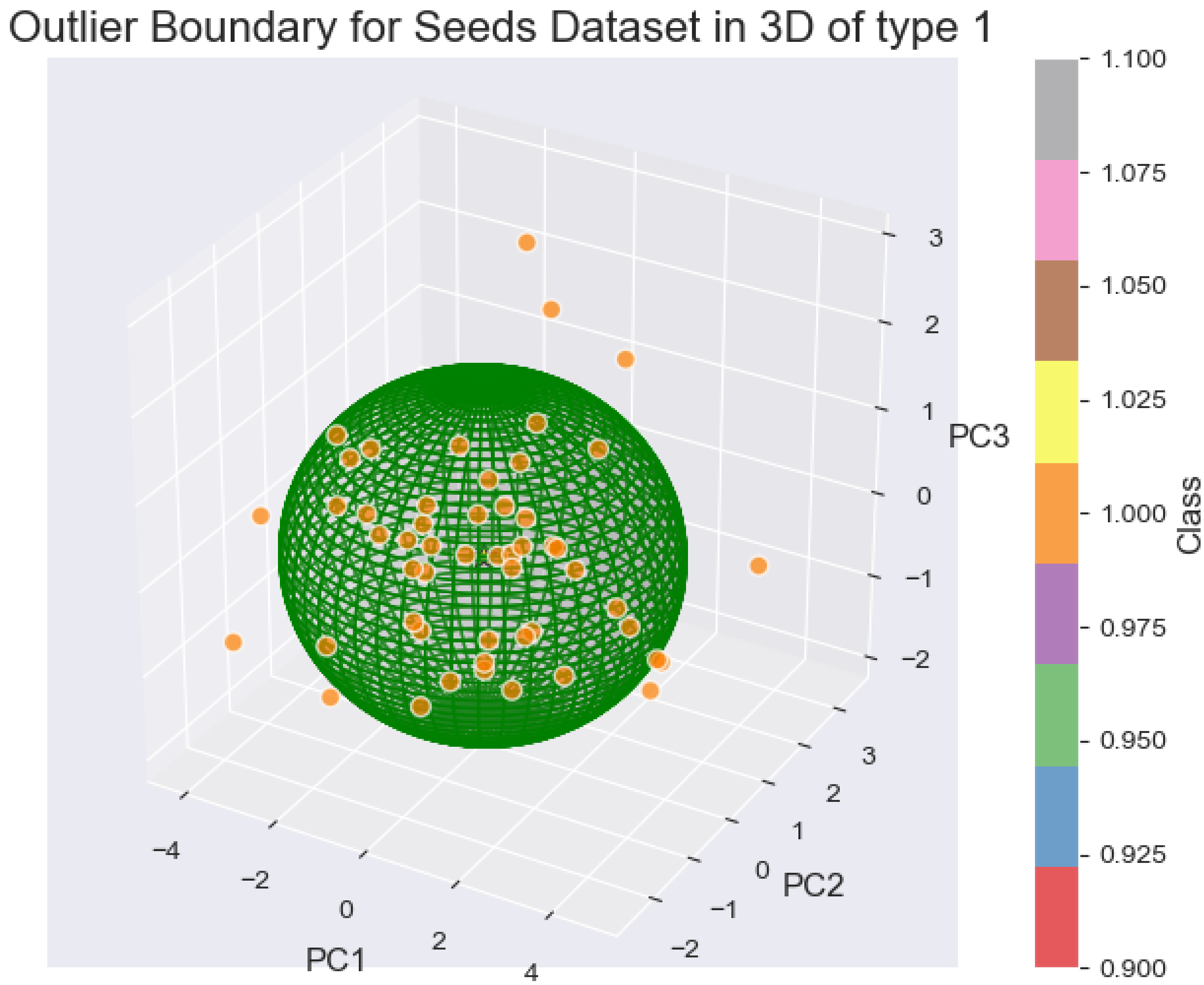


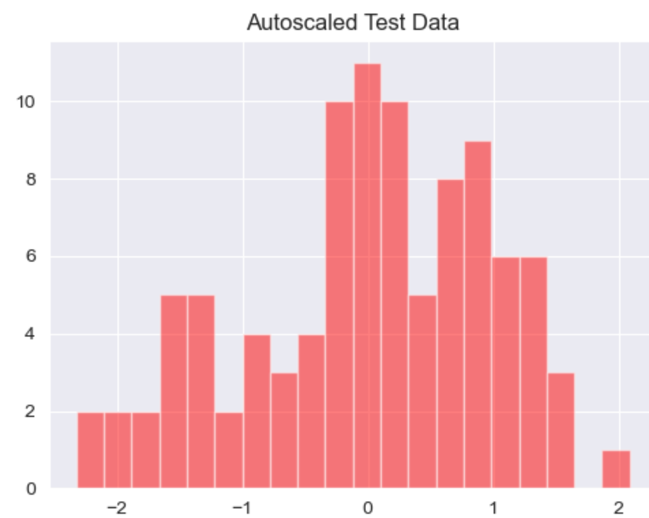

```
Explained Variance Ratio:
Principal Component 1: 0.5823
Principal Component 2: 0.2390
Principal Component 3: 0.1402
Principal Component 4: 0.0276
Principal Component 5: 0.0076
Principal Component 6: 0.0033
Principal Component 7: 0.0001

Cumulative Explained Variance:
Principal Components 1: 0.5823
Principal Components 2: 0.8213
Principal Components 3: 0.9615
Principal Components 4: 0.9891
Principal Components 5: 0.9967
```

```
Principal Components 6: 0.9999
Principal Components 7: 1.0000
array([[ 1.01960784,  0.98926744,  0.35175141,  0.82120606,  0.8925949 ,
        -0.03288472,  0.71765183],
       [ 0.98926744,  1.01960784,  0.11166391,  0.92816604,  0.76448611,
        -0.0636939 ,  0.81091111],
       [ 0.35175141,  0.11166391,  1.01960784, -0.22245547,  0.69509785,
         0.13349525, -0.19458253],
       [ 0.82120606,  0.92816604, -0.22245547,  1.01960784,  0.46802707,
        -0.08693783,  0.89786016],
       [ 0.8925949 ,  0.76448611,  0.69509785,  0.46802707,  1.01960784,
         0.00114736,  0.37920914],
       [-0.03288472, -0.0636939 ,  0.13349525, -0.08693783,  0.00114736,
         1.01960784, -0.01442654],
       [ 0.71765183,  0.81091111, -0.19458253,  0.89786016,  0.37920914,
        -0.01442654,  1.01960784]])
Covariance matrix shape: (7, 7)
Eigen Vector shape: (7, 7)
Eigen Value shape: (7,)
Eigen Vector: [[ 4.86160122e-01  1.24119043e-01 -2.74144610e-02  1.66107410e-01
  -7.25853912e-01 -4.35038767e-01 -6.14568465e-02]
 [ 4.88721972e-01 -5.71232379e-02 -7.62770952e-04  2.83174421e-01
   6.68659120e-01 -4.79925281e-01  1.63138335e-02]
 [ 1.02001280e-01  7.34169928e-01 -8.79952986e-02 -4.31190469e-01
   1.58836146e-01 -3.28175236e-02 -4.80224897e-01]
 [ 4.40250806e-01 -3.23086852e-01  6.16900977e-02  1.66587957e-01
  -6.54503712e-03  5.55408132e-01 -6.01428190e-01]
 [ 3.94754649e-01  4.38984325e-01 -1.08261584e-01  1.92216236e-01
   2.69136836e-02  5.20389271e-01  5.75555851e-01]
 [-2.46029682e-02  1.90723679e-01  9.75889070e-01  1.01917607e-01
  -2.95319024e-03  7.20957194e-03  1.45532454e-02]
 [ 4.05138985e-01 -3.29936423e-01  1.53684666e-01 -7.94486959e-01
   5.12375195e-03 -9.17280936e-04  2.68605214e-01]]
Eigen Value: [4.15603589e+00 1.70603001e+00 1.00064933e+00 1.96773412e-01
 4.27673791e-04 2.34026124e-02 5.39359824e-02]
Lambda : [[4.15603589e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 1.70603001e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 1.00064933e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 1.96773412e-01
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  5.39359824e-02 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 2.34026124e-02 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 4.27673791e-04]] & Lambda Incerse : [[2.40613899e-01
0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 5.86156161e-01 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 9.99351095e-01 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 5.08198739e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  1.85404985e+01 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 4.27302723e+01 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 2.33823073e+03]]
T_squared statistic : [ 1.23373886  1.63810081  1.53234106  4.19149616  5.23451515
1.11615806
```

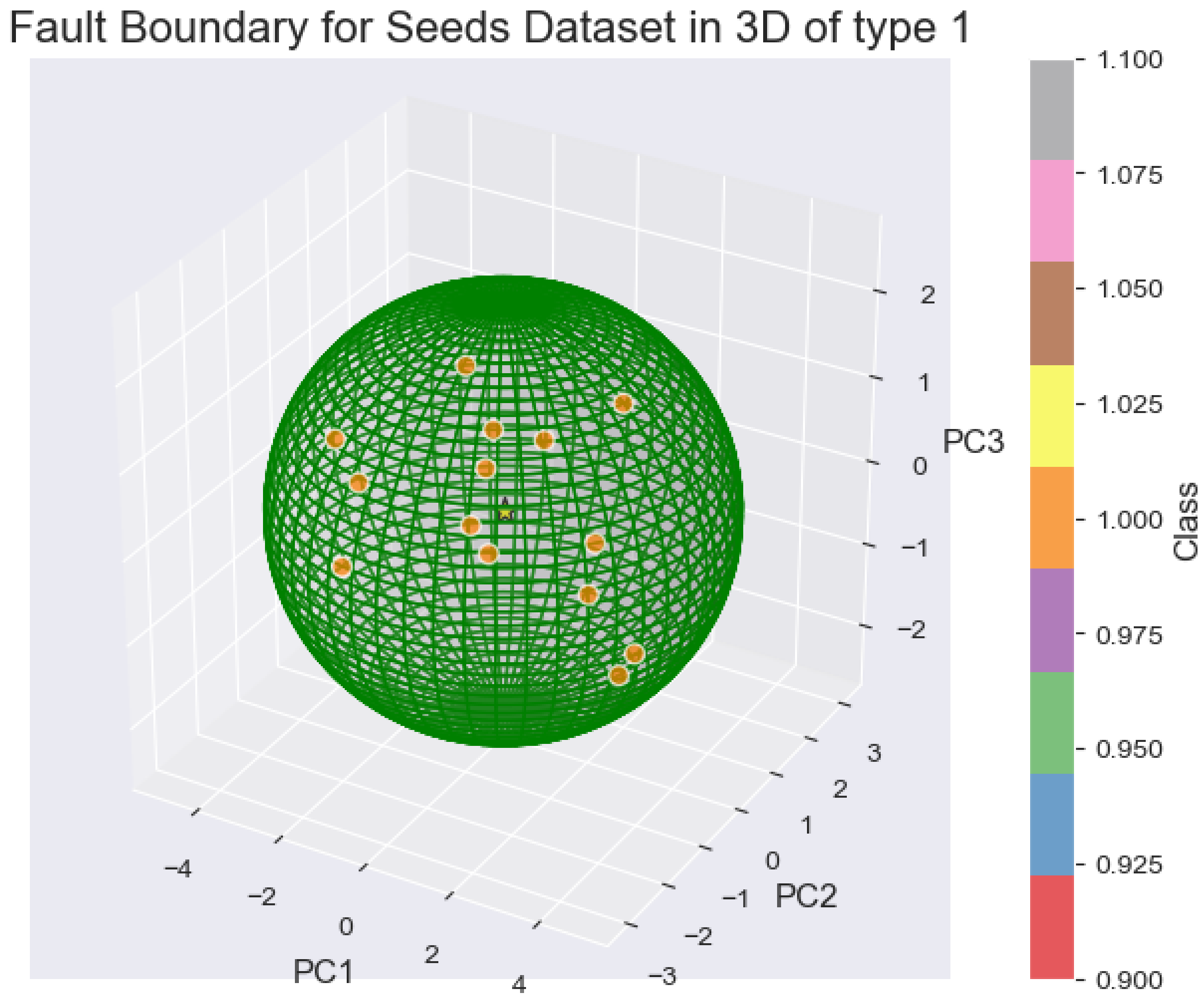
```
  4.51205455  0.22373134  3.23847564  4.19443569  2.9412283   1.16242314
  2.2435211   0.93712763  0.58813345  3.83273885  2.10821125  2.82890186
  6.76319178  2.0620459   0.91827338  0.53577968  0.35819359  4.89547825
  9.28168284  1.45568745  1.10183677  0.05036428  0.49639803  4.53970467
  2.55571481  0.44223499  1.17888849  3.25425429  6.70450201  3.64940154
  6.07749886  2.64021354  6.53667015  4.55810176  2.47830263  0.09633501
  7.95999922  1.93350334  2.86238874  1.43339465  0.41569832  4.0212082
  1.68929047  0.47622034  5.80793937 10.01226974]
Outlier Threhold : 6.477758924920254
```





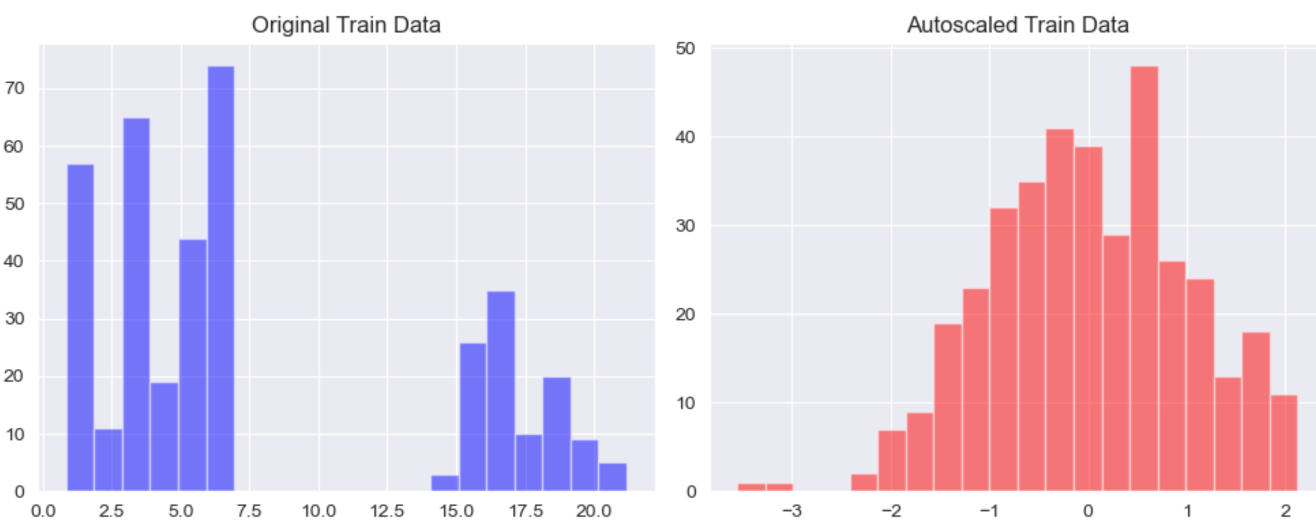



```
Fault Threhold : 10.105414155861743
T_squared statistic [0.30086346 2.64237014 2.84280146 1.2421455  4.17202916 5.3537633
8
 8.57669644 1.04922049 2.85543364 4.91957729 0.68285452 2.5199176
 0.26563116 3.10970974]
```

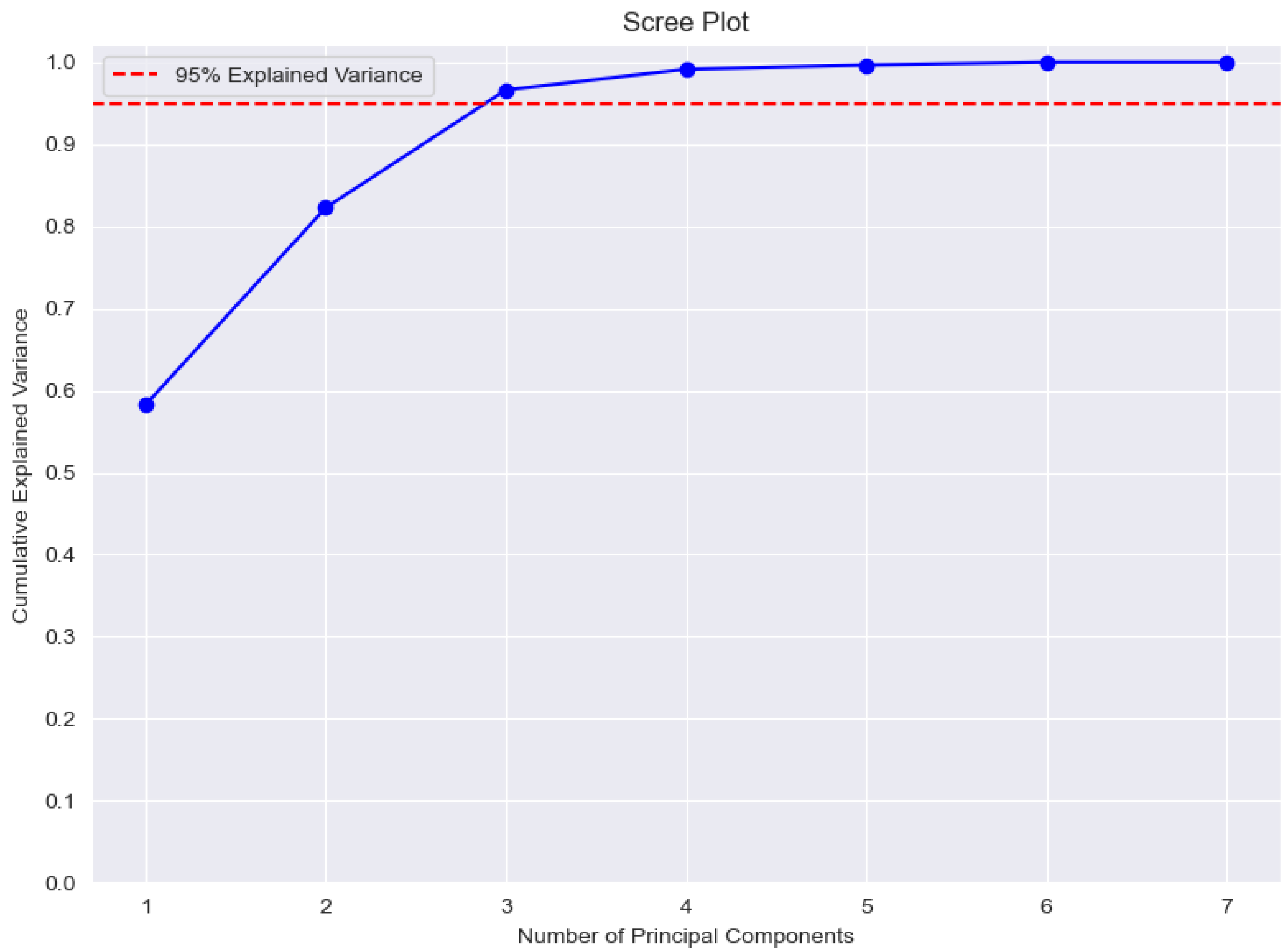


For Type 2 - Fault & Outlier Analysis

In [22]:
```
OutlierAndFaultAnalysis(dataset_whole, unique_type[1], alpha_90)
```

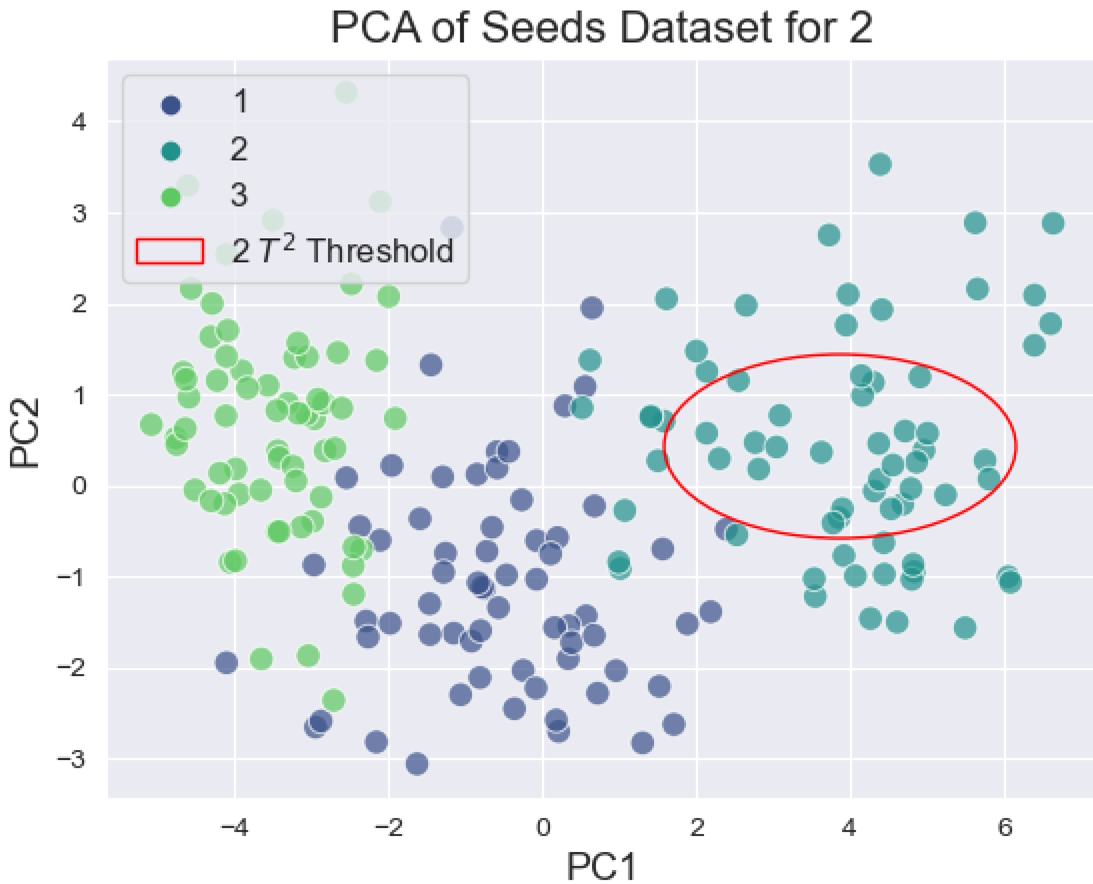



```
Number of total component : 7
Considerable Principle Component :  3
```

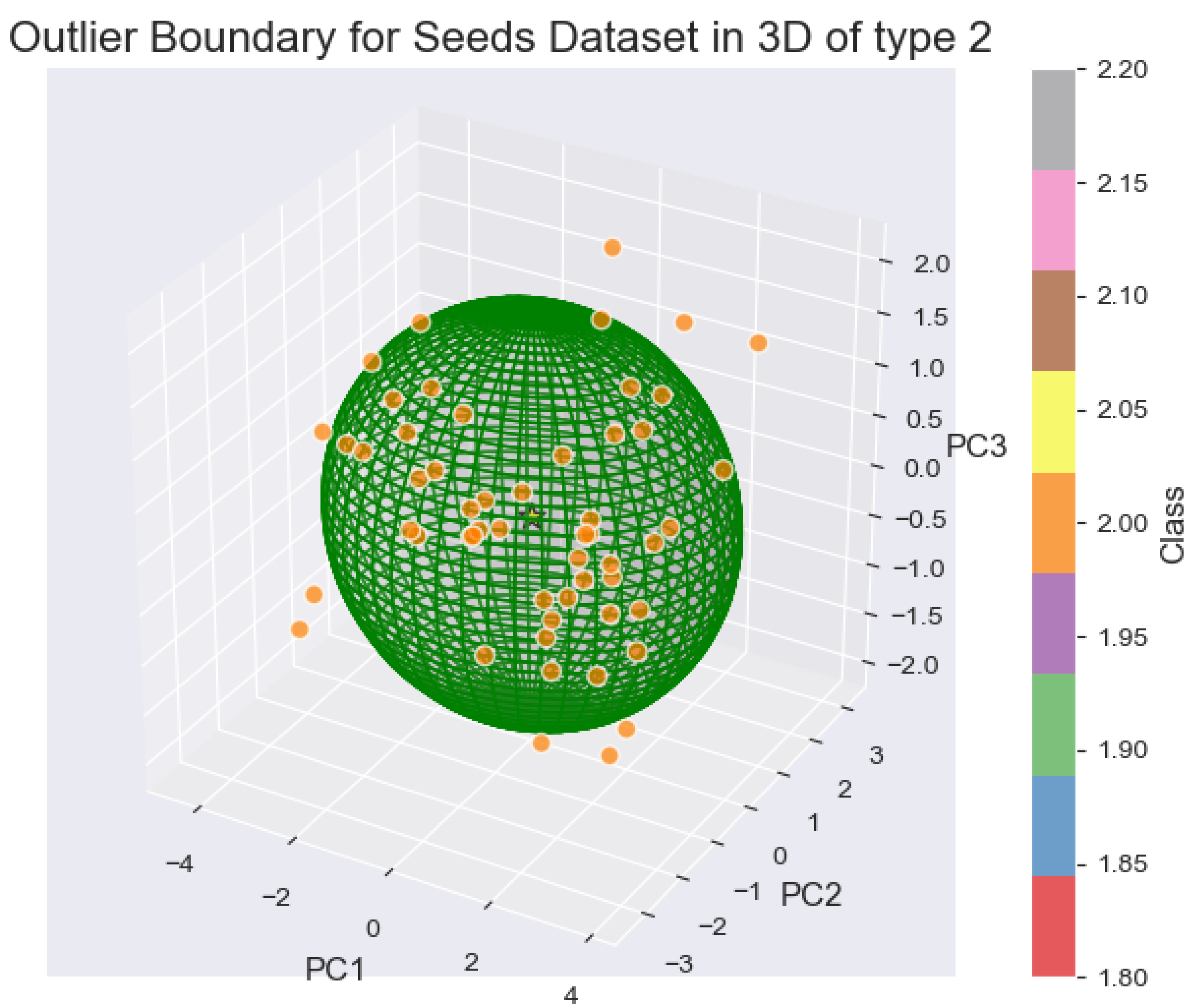



```
Explained Variance Ratio:
Principal Component 1: 0.5824
Principal Component 2: 0.2401
Principal Component 3: 0.1436
Principal Component 4: 0.0252
Principal Component 5: 0.0051
Principal Component 6: 0.0035
Principal Component 7: 0.0000

Cumulative Explained Variance:
Principal Components 1: 0.5824
Principal Components 2: 0.8225
Principal Components 3: 0.9661
Principal Components 4: 0.9913
Principal Components 5: 0.9965
Principal Components 6: 1.0000
Principal Components 7: 1.0000
array([[ 1.01886792,  0.99361793,  0.34390953,  0.81302107,  0.89805514,
        -0.01682255,  0.69739508],
       [ 0.99361793,  1.01886792,  0.12481932,  0.90405923,  0.78236247,
        -0.0134955 ,  0.79364183],
       [ 0.34390953,  0.12481932,  1.01886792, -0.19980834,  0.70203192,
        -0.05150407, -0.24579297],
       [ 0.81302107,  0.90405923, -0.19980834,  1.01886792,  0.48877586,
         0.00591962,  0.94886106],
       [ 0.89805514,  0.78236247,  0.70203192,  0.48877586,  1.01886792,
         0.03872785,  0.35903265],
       [-0.01682255, -0.0134955 , -0.05150407,  0.00591962,  0.03872785,
         1.01886792, -0.03354219],
       [ 0.69739508,  0.79364183, -0.24579297,  0.94886106,  0.35903265,
        -0.03354219,  1.01886792]])
Covariance matrix shape: (7, 7)
Eigen Vector shape: (7, 7)
Eigen Value shape: (7,)
```

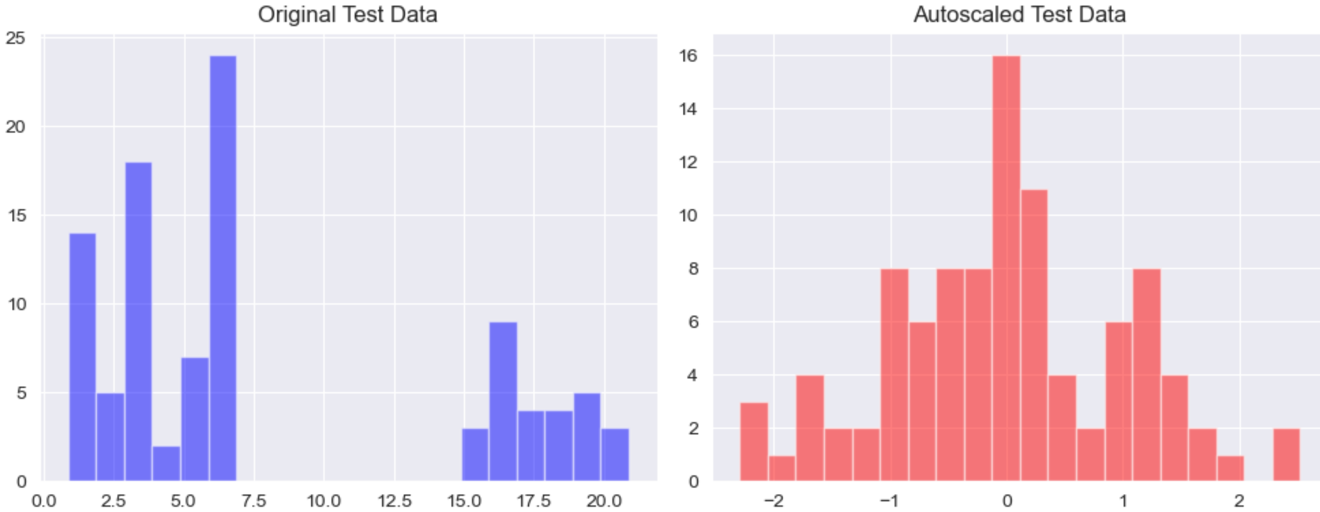
```
Eigen Vector: [[ 4.84352604e-01  1.27626025e-01 -1.41587935e-03 -2.54677935e-01
   7.15889754e-01 -3.72725654e-01  1.81187043e-01]
 [ 4.86952210e-01 -3.70862039e-02 -1.30671548e-03 -3.87733362e-01
  -6.79859151e-01 -3.07198201e-01  2.33632385e-01]
 [ 1.01941228e-01  7.33818040e-01 -3.35602406e-02  5.18520720e-01
  -1.58925662e-01 -3.57310380e-01 -1.67931445e-01]
 [ 4.43609074e-01 -3.19341024e-01  5.48540492e-03  9.23124021e-02
  -1.74349735e-03 -3.90155729e-03 -8.32263401e-01]
 [ 3.98355797e-01  4.43207223e-01  6.06284094e-02 -1.52827839e-01
   7.28750738e-04  7.85723774e-01  2.20337062e-02]
 [-4.92294700e-03 -1.64261602e-02  9.96693518e-01  5.46230720e-02
  -5.15838192e-03 -5.49813971e-02  1.65750940e-02]
 [ 4.02973322e-01 -3.81006752e-01 -4.20254107e-02  6.93596889e-01
   2.41867492e-03  1.36506850e-01  4.36993830e-01]]
Eigen Value: [4.15382873e+00 1.71210537e+00 1.02444642e+00 1.79919498e-01
 3.23129411e-04 2.49592084e-02 3.64931232e-02]
Lambda : [[4.15382873e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 1.71210537e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 1.02444642e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 1.79919498e-01
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  3.64931232e-02 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 2.49592084e-02 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 3.23129411e-04]] & Lambda Incerse : [[2.40741751e-01
0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 5.84076201e-01 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 9.76136950e-01 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 5.55804131e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  2.74024231e+01 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 4.00653733e+01 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 3.09473531e+03]]
T_squared statistic : [ 0.37901168  3.64130249  8.13497476  0.10107191  3.06548708
2.66750466
  0.89383902  0.76422453  0.38975618  2.75226731  1.90534414  1.55185129
  1.33867389  1.9155648   2.65919647  4.05965768  4.78575106  3.57169661
  0.94159863  1.21421419  4.10233584  2.30380734  1.07766653  4.84918728
  0.21302546  3.9625555   1.34501884  3.65229826  0.76479274  4.50782358
  1.61341254  3.96122256  2.5582729   3.05857211  3.71449386  7.43080565
  1.77618393  0.25509732  5.6485883   2.05021169  3.71793879  3.90469522
  2.7721829   0.84333246  3.77531506 10.80788527  1.0871005   6.4170714
  3.03142486  2.50548522  5.8581722   3.61042547  1.40243627  3.68817376]
Outlier Threhold : 6.468148729842601
```



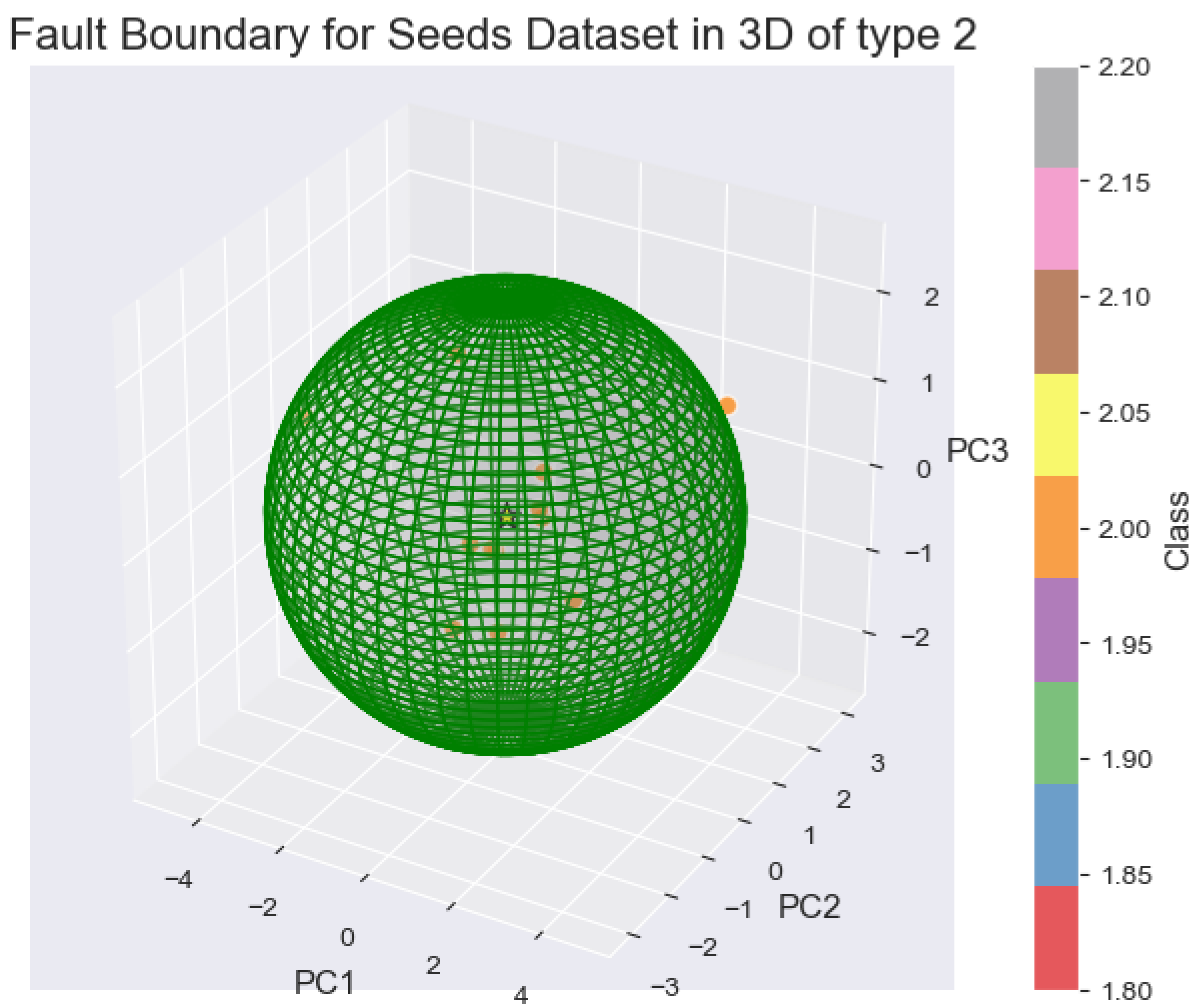
PCA of Seeds Dataset for 2
1
2
3
2 T^2 Threshold
PC2
PC1



Outlier Boundary for Seeds Dataset in 3D of type 2
PC1
PC2
PC3
Class

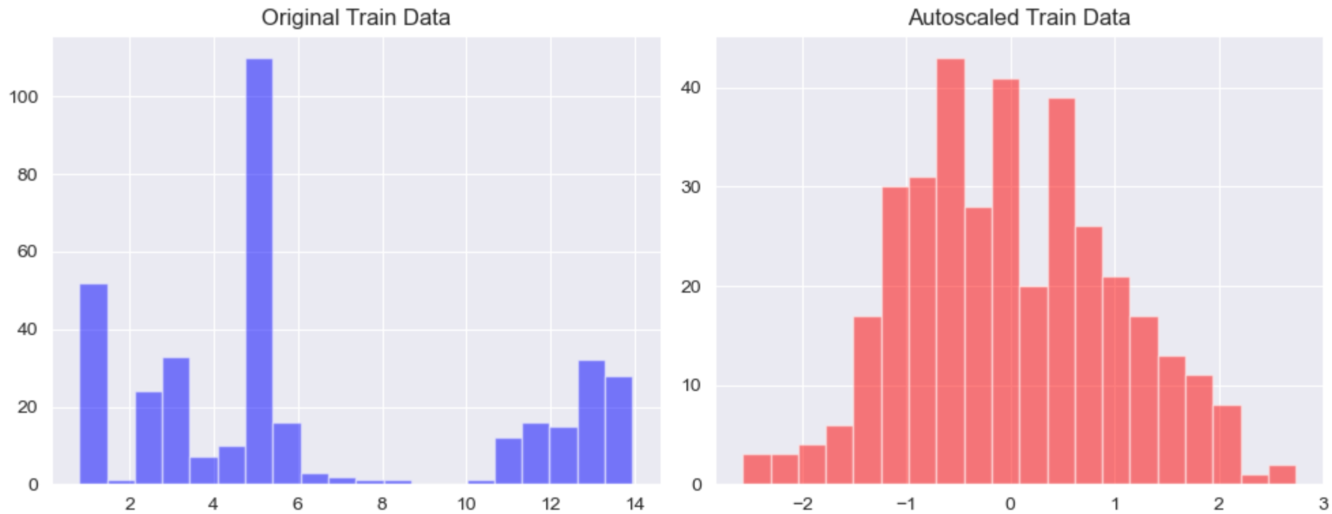



```
Fault Threhold : 10.105414155861743
T_squared statistic [6.18008886 2.02912177 5.07005525 0.58355396 0.47800707 1.4065473
8
 7.0315417  5.5454263  1.54597851 0.56926166 5.29676109 1.22412648
 1.93409028 0.35326894]
```

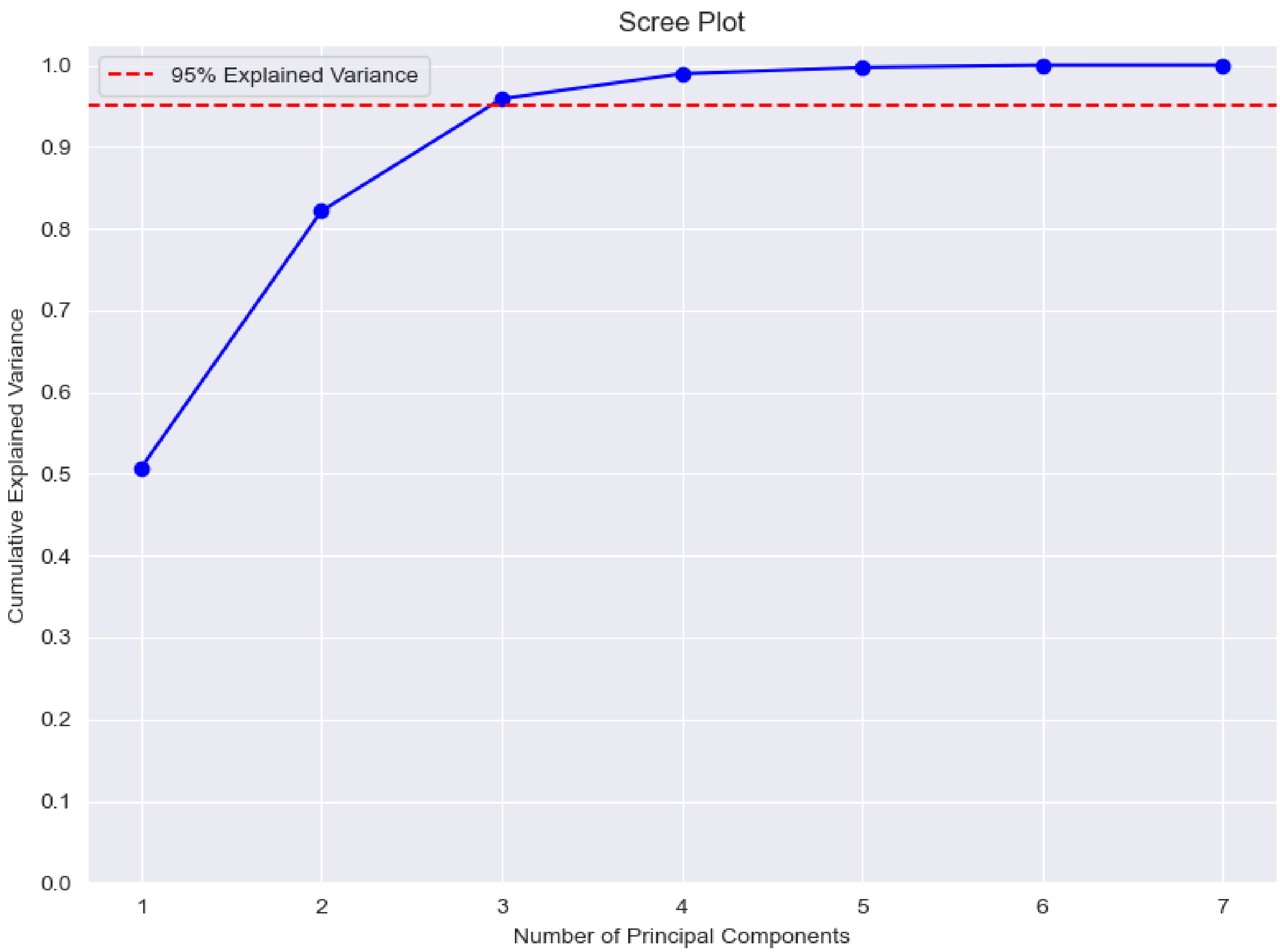


For Type 3 - Fault & Outlier Analysis

In [23]:
```
OutlierAndFaultAnalysis(dataset_whole, unique_type[2], alpha_90)
```



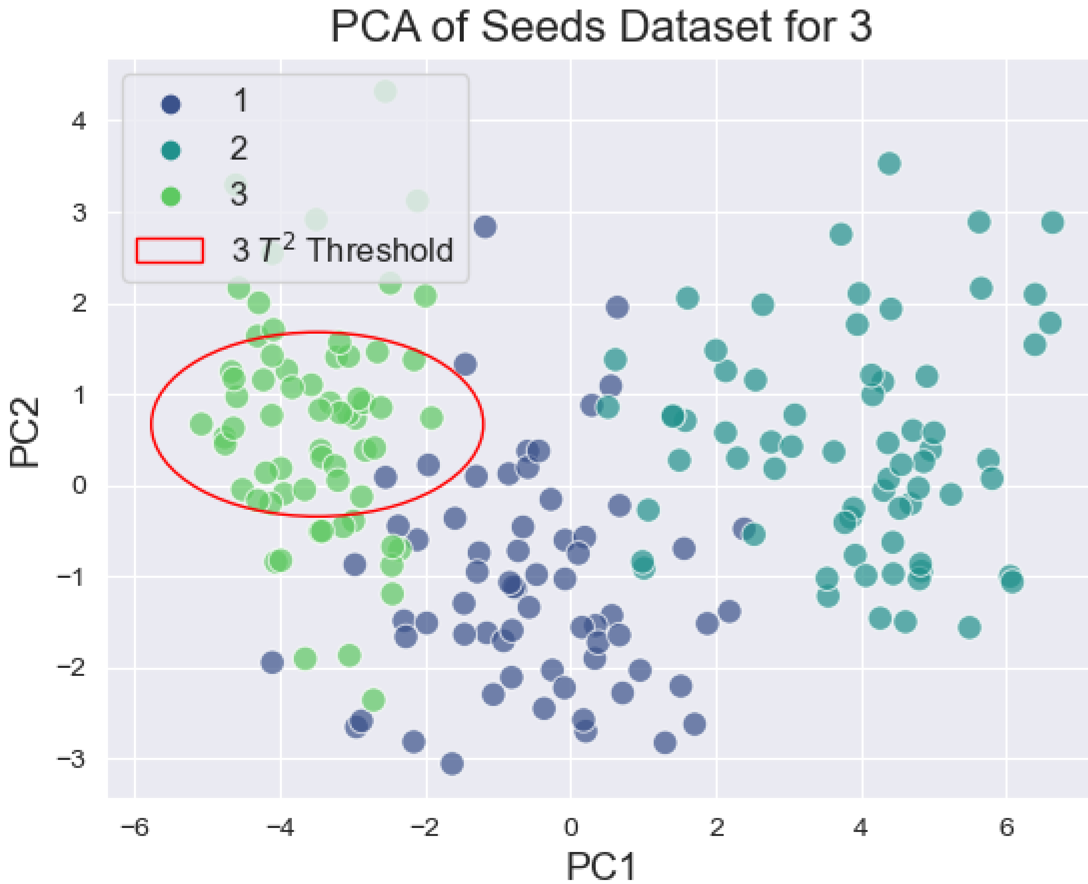

```
Number of total component : 7
Considerable Principle Component :  3
```

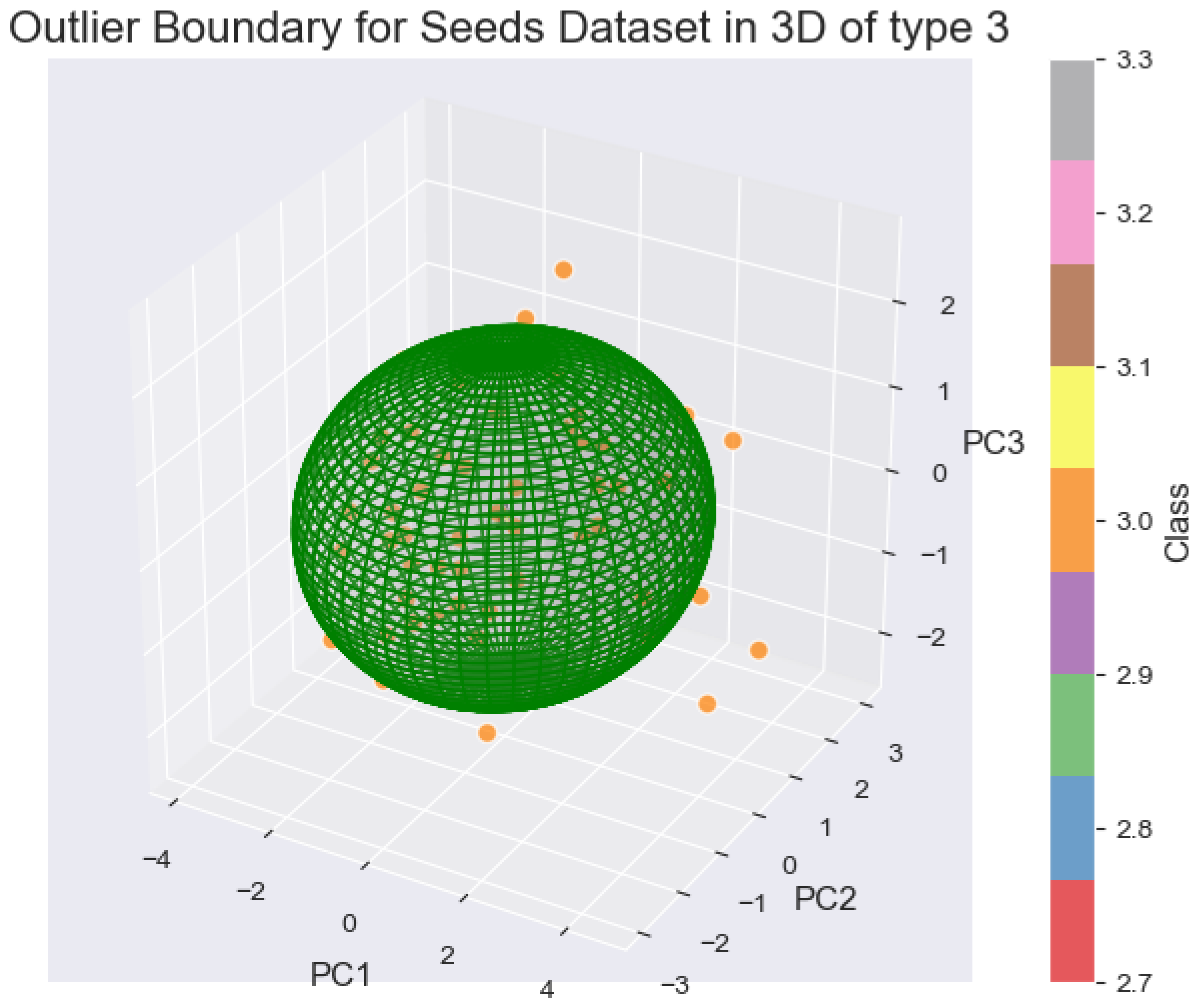


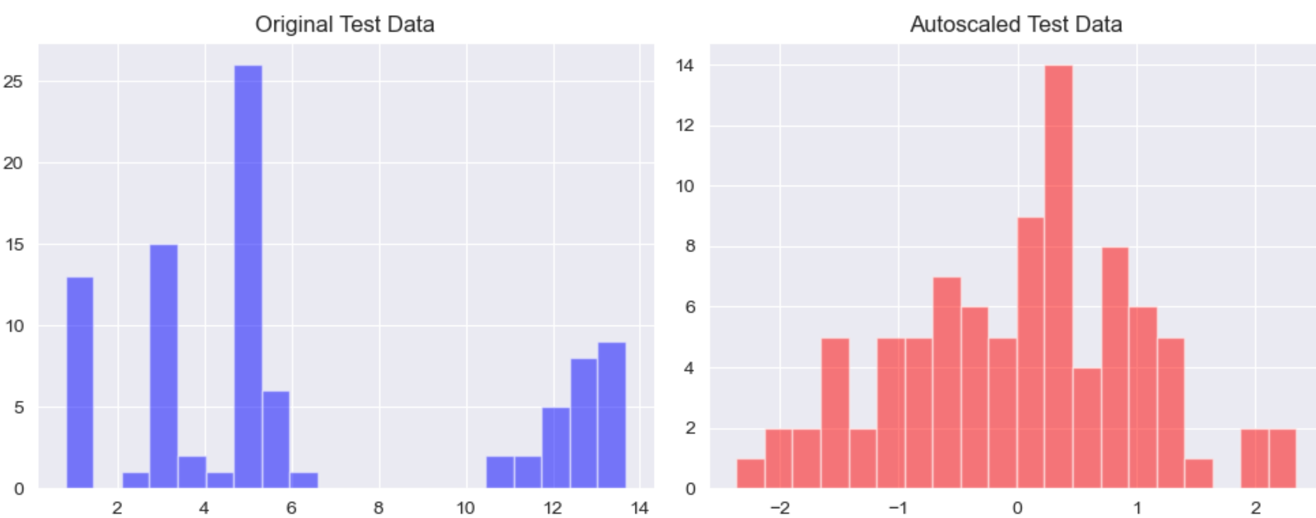

```
Explained Variance Ratio:
Principal Component 1: 0.5077
Principal Component 2: 0.3138
Principal Component 3: 0.1375
Principal Component 4: 0.0306
Principal Component 5: 0.0078
Principal Component 6: 0.0026
Principal Component 7: 0.0000

Cumulative Explained Variance:
Principal Components 1: 0.5077
Principal Components 2: 0.8215
Principal Components 3: 0.9589
Principal Components 4: 0.9895
Principal Components 5: 0.9973
```

```
Principal Components 6: 1.0000
Principal Components 7: 1.0000
array([[ 1.01960784,  0.93297416,  0.5316857 ,  0.6183236 ,  0.89144139,
         0.15443826,  0.39479059],
       [ 0.93297416,  1.01960784,  0.13629352,  0.86052995,  0.6299891 ,
         0.14738729,  0.6481973 ],
       [ 0.5316857 ,  0.13629352,  1.01960784, -0.30510417,  0.85533853,
         0.04961454, -0.40342984],
       [ 0.6183236 ,  0.86052995, -0.30510417,  1.01960784,  0.21144354,
         0.14325732,  0.85538037],
       [ 0.89144139,  0.6299891 ,  0.85533853,  0.21144354,  1.01960784,
         0.19298289,  0.01887418],
       [ 0.15443826,  0.14738729,  0.04961454,  0.14325732,  0.19298289,
         1.01960784,  0.092182  ],
       [ 0.39479059,  0.6481973 , -0.40342984,  0.85538037,  0.01887418,
         0.092182  ,  1.01960784]])
Covariance matrix shape: (7, 7)
Eigen Vector shape: (7, 7)
Eigen Value shape: (7,)
Eigen Vector: [[ 5.08665847e-01  1.68955377e-01  8.98949622e-02  1.56632310e-01
   2.38484086e-01 -7.34898414e-01  2.88353974e-01]
 [ 5.12228576e-01 -9.90736910e-02  8.50687707e-02  3.61328115e-01
   4.41684266e-01  6.14375676e-01  1.32170816e-01]
 [ 1.64903256e-01  6.25655364e-01  5.91062968e-02 -3.75787119e-01
  -3.05991738e-01  2.86295408e-01  5.10937143e-01]
 [ 4.16142221e-01 -3.92748933e-01  2.68769416e-02  2.28870768e-01
  -7.86187843e-01  8.83124179e-03  3.60612485e-02]
 [ 3.97728059e-01  4.39174550e-01  1.02255461e-02 -9.91548593e-02
  -7.36572049e-02  2.02553220e-02 -7.95717409e-01]
 [ 1.26118657e-01  2.25703096e-02 -9.89598117e-01  1.71947907e-03
   2.49593015e-02  3.57625617e-03  6.03449964e-02]
 [ 3.23140813e-01 -4.71760979e-01  3.25158418e-02 -8.00921895e-01
   1.73981985e-01 -8.55026286e-04 -1.47637877e-02]]
Eigen Value: [3.62344893e+00 2.23951679e+00 9.81031721e-01 2.18392128e-01
 5.58123887e-02 2.18575163e-04 1.88343659e-02]
Lambda : [[3.62344893e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 2.23951679e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 9.81031721e-01 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 2.18392128e-01
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  5.58123887e-02 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 1.88343659e-02 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 2.18575163e-04]] & Lambda Incerse : [[2.75980155e-01
0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 4.46524895e-01 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 1.01933503e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 4.57891963e+00
  0.00000000e+00 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  1.79171690e+01 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 5.30944341e+01 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 4.57508524e+03]]
T_squared statistic : [ 0.02201934  0.99187911  1.9057823   2.03846002  3.01717576
0.78339786
  7.26092438  1.12702006  2.26326231  3.67621363  1.15967323  2.44055409
```

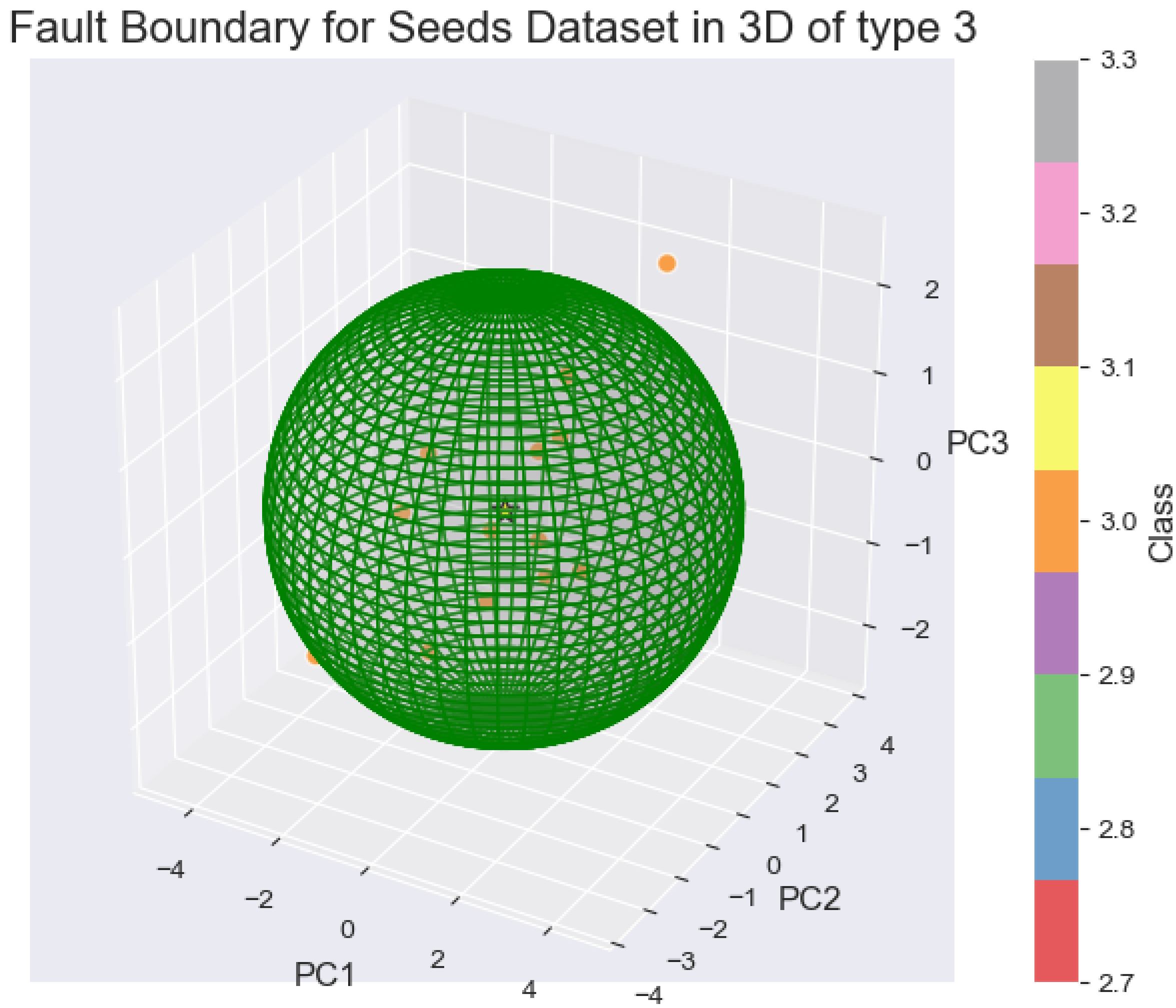
```
 3.55540862  2.91392409  2.25842208  2.18066918  3.89284424  6.23069916
 0.83743248  0.46898919  1.06817528  1.06301782  2.12643668  3.98913581
 2.35140649  4.46697904  3.90493882  2.46499357  4.49325233  2.61997302
 1.39724409  1.19209871  4.74804708  4.13547871  1.32834844  1.02043801
 2.21311197  7.32645785  1.26814388  3.64244674  0.64725521  6.95348061
 2.64119622  3.00019647  4.08284392  1.12589057  2.07818541  4.66554792
11.78601017  6.91781016  1.20431737  2.05239048]
Outlier Threhold : 6.477758924920254
```








```
Fault Threhold : 10.574978947286116
T_squared statistic [2.89323945 2.8032127  0.23281619 5.69994453 6.16830164 1.4804473
2
 5.99367776 3.16279648 1.22292409 0.83350819 9.91110472 1.00492211
 0.90816847]
```



Conclusion on Outlier Detection :

1. We have performed the outlier detection on type wise Train dataset.

2. In the context of Principal Component Analysis (PCA), $T2$ statistic is an effective tool for detecting outliers. This is essentially a multivariate generalization of Student's t-statistic and it measures the distance of a data point in the transformed space from the origin.

3. By projecting our multi-dimensional dataset into a lower-dimensional space via PCA, we created a scatter plot of the transformed data. As seen in our visualizations, the elliptical boundary (illustrated in green) encapsulates the majority of our data points. This boundary represents the calculated $T2$ statistic threshold, beyond which points are considered unusual with respect to the multivariate distribution of our dataset.

```
- PCA analysis on the Type 1 data reveals that 3 PC is needed to maintain 95%
information (explained variance) in the given data.
- Considering the fact we have used 3D plot to show the outlier for different
types of data.
- All the point outside the green elliptical boundary, considered as outlier.
- These points deviate significantly from the overall distribution thus
placed outside the boundary.
```

Conclusion on Fault Identification :

1. We have performed the outlier detection on type wise Test dataset.

2. In the world of multivariate process monitoring, PCA combined with Hotelling's T^2 statistic is a powerful methodology for detecting faults or anomalies in the system. In essence, PCA reduces the dimensionality of the data, thereby eliminating the potential issues caused by multicollinearity and helping to clarify the structure of the data. Hotelling's T^2 statistic, on the other hand, is a multivariate measure of the deviation of a given observation from the mean of the observations, serving as a generalized form of the t-statistic for multivariate data.

```
- PCA analysis on the Type 1 data reveals that 3 PC is needed to maintain 95%
information (explained variance) in the given data.
- Considering the fact we have used 3D plot to show the outlier for different
types of data.
- All the point outside the green elliptical boundary, considered as fault.
- These points deviate significantly from the overall distribution thus
placed outside the boundary.
```

3. In essence, the points lying outside this boundary represent conditions or states where the system behaves differently than usual. Identifying these states is crucial in process monitoring and control to prevent suboptimal operation or even system failure.

In [ ]: