CSE 2794 - Machine Learning Workshop 2

LAB ASSIGNMENT-1: PREPROCESSING TECHNIQUES FOR NEURAL NETWORKS

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Section: 23412C3

1. Data Exploration and Visualization

- Load the dataset and analyze its structure.
- · Generate summary statistics and check for missing values.
- Visualize feature distributions (histograms, boxplots) to identify outliers.

import pandas as pd
import seaborn as sns

data = pd.read_csv('winequality-red.csv', delimiter=';')
data.describe().T

	count	mean	std	min	25%	50%	75%	max	
fixed acidity	1599.0	8.319637	1.741096	4.60000	7.1000	7.90000	9.200000	15.90000	ılı
volatile acidity	1599.0	0.527821	0.179060	0.12000	0.3900	0.52000	0.640000	1.58000	
citric acid	1599.0	0.270976	0.194801	0.00000	0.0900	0.26000	0.420000	1.00000	
residual sugar	1599.0	2.538806	1.409928	0.90000	1.9000	2.20000	2.600000	15.50000	
chlorides	1599.0	0.087467	0.047065	0.01200	0.0700	0.07900	0.090000	0.61100	
free sulfur dioxide	1599.0	15.874922	10.460157	1.00000	7.0000	14.00000	21.000000	72.00000	
total sulfur dioxide	1599.0	46.467792	32.895324	6.00000	22.0000	38.00000	62.000000	289.00000	
density	1599.0	0.996747	0.001887	0.99007	0.9956	0.99675	0.997835	1.00369	
pН	1599.0	3.311113	0.154386	2.74000	3.2100	3.31000	3.400000	4.01000	
sulphates	1599.0	0.658149	0.169507	0.33000	0.5500	0.62000	0.730000	2.00000	
alcohol	1599.0	10.422983	1.065668	8.40000	9.5000	10.20000	11.100000	14.90000	
quality	1599.0	5.636023	0.807569	3.00000	5.0000	6.00000	6.000000	8.00000	
	volatile acidity citric acid residual sugar chlorides free sulfur dioxide total sulfur dioxide density pH sulphates alcohol	fixed acidity 1599.0 volatile acidity 1599.0 citric acid 1599.0 residual sugar 1599.0 chlorides 1599.0 free sulfur dioxide 1599.0 total sulfur dioxide 1599.0 pH 1599.0 sulphates 1599.0 alcohol 1599.0	fixed acidity 1599.0 8.319637 volatile acidity 1599.0 0.527821 citric acid 1599.0 0.270976 residual sugar 1599.0 2.538806 chlorides 1599.0 0.087467 free sulfur dioxide 1599.0 15.874922 total sulfur dioxide 1599.0 0.996747 pH 1599.0 3.311113 sulphates 1599.0 0.658149 alcohol 1599.0 10.422983	fixed acidity 1599.0 8.319637 1.741096 volatile acidity 1599.0 0.527821 0.179060 citric acid 1599.0 0.270976 0.194801 residual sugar 1599.0 2.538806 1.409928 chlorides 1599.0 0.087467 0.047065 free sulfur dioxide 1599.0 15.874922 10.460157 total sulfur dioxide 1599.0 46.467792 32.895324 density 1599.0 0.996747 0.001887 pH 1599.0 3.311113 0.154386 sulphates 1599.0 0.658149 0.169507 alcohol 1599.0 10.422983 1.065668	fixed acidity 1599.0 8.319637 1.741096 4.60000 volatile acidity 1599.0 0.527821 0.179060 0.12000 citric acid 1599.0 0.270976 0.194801 0.00000 residual sugar 1599.0 2.538806 1.409928 0.90000 chlorides 1599.0 0.087467 0.047065 0.01200 free sulfur dioxide 1599.0 15.874922 10.460157 1.00000 total sulfur dioxide 1599.0 0.996747 0.001887 0.99007 pH 1599.0 3.311113 0.154386 2.74000 sulphates 1599.0 0.658149 0.169507 0.33000 alcohol 1599.0 10.422983 1.065668 8.40000	fixed acidity 1599.0 8.319637 1.741096 4.60000 7.1000 volatile acidity 1599.0 0.527821 0.179060 0.12000 0.3900 citric acid 1599.0 0.270976 0.194801 0.00000 0.0900 residual sugar 1599.0 2.538806 1.409928 0.90000 1.9000 chlorides 1599.0 0.087467 0.047065 0.01200 0.0700 free sulfur dioxide 1599.0 45.874922 10.460157 1.00000 7.0000 total sulfur dioxide 1599.0 46.467792 32.895324 6.00000 22.0000 pH 1599.0 0.996747 0.001887 0.99007 0.9956 pH 1599.0 0.658149 0.169507 0.33000 0.5500 sulphates 1599.0 10.422983 1.065668 8.40000 9.5000	fixed acidity 1599.0 8.319637 1.741096 4.60000 7.1000 7.90000 volatile acidity 1599.0 0.527821 0.179060 0.12000 0.3900 0.52000 citric acid 1599.0 0.270976 0.194801 0.00000 0.0900 0.26000 residual sugar 1599.0 2.538806 1.409928 0.90000 1.9000 2.20000 chlorides 1599.0 0.087467 0.047065 0.01200 0.0700 0.07900 free sulfur dioxide 1599.0 15.874922 10.460157 1.00000 7.0000 14.00000 total sulfur dioxide 1599.0 46.467792 32.895324 6.0000 22.0000 38.00000 pH 1599.0 3.311113 0.154386 2.74000 3.2100 3.31000 sulphates 1599.0 10.422983 1.065668 8.40000 9.5000 10.20000	fixed acidity 1599.0 8.319637 1.741096 4.60000 7.1000 7.90000 9.200000 volatile acidity 1599.0 0.527821 0.179060 0.12000 0.3900 0.52000 0.640000 citric acid 1599.0 0.270976 0.194801 0.00000 0.0900 0.26000 0.420000 residual sugar 1599.0 2.538806 1.409928 0.90000 1.9000 2.20000 2.600000 chlorides 1599.0 0.087467 0.047065 0.01200 0.0700 0.07900 0.09000 free sulfur dioxide 1599.0 15.874922 10.460157 1.00000 7.0000 14.00000 21.000000 total sulfur dioxide 1599.0 46.467792 32.895324 6.0000 22.0000 38.0000 62.000000 pH 1599.0 3.311113 0.154386 2.74000 3.2100 3.31000 3.400000 sulphates 1599.0 0.658149 0.169507 0.33000 0.5500 0.62000 0.730000	fixed acidity 1599.0 8.319637 1.741096 4.60000 7.1000 7.90000 9.20000 15.90000 volatile acidity 1599.0 0.527821 0.179060 0.12000 0.3900 0.52000 0.640000 1.58000 citric acid 1599.0 0.270976 0.194801 0.00000 0.0900 0.26000 0.420000 1.00000 residual sugar 1599.0 2.538806 1.409928 0.99000 1.9000 2.20000 2.60000 15.50000 chlorides 1599.0 0.087467 0.047065 0.01200 0.0700 0.07900 0.099000 0.61100 free sulfur dioxide 1599.0 15.874922 10.460157 1.00000 7.0000 14.0000 21.00000 72.00000 density 1599.0 0.996747 0.001887 0.99007 0.9956 0.99675 0.997835 1.00369 pH 1599.0 0.658149 0.169507 0.33000 0.5500 0.62000 0.730000 2.00000 sulphates <t< th=""></t<>

data.info()

<class 'pandas.core.frame.DataFrame'>
 RangeIndex: 1599 entries, 0 to 1598
 Data columns (total 12 columns):

#	Column	Non-Null Count	Dtype
0	fixed acidity	1599 non-null	float64
1	volatile acidity	1599 non-null	float64
2	citric acid	1599 non-null	float64
3	residual sugar	1599 non-null	float64
4	chlorides	1599 non-null	float64
5	free sulfur dioxide	1599 non-null	float64
6	total sulfur dioxide	1599 non-null	float64
7	density	1599 non-null	float64
8	pH	1599 non-null	float64
9	sulphates	1599 non-null	float64
10	alcohol	1599 non-null	float64
11	quality	1599 non-null	int64

dtypes: float64(11), int64(1)
memory usage: 150.0 KB

2. Data Cleaning

- Handle Missing Values (if present; else, explain potential methods).
- Outlier Treatment: Use IQR or Z-score to detect and handle outliers (e.g., capping).

```
def handle_outliers_iqr(df, column):
    Q1 = df[column].quantile(0.25)
    Q3 = df[column].quantile(0.75)
    IQR = Q3 - Q1
    lower\_bound = Q1 - 1.5 * IQR
    upper_bound = Q3 + 1.5 * IQR
# Capping outliers
    df[column] = df[column].clip(lower=lower_bound, upper=upper_bound)
# Apply IQR outlier treatment to all numerical columns
numerical_cols = data.select_dtypes(include=['number']).columns
for col in numerical_cols:
    data = handle_outliers_iqr(data, col)
# Display the updated data
print(data.describe().T)
                             count
                                         mean
                                                     std
                                                               min
                                                                         25%
     fixed acidity
                           1599.0
                                    8.290901
                                                1.655860
                                                          4.600000
                                                                      7.1000
     volatile acidity
                            1599.0
                                     0.526429
                                                0.174045
                                                          0.120000
                                                                      0.3900
     citric acid
                           1599.0
                                     0.270922
                                                0.194614
                                                          0.000000
                                                                      0.0900
     residual sugar
                           1599.0
                                     2.322358
                                                0.609493
                                                          0.900000
                                                                      1.9000
                                                0.017822
     chlorides
                           1599.0
                                    0.081194
                                                          0.040000
                                                                      0.0700
     free sulfur dioxide
                           1599.0
                                   15.689181
                                                9.837494
                                                          1.000000
                                                                      7.0000
     total sulfur dioxide
                           1599.0
                                   45.714822
                                               30.374029
                                                          6.000000
                                                                     22,0000
     density
                           1599.0
                                     0.996742
                                                0.001806
                                                          0.992248
                                                                      0.9956
     рΗ
                           1599.0
                                     3.310353
                                                0.149851
                                                          2.925000
                                                                      3.2100
     sulphates
                           1599.0
                                     0.649831
                                                0.137086
                                                          0.330000
                                                                      0.5500
     alcohol
                            1599.0
                                   10.419627
                                                1.054808
                                                          8.400000
                                                                      9.5000
                           1599.0
                                                0.783211
     quality
                                    5.633521
                                                          3.500000
                                                                      5.0000
                                 50%
                                            75%
                                                        max
     fixed acidity
                            7.90000
                                       9.200000
                                                  12.350000
     volatile acidity
                            0.52000
                                                   1.015000
                                       0.640000
                            0.26000
                                       0.420000
                                                   0.915000
     citric acid
                            2.20000
                                                   3.650000
     residual sugar
                                       2,600000
     chlorides
                             0.07900
                                       0.090000
                                                   0.120000
     free sulfur dioxide
                            14.00000
                                      21.000000
                                                  42.000000
                           38.00000
                                      62.000000
                                                 122.000000
     total sulfur dioxide
     density
                             0.99675
                                       0.997835
                                                   1.001187
                             3.31000
                                       3,400000
                                                   3.685000
     sulphates
                             0.62000
                                       0.730000
                                                   1.000000
     alcohol
                            10.20000
                                     11.100000
                                                  13.500000
                            6.00000
     aualitv
                                       6.000000
                                                   7.500000
```

3. Feature Engineering

- Create a Categorical Feature: Bin a numerical column (e.g., alcohol into low, medium, high).
- Encode Categorical Features: Apply one-hot encoding and label encoding.

```
# Define bins and labels for alcohol content
bins = [0, 9, 11, 100] # Adjust these bins as needed
labels = ['low', 'medium', 'high']
# Create the categorical feature
data['alcohol_category'] = pd.cut(data['alcohol'], bins=bins, labels=labels, right=False)
# Display the updated data with the new feature
print(data.head())
        fixed acidity volatile acidity citric acid residual sugar
                                                                         chlorides \
<del>∑</del>•
     0
                  7.4
                                    0.70
                                                  0.00
                                                                   1.9
                                                                             0.076
                  7.8
                                    0.88
                                                  0.00
                                                                    2.6
                                                                             0.098
     1
                                                                             0.092
     2
                  7.8
                                    0.76
                                                  0.04
                                                                   2.3
                                                                             0.075
     3
                 11.2
                                    0.28
                                                  0.56
                                                                   1.9
     4
                                                                             0.076
                  7.4
                                    0.70
                                                  0.00
                                                                   1.9
        free sulfur dioxide total sulfur dioxide
                                                     density
                                                                рΗ
                                                                    sulphates \
     0
                        11.0
                                               34.0
                                                      0.9978
                                                              3.51
                                                                          0.56
                        25.0
                                               67.0
                                                      0.9968
                                                              3.20
     2
                        15.0
                                                      0.9970
                                                              3.26
                                                                          0.65
                        17.0
                                               60.0
                                                      0.9980
                                                              3.16
                                                                          0.58
     4
                        11.0
                                               34.0
                                                      0.9978
                                                                          0.56
                                                              3.51
                 quality alcohol_category
        alcohol
     0
            9.4
                     5.0
                                    medium
     1
            9.8
                     5.0
                                    medium
     2
            9.8
                     5.0
                                    medium
     3
            9.8
                     6.0
                                    medium
            9.4
                                    medium
                     5.0
```

```
import seaborn as sns
from sklearn.preprocessing import OneHotEncoder, LabelEncoder
# Define bins and labels for alcohol content
bins = [0, 9, 11, 100] # Adjust these bins as needed
labels = ['low', 'medium', 'high']
# Create the categorical feature
data['alcohol_category'] = pd.cut(data['alcohol'], bins=bins, labels=labels, right=False)
# One-hot encoding
encoder = OneHotEncoder(handle_unknown='ignore', sparse_output=False) # sparse=False for direct array access
encoded data = encoder.fit transform(data[['alcohol category']])
encoded_df = pd.DataFrame(encoded_data, columns=encoder.get_feature_names_out(['alcohol_category']))
data = pd.concat([data, encoded_df], axis=1)
# Label encoding
label_encoder = LabelEncoder()
data['alcohol_category_label'] = label_encoder.fit_transform(data['alcohol_category'])
# Display the updated data with encoded features
print(data.head())
        fixed acidity volatile acidity citric acid residual sugar
\overline{2}
                                                                      chlorides \
                  7.4
                                   0.70
                                                0.00
                                                                  1.9
                                                                           0.076
                  7.8
                                   0.88
                                                0.00
                                                                           0.098
     1
                                                                  2.6
                                                                           0.092
                                   9.76
     2
                  7.8
                                                0.04
                                                                  2.3
     3
                 11.2
                                   0.28
                                                0.56
                                                                  1.9
                                                                           0.075
     4
                  7.4
                                   0.70
                                                0.00
                                                                  1.9
                                                                           0.076
        free sulfur dioxide total sulfur dioxide density
                                                               pH sulphates \
     0
                       11.0
                                              34.0
                                                    0.9978
                                                            3.51
     1
                                              67.0
                                                    0.9968
                                                            3.20
     2
                       15.0
                                              54.0
                                                    0.9970
                                                                        0.65
                                                            3.26
                       17.0
                                              60.0
                                                    0.9980
                                                                        0.58
     3
                                                            3.16
     4
                                                    0.9978
                                             34.0
                       11.0
                                                            3.51
                                                                        0.56
        alcohol quality alcohol_category alcohol_category_high
     0
            9.4
                     5.0
                                   medium
                                                              0.0
     1
            9.8
                     5.0
                                   medium
                                                              0.0
     2
            9.8
                     5.0
                                   medium
                                                              0.0
     3
            9.8
                     6.0
                                   medium
                                                              0.0
     4
                     5.0
                                   medium
        alcohol_category_low alcohol_category_medium alcohol_category_label
     0
                         0.0
                                                  1.0
                                                                             2
     1
                         0.0
                                                  1.0
     2
                         0.0
                                                  1.0
                                                                             2
     3
                         9.9
                                                  1.0
                                                                             2
     4
                         0.0
                                                  1.0
                                                                             2
```

4. Feature Scaling

- · Normalization: Scale features to [0, 1] using MinMaxScaler.
- Standardization: Use StandardScaler to transform data to mean=0, variance=1.

```
from \ sklearn.preprocessing \ import \ MinMaxScaler
# Assuming 'data' is your DataFrame from the previous code
# Create a MinMaxScaler object
scaler = MinMaxScaler()
# Select numerical features to scale (exclude the newly created categorical features)
numerical_cols_to_scale = ['fixed acidity', 'volatile acidity', 'citric acid', 'residual sugar', 'chlorides', 'free sulfur dioxide', 'to
\ensuremath{\text{\#}} Fit the scaler on the numerical features and transform them
data[numerical cols to scale] = scaler.fit transform(data[numerical cols to scale])
# Display the updated data with scaled features
print(data.head())
\overline{2}
        fixed acidity volatile acidity citric acid residual sugar
                                                                       chlorides \
             0.361290
                                0.648045
                                             0.000000
                                                              0.363636
                                                                            0.4500
     1
             0.412903
                                0.849162
                                              0.000000
                                                              0.618182
                                                                            0.7250
             0.412903
                                0.715084
                                             0.043716
                                                              0.509091
                                                                            0.6500
     2
                                                              0.363636
             0.851613
                                0.178771
                                             0.612022
                                                                            0.4375
     3
     4
                                0.648045
             0.361290
                                             0.000000
                                                              0.363636
                                                                            0.4500
        free sulfur dioxide total sulfur dioxide
                                                     density
                                                                          sulphates
     0
                   0.243902
                                          0.241379 0.621085 0.769737
                                                                           0.343284
                   0.585366
                                          0.525862 0.509228 0.361842
     1
                                                                           0.522388
```

```
2
             0.341463
                                   0.413793 0.531600 0.440789
                                                                  0.477612
3
             0.390244
                                   0.465517 0.643456 0.309211
                                                                  0.373134
                                                                  0.343284
4
             0.243902
                                   0.241379 0.621085 0.769737
    alcohol
            quality alcohol_category alcohol_category_high
  0.196078
               5.0
                              medium
                                                        0.0
  0.274510
                5.0
                                                        0.0
                              medium
2 0.274510
                5.0
                              medium
                                                        0.0
  0.274510
                              medium
3
                 6.0
                                                        0.0
4
  0.196078
                5.0
                              medium
                                                        0.0
   alcohol_category_low alcohol_category_medium alcohol_category_label
0
                   0.0
                                            1.0
1
                   0.0
                                            1.0
3
                   0.0
                                            1.0
                   0.0
                                            1.0
```

5. Feature Selection

• Principal Component Analysis (PCA): Apply PCA to reduce the number of features.

```
from sklearn.decomposition import PCA
import pandas as pd
# Assuming 'data' is your DataFrame from the previous code
# and numerical_cols_to_scale contains the numerical features
# Select numerical features for PCA
pca_features = data[numerical_cols_to_scale]
# Apply PCA with the desired number of components (e.g., 5 components)
pca = PCA(n_components=5) # Adjust n_components as needed
pca_result = pca.fit_transform(pca_features)
# Create a DataFrame from the PCA results
pca df = pd.DataFrame(data=pca result, columns=[f'PC{i+1}' for i in range(5)])
# Concatenate the PCA results with the original DataFrame
data = pd.concat([data, pca_df], axis=1)
# Display the updated DataFrame
print(data.head())
# Explained variance ratio
explained_variance_ratio = pca.explained_variance_ratio_
print("Explained Variance Ratio:", explained_variance_ratio)
print("Total Variance Explained:", sum(explained_variance_ratio))
<del>____</del>
        fixed acidity volatile acidity citric acid residual sugar chlorides \
     0
                                            0.000000
             0.361290
                               0.648045
                                                            0.363636
                                                                         0.4500
     1
             0.412903
                               0.849162
                                            0.000000
                                                            0.618182
                                                                          0.7250
     2
             0.412903
                               0.715084
                                            0.043716
                                                            0.509091
                                                                         0.6500
     3
             0.851613
                               0.178771
                                            0.612022
                                                            0.363636
                                                                         0.4375
     4
             0.361290
                               0.648045
                                            0.000000
                                                            0.363636
                                                                         0.4500
        free sulfur dioxide total sulfur dioxide
                                                    density
                                                                       sulphates
                                        0.241379 0.621085 0.769737
     0
                  0.243902
                                                                        0.343284
                   0.585366
                                         0.525862 0.509228 0.361842
                                                                        0.522388
     1
     2
                   0.341463
                                         0.413793 0.531600 0.440789
                                                                        0.477612
                   0.390244
                                         0.465517 0.643456 0.309211
     3
                                                                        0.373134
     4
                   0.243902
                                         0.241379 0.621085 0.769737
                                                                        0.343284
             alcohol_category alcohol_category_high alcohol_category_low \
     0
                       medium
                                                 0.0
                                                                      0.0
       . . .
     1
                       medium
                                                 0.0
                                                                      0.0
        . . .
     2
                       medium
                                                 0.0
       . . .
     3
                       medium
                                                 0.0
                                                                      0.0
        . . .
     4
                       medium
                                                 0.0
                                                                      0.0
        alcohol_category_medium alcohol_category_label
                                                              PC1
     0
                                                      2 -0.334066 -0.044274
                            1.0
     1
                            1.0
                                                      2 -0.081086 0.415474
     2
                            1.0
                                                      2 -0.103170 0.148488
     3
                            1.0
                                                      2 0.454986 0.010979
     4
                                                      2 -0.334066 -0.044274
                       PC4
     0 -0.379685 -0.078170 -0.012338
     1 -0.311652 0.062130 0.126833
     2 -0.313668 -0.015201 0.087897
     3 0.178805 -0.326279 -0.266847
     4 -0.379685 -0.078170 -0.012338
```

[5 rows x 22 columns]
Explained Variance Ratio: [0.26734621 0.21923543 0.14619164 0.09807839 0.07608929]
Total Variance Explained: 0.8069409592967512

6. Train Test Splitting

• Split the dataset so that 80% of the samples will be used for training and rest will be used for testing.

```
from sklearn.model_selection import train_test_split

# Assuming 'data' is your DataFrame and 'quality' is your target variable
X = data.drop('quality', axis=1)
y = data['quality']

# Split the data into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42) # random_state for reproducibility

# Now you have X_train, X_test, y_train, and y_test
print(X_train.shape, X_test.shape, y_train.shape, y_test.shape)

1 (1279, 21) (320, 21) (1279,) (320,)
```