Data Analysis and Knowledge Discovery Exercise Work 1

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1 Task 1: Histograms

Histograms were plotted using python and matplotlib. Freedman-Diaconis rule, Sturges' rule and Square-root choice was used to calculate the number of bins in the histograms. These three histograms were plotted for all of the attributes. However, only plots for alcohol are shown in this documents to demonstrate the results.

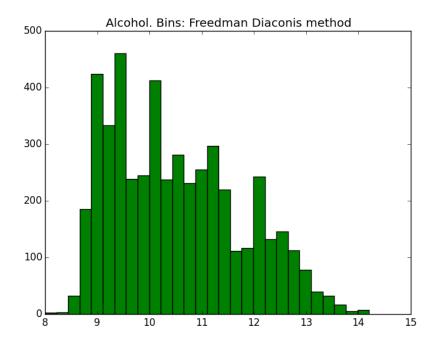


Figure 1: Histogram of alcohol attribute. Number of bins selected with Freedman-Diaconis rule.

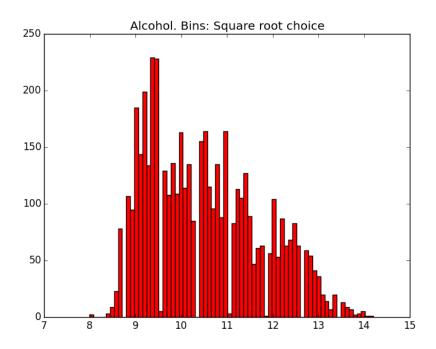


Figure 2: Histogram of alcohol attribute. Number of bins selected with Square-root choice.

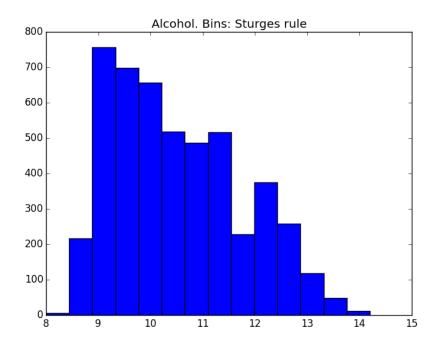


Figure 3: Histogram of alcohol attribute. Number of bins selected with Sturges' rule.

Figures 1, 2, 3 show the plotted histograms for alcohol attribute. Square-root choice produced 70 bins with this dataset. Respectively, Freedman-Diaconis rule produced 28 bins and

Sturges' 14 bins. Histograms with lower number of bins show that majority of samples have alcohol around 10. Figure 2 shows that higher number of bins reveal that some tenths have very low number of samples, even though the next tenth has 50 or more samples.

2 Task 2: Scatter Plots and Parallel Coordinates Representation

Scatter plot were produced using matplotlib's scatter function. Attributes were plotted against each other, but only three are added to this document.

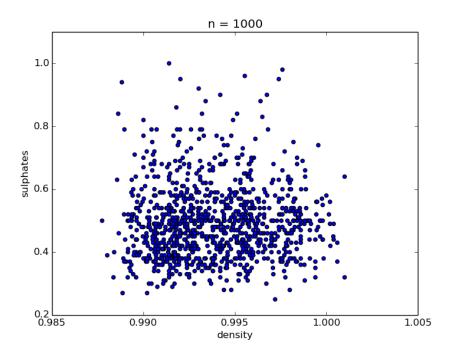


Figure 4: Scatter plot of density and sulphates

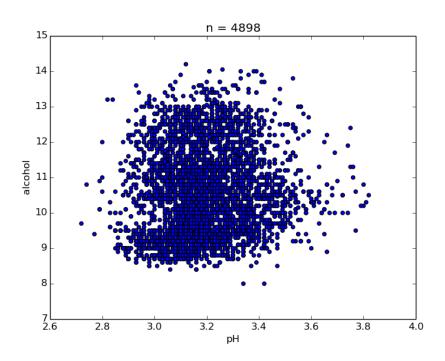


Figure 5: Scatter plot of pH and alcohol

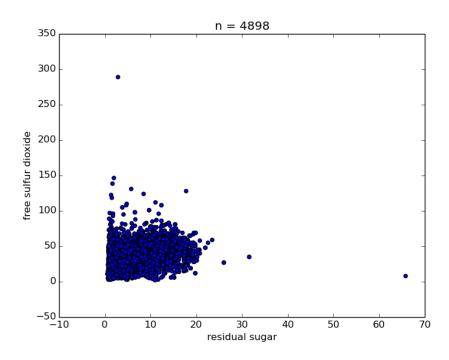


Figure 6: Scatter plot of residual sugar and free sulfur dioxide

Figure 4 shows how samples are omitted to make the density variations more visible. Figure 5 shows how samples have quite evenly scatted pH values relative to alcohol. Figure 6 shows

some outliers.

3 Task 3: Principal Component Analysis

PCA component analysis was done using numpy's cov method to calculate covariance matrix and linalg.eig to calculate eigen vectors and eigen values.

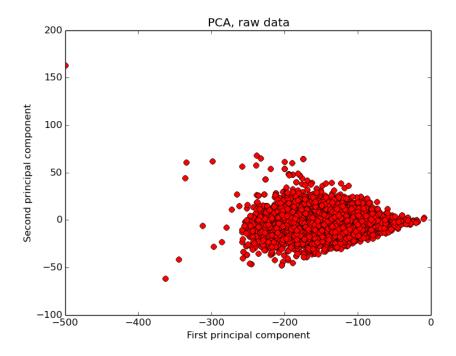


Figure 7: PCA with raw data

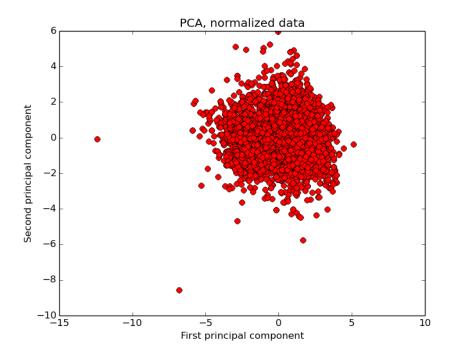


Figure 8: PCA with z-score normalized data

Figure 7 shows scatter plot of the first principal components computed with raw data. Figure 8 shows the same scatter plot with normalized data. With normalization, the scatter plot shows more rounded figure compared to raw data which has kind of triangle shape.

4 Task 4: 2D Multidimensional Scaling

2D MDS was calculated with MDS function from scikit-learn.

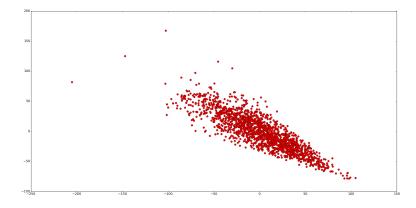


Figure 9: 2D MDS

Figure 9 shows 2D MDS scatter plot. The figure has some resemblence to PCA scatter plot with raw data.

5 Task 5: Pearson and Kendall's Tau Correlation Tables

Correlation tables were calculated with Pandas' "corr" method.

5.1 Pearson Correlation Table

| | fixed acidity | volatile acidity | citric acid | residual sugar | chlorides | free sulfur dioxide | total sulfur dioxide | density | pH | sulphates | alcohol | quality |
|----------------------|---------------|------------------|-------------|----------------|-----------|---------------------|----------------------|-----------|-----------|-----------|-----------|-----------|
| fixed acidity | 1.000000 | -0.022697 | 0.289181 | 0.089021 | 0.023086 | -0.049396 | 0.091070 | 0.265331 | -0.425858 | -0.017143 | -0.120881 | -0.113663 |
| volatile acidity | -0.022697 | 1.000000 | -0.149472 | 0.064286 | 0.070512 | -0.097012 | 0.089261 | 0.027114 | -0.031915 | -0.035728 | 0.067718 | -0.194723 |
| citric acid | 0.289181 | -0.149472 | 1.000000 | 0.094212 | 0.114364 | 0.094077 | 0.121131 | 0.149503 | -0.163748 | 0.062331 | -0.075729 | -0.009209 |
| residual sugar | 0.089021 | 0.064286 | 0.094212 | 1.000000 | 0.088685 | 0.299098 | 0.401439 | 0.838966 | -0.194133 | -0.026664 | -0.450631 | -0.097577 |
| chlorides | 0.023086 | 0.070512 | 0.114364 | 0.088685 | 1.000000 | 0.101392 | 0.198910 | 0.257211 | -0.090439 | 0.016763 | -0.360189 | -0.209934 |
| free sulfur dioxide | -0.049396 | -0.097012 | 0.094077 | 0.299098 | 0.101392 | 1.000000 | 0.615501 | 0.294210 | -0.000618 | 0.059217 | -0.250104 | 0.008158 |
| total sulfur dioxide | 0.091070 | 0.089261 | 0.121131 | 0.401439 | 0.198910 | 0.615501 | 1.000000 | 0.529881 | 0.002321 | 0.134562 | -0.448892 | -0.174737 |
| density | 0.265331 | 0.027114 | 0.149503 | 0.838966 | 0.257211 | 0.294210 | 0.529881 | 1.000000 | -0.093591 | 0.074493 | -0.780138 | -0.307123 |
| pH | -0.425858 | -0.031915 | -0.163748 | -0.194133 | -0.090439 | -0.000618 | 0.002321 | -0.093591 | 1.000000 | 0.155951 | 0.121432 | 0.099427 |
| sulphates | -0.017143 | -0.035728 | 0.062331 | -0.026664 | 0.016763 | 0.059217 | 0.134562 | 0.074493 | 0.155951 | 1.000000 | -0.017433 | 0.053678 |
| alcohol | -0.120881 | 0.067718 | -0.075729 | -0.450631 | -0.360189 | -0.250104 | -0.448892 | -0.780138 | 0.121432 | -0.017433 | 1.000000 | 0.435575 |
| quality | -0.113663 | -0.194723 | -0.009209 | -0.097577 | -0.209934 | 0.008158 | -0.174737 | -0.307123 | 0.099427 | 0.053678 | 0.435575 | 1.000000 |

5.2 Kendall's Tau Correlation Table

| | fixed acidity | volatile acidity | citric acid | residual sugar | chlorides | free sulfur dioxide | total sulfur dioxide | density | pН | sulphates | alcohol | quality |
|----------------------|---------------|------------------|-------------|----------------|-----------|---------------------|----------------------|-----------|-----------|-----------|-----------|-----------|
| fixed acidity | 1.000000 | -0.029565 | 0.208569 | 0.074946 | 0.065361 | -0.016940 | 0.077272 | 0.185510 | -0.294796 | -0.008724 | -0.073241 | -0.065474 |
| volatile acidity | -0.029565 | 1.000000 | -0.104012 | 0.072757 | -0.003523 | -0.054751 | 0.081319 | 0.006600 | -0.030385 | -0.011580 | 0.023495 | -0.154787 |
| citric acid | 0.208569 | -0.104012 | 1.000000 | 0.015329 | 0.022292 | 0.060809 | 0.062188 | 0.061542 | -0.101307 | 0.054489 | -0.019981 | 0.014557 |
| residual sugar | 0.074946 | 0.072757 | 0.015329 | 1.000000 | 0.155274 | 0.236748 | 0.293319 | 0.588989 | -0.125553 | -0.002545 | -0.305601 | -0.063087 |
| chlorides | 0.065361 | -0.003523 | 0.022292 | 0.155274 | 1.000000 | 0.113851 | 0.257075 | 0.349119 | -0.037891 | 0.062555 | -0.404039 | -0.244856 |
| free sulfur dioxide | -0.016940 | -0.054751 | 0.060809 | 0.236748 | 0.113851 | 1.000000 | 0.444696 | 0.217295 | -0.005229 | 0.035621 | -0.182539 | 0.017164 |
| total sulfur dioxide | 0.077272 | 0.081319 | 0.062188 | 0.293319 | 0.257075 | 0.444696 | 1.000000 | 0.388378 | -0.008421 | 0.108697 | -0.325826 | -0.151230 |
| density | 0.185510 | 0.006600 | 0.061542 | 0.588989 | 0.349119 | 0.217295 | 0.388378 | 1.000000 | -0.075630 | 0.064202 | -0.635104 | -0.266598 |
| pH | -0.294796 | -0.030385 | -0.101307 | -0.125553 | -0.037891 | -0.005229 | -0.008421 | -0.075630 | 1.000000 | 0.095823 | 0.102631 | 0.084441 |
| sulphates | -0.008724 | -0.011580 | 0.054489 | -0.002545 | 0.062555 | 0.035621 | 0.108697 | 0.064202 | 0.095823 | 1.000000 | -0.026410 | 0.026403 |
| alcohol | -0.073241 | 0.023495 | -0.019981 | -0.305601 | -0.404039 | -0.182539 | -0.325826 | -0.635104 | 0.102631 | -0.026410 | 1.000000 | 0.346672 |
| quality | -0.065474 | -0.154787 | 0.014557 | -0.063087 | -0.244856 | 0.017164 | -0.151230 | -0.266598 | 0.084441 | 0.026403 | 0.346672 | 1.000000 |