

**Postgraduate Certificate in Software Design with Artificial Intelligence**

**Data Mining and Machine Learning**

**Assignment 1**

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*Brief Description: This paper evaluates different data sets using regression, decision trees and kNN algorithms. Models are created and predictions are made using the test data from the data sets.*

Git: <https://github.com/DanielsHappyWorks/DM-ML-Module-Assignment>

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# Introduction

# Regression

## Overview of the Problem

For regression, a data set that describes characteristics of wine will be used. The data is called Wine Quality and was originally sourced by Paulo Cortez, Antonio Cerdeira, Fernando Almeida, Telmo Matos and Jose Reis.

The data contains two sets:

1. red wine with 1599 rows
2. white wine with 4898 rows

The data set has 12 features which include:

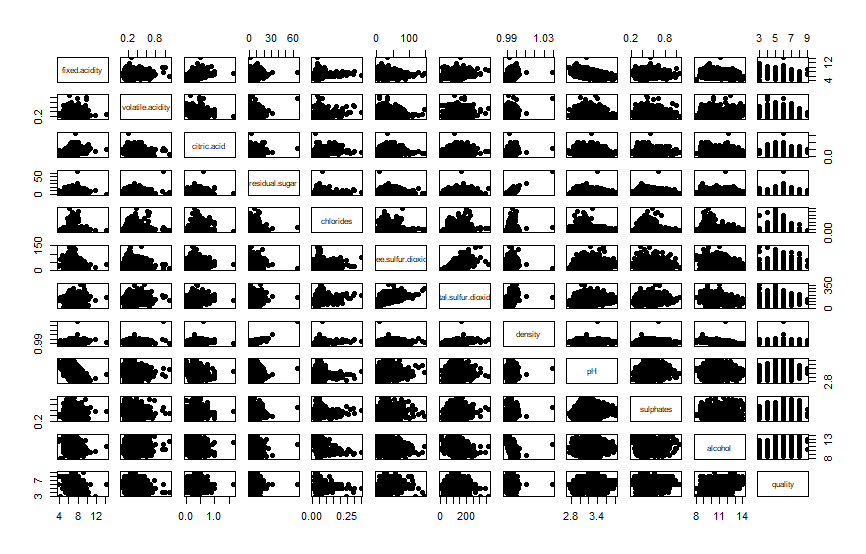
1. fixed acidity
2. volatile acidity
3. citric acid
4. residual sugar
5. chlorides
6. free sulfur dioxide
7. total sulfur dioxide
8. density
9. pH
10. sulphates
11. alcohol
12. quality (score between 0 and 10)

For this specific problem only the white wine data set will be used. Using regression algorithms, all the features will be analysed and correlated together to try and predict the quality of the wine.

## Data Exploration (tables and graphs)

The data has no missing features which was double checked when the csv was loaded into R. No clean up was needed to handle missing fields

The first graph created was one with all columns plotted against each other. Its hard to see the output because of how small the graphs are.



To get a better image of how all the attributes effect quality, they were plotted against each other and exported as pdf files using R.

Plots:

|  |  |  |
| --- | --- | --- |
| Feature | Scatter | Histogram |
| fixed acidity |  |  |
| volatile acidity |  |  |
| citric acid |  |  |
| residual sugar |  |  |
| chlorides |  |  |
| free sulfur dioxide |  |  |
| total sulfur dioxide |  |  |
| density |  |  |
| pH |  |  |
| sulphates |  |  |
| alcohol |  |  |

Larger versions of the plots can be seen within the R project. Please note that for some graphs the Linear Regression line doesn’t do a good job at predicting very high and very low values with the data present which is probably due to linear regression not being the best fit for the data. This could also be because there are more mid ranged values which might be degrading the performance.

The quality was also used against all features separately to get a linear regression models so they could be compared. The performance is described in section 1.4 Model Generation and Information

## Definition of Training and Testing Set

The entire data set with 12 features and 4898 was used for Training models.

14 rows were chosen randomly by hand so they can be used to validate how well the models would predict quality. The validation sample has two of each type of quality to be tested against.

Validation Sample:

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ID | quality | volatile acidity | citric acid | residual sugar | chlorides | free sulfur dioxide | total sulfur dioxide | density | pH | sulphates | alcohol | fixed acidity |
| 1 | 3 | 0.26 | 0.21 | 16.2 | 0.074 | 41 | 197 | 0.998 | 3.02 | 0.5 | 9.8 | 8.5 |
| 2 | 3 | 0.17 | 0.47 | 1.4 | 0.037 | 5 | 33 | 0.9939 | 2.89 | 0.28 | 9.6 | 10.3 |
| 3 | 4 | 0.485 | 0 | 1.5 | 0.065 | 8 | 103 | 0.994 | 3.63 | 0.4 | 9.7 | 5.5 |
| 4 | 4 | 0.31 | 0.31 | 9.9 | 0.04 | 10 | 175 | 0.9953 | 3.46 | 0.55 | 11.4 | 6.7 |
| 5 | 5 | 0.36 | 0.04 | 5.7 | 0.046 | 21 | 87 | 0.9934 | 3.22 | 0.51 | 10.2 | 5.9 |
| 6 | 5 | 0.37 | 0.51 | 11.8 | 0.044 | 62 | 163 | 0.9976 | 3.19 | 0.44 | 8.8 | 6.8 |
| 7 | 6 | 0.34 | 0.39 | 7.6 | 0.04 | 45 | 215 | 0.9965 | 3.11 | 0.53 | 9.2 | 7.6 |
| 8 | 6 | 0.3 | 0.27 | 11.6 | 0.028 | 22 | 97 | 0.99314 | 2.96 | 0.38 | 11.7 | 6.8 |
| 9 | 7 | 0.23 | 0.39 | 2.3 | 0.033 | 29 | 102 | 0.9908 | 3.26 | 0.54 | 12.3 | 7.2 |
| 10 | 7 | 0.41 | 0.37 | 4.5 | 0.03 | 40 | 114 | 0.992 | 3.17 | 0.54 | 12.4 | 7.9 |
| 11 | 8 | 0.19 | 0.27 | 13.9 | 0.057 | 45 | 155 | 0.99807 | 2.94 | 0.41 | 8.8 | 7.3 |
| 12 | 8 | 0.28 | 0.34 | 2.2 | 0.037 | 24 | 125 | 0.98986 | 3.36 | 0.33 | 12.8 | 5.8 |
| 13 | 9 | 0.27 | 0.45 | 10.6 | 0.035 | 28 | 124 | 0.997 | 3.2 | 0.46 | 10.4 | 9.1 |
| 14 | 9 | 0.36 | 0.34 | 4.2 | 0.018 | 57 | 119 | 0.9898 | 3.28 | 0.36 | 12.7 | 6.9 |

## Model Generation and Information

There were 14 models created. 11 with only one feature each. 3 with all the features of which two were polynomial regression models.

Single Feature models:

|  |  |
| --- | --- |
| Model | R-squared |
| Model 1: quality ~ fixed.acidity | Multiple R-squared: 0.01292  Adjusted R-squared: 0.01272 |
| Model 2: quality ~ volatile.acidity | Multiple R-squared: 0.03792  Adjusted R-squared: 0.03772 |
| Model 3: quality ~ citric.acid | Multiple R-squared: 8.481e-05  Adjusted R-squared: -0.0001194 |
| Model 4: quality ~ residual.sugar | Multiple R-squared: 0.009521  Adjusted R-squared: 0.009319 |
| Model 5: quality ~ chlorides | Multiple R-squared: 0.04407  Adjusted R-squared: 0.04388 |
| Model 6: quality ~ free.sulfur.dioxide | Multiple R-squared: 6.655e-05  Adjusted R-squared: -0.0001377 |
| Model 7: quality ~ total.sulfur.dioxide | Multiple R-squared: 0.03053  Adjusted R-squared: 0.03034 |
| Model 8: quality ~ density | Multiple R-squared: 0.09432  Adjusted R-squared: 0.09414 |
| Model 9: quality ~ pH | Multiple R-squared: 0.009886  R-squared: 0.009684 |
| Model 10: quality ~ sulphates | Multiple R-squared: 0.002881  Adjusted R-squared: 0.002678 |
| Model 11: quality ~ alcohol | Multiple R-squared: 0.1897  Adjusted R-squared: 0.1896 |

Multiple Feature Models:

|  |  |
| --- | --- |
| Model | R-squared |
| All Features | Multiple R-squared: 0.2819  Adjusted R-squared: 0.2803 |
| All Features to degree 2 | Multiple R-squared: 0.3679  Adjusted R-squared: 0.3578 |
| All Features to degree 3 | Multiple R-squared: 0.4612  Adjusted R-squared: 0.4181 |

A few other models with just a select few parameters were tried but they were usually worse than the three listed above.

## Predictions for the test data

For predictions I chose to do them on the models with all features and polynomial degrees 2 and 3 degree using the 14 rows listed in section 1.3. Anything beyond polynomial degree 3 caused R-Studio to freeze as it required too much memory so testing for overfitting couldn’t be performed.

To this point the models weren’t great based on the r values. So, when the predictions are made, they will be rounded to the nearest whole number to see how accurate they are since regression can predict values between whole numbers.

Output from predictions:



The predictions as seen above are very bad compared to the actual values. The best performing one is the model with all the features even then the quality of the wine isn’t predicted accurately.

## Evaluation of the model(s) and conclusion.

Overall the predictions for this data set using the models were very inaccurate.

The predictions with all the features were only capable of really predicting quality from 5-7 even though the data set started at 3 and ended at 9. This was kind of expected since if we look at all the one feature regression graph the estimates are mostly within the quality of 5-7

The polynomial models, which seemed more accurate due to the R-Values, performed even worse. The estimates were unreasonable at best. We would probably get more accurate results by just using one feature which is unfortunate.

There is a high possibility that the models could be improved by having a wider range of data. If we look at the data, most of the 4k entries are usually within the 6-7 quality rating. In the next iteration it could be worth while creating a data set that has a better balance of entries for predictions.

In conclusion the data set wasn’t fit for linear regression in the way it was utilised. More Data Exploration could be done to see if the results could improve but this is out of scope of the project. It’s a possibility that predicting something like this is near impossible as the quality of wine could be subjective, and the data might be degraded because of it. More investigation into the source of the data could give us a better look into this.

# Decision Trees

## Overview of the Problem

## Data Exploration (tables and graphs)

## Definition of Training and Testing Set

## Model Generation and Information

## Predictions for the test data

## Evaluation of the model(s) and conclusion.

# kNN

## Overview of the Problem

## Data Exploration (tables and graphs)

## Definition of Training and Testing Set

## Model Generation and Information

## Predictions for the test data

## Evaluation of the model(s) and conclusion.

# Citations

* P. Cortez, A. Cerdeira, F. Almeida, T. Matos and J. Reis. Modeling wine preferences by data mining from physicochemical properties. In Decision Support Systems, Elsevier, 47(4):547-553. ISSN: 0167-9236.