inferential_stats_project

February 15, 2015

1 Researching Wine Quality from physiochemical properties.

1.1 Introduction

We look at two datasets related to red and white vinho verde wine samples, from the north of Portugal. The goal is to model wine quality based on physicochemical tests.

Vinho verde is a unique product from the Minho (northwest) region of Portugal. Medium in alcohol, is it particularly appreciated due to its freshness (specially in the summer).

The source states that these datasets can be viewed as *classification* or *regression* tasks. The classes are ordered and not balanced (e.g. there are much more normal wines than excellent or poor ones).

If we can establish this relationship, then of significance would be the sommeliers' reputation who perform wine tasting all the time and providing a certificate of merit or grading to sommeliers such that based on the correlation as stated previously, one could establish the quality of wine and wine quality as set by the taster.

This is really interesting to the massive wine market, wine consumers, wine tasters and to the reputation of esteemed wine-breweries! A predictive model developed on this data is expected to provide guidance to vineyards regarding quality and price expected on their produce without heavy reliance on volatility of wine tasters.

1.2 Research Question and Hypothesis

1.2.1 Research Question

A research question relevant to the topic is: Is there a correlation between physiochemical makeup of the wine and quality of wine?

For this, we need to explore the physiochemical attributes given in the dataset and analysis the statistical variables to find out if there is any possibility of a strong correlation. If not, we reject the proposition that there is any correlation. Which brings us close to framing the hypothesis.

1.2.2 Framing the Hypothesis

Null Hypothesis H0: There is no significant relationship between any of the physiochemical constituents and the quality of Red Wine.

Which means the alternative hypothesis should be:

Alternative Hypothesis HA: There is evidence from Pearson's R values that there is a significant relation between any of the physiochemical constituents of and the quality of Red Wine. We accept the alternative hypothesis HA if we get a Pearson's R of atleast 0.60.

1.3 Experimental Design

The Dataset contains the following two samples (with sample size):

1. red wine - 1599;

2. white wine - 4898;

We note that specific attributes have been included per sample as given here: Input variables (based on physicochemical tests):

- 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

Output variable (based on sensory data):

12. quality (score between 0 and 10)

We also observe that:

- 1. Quality is an ordinal variable with possible ranking from 1 (worst) to 10 (best)
- 2. The attribute data across all samples is a continuous variable including the Quality attribute

Lets first sort the tables in a proper format and analyze the data afterwards.

```
In [108]: #import matplotlib
          %automagic
          %matplotlib inline
          import numpy as np
          import pandas
          from pandas import DataFrame
          import os
          import csv
          def read_write_wine_csv(fpath_name, fpath_new_name):
              Takes a raw unformatted csv file as input.
              Returns a sorted by column, formatted csv file as output
              #open the input file for reading csv
              with open(fpath_name) as f:
                  wine = csv.reader(f, delimiter = ';', quoting=csv.QUOTE_NONNUMERIC)
                  #open output file for writing to csv
                  with open(fpath_new_name, 'wb+') as new_wine_file:
                      #qet headers with serial no. as first column
                      headers = ['sno'] + list(wine.next())
                      #write the new file with headers as first row using DictWriter
                      csv_dct_writer = csv.DictWriter(new_wine_file, fieldnames = headers)
                      csv_dct_writer.writerow({col:col for col in headers})
```

Now that we have the data in our comfortable format, it will be interesting to show that there is a relation between physiochemical attributes of wine and quality of wine based on wine tasting.

We take into account all indicators per sample and perform the following exploratory analysis:

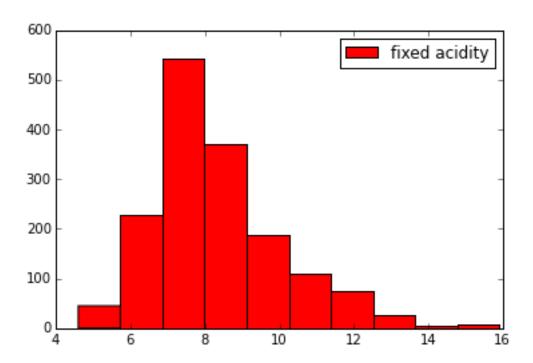
- 1. Univariate Analysis Finding descriptive statistics for each attribute with plots across samples of all tables:
- 2. Removing outliers;
- 3. Pearson's Correlation;
- 4. Scatterplot among all attributes;

1.4 Results

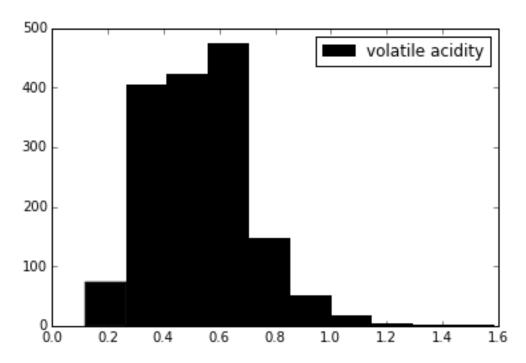
1.4.1 Exploratory Analysis

We take the histogram plots of each attribute in the **Red Wine** dataset.

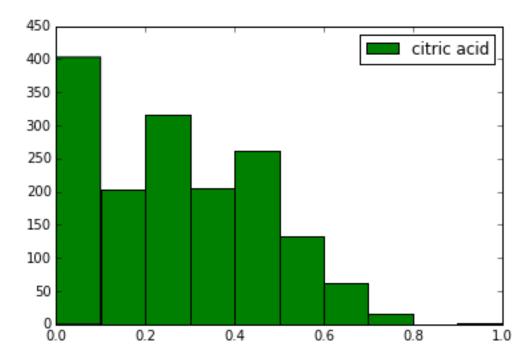
Alongwith taking histogram plots of each attribute, we will clean out any outliers from all the attributes to find out unbiased standard deviation.

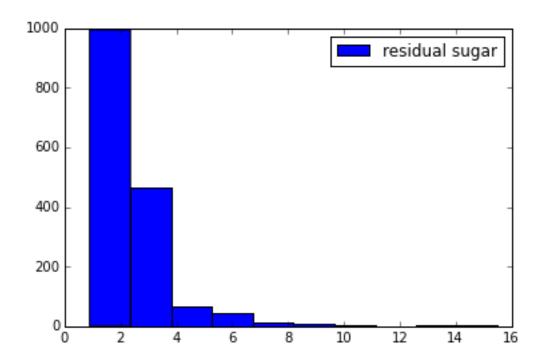


Out[190]: <matplotlib.legend.Legend at 0x130eb358>

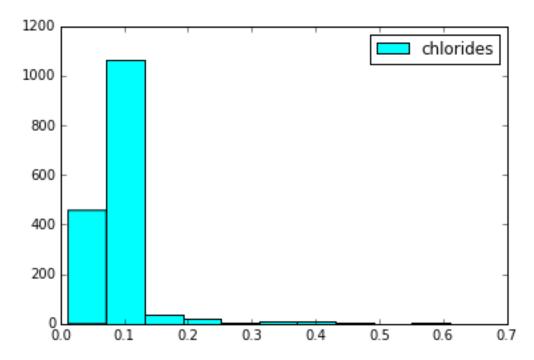


Out[191]: <matplotlib.legend.Legend at 0x1355b668>

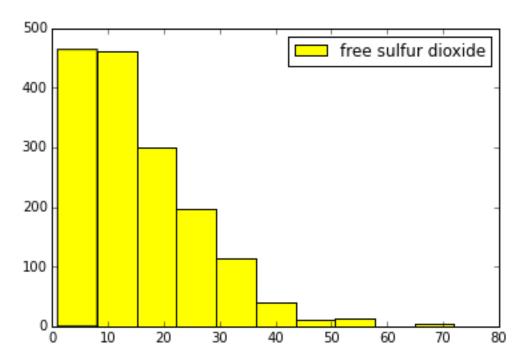


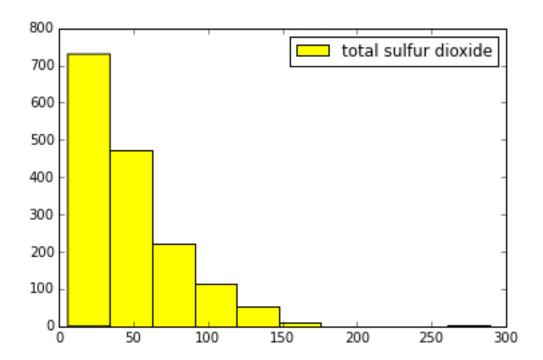


Out[193]: <matplotlib.legend.Legend at 0x134380b8>

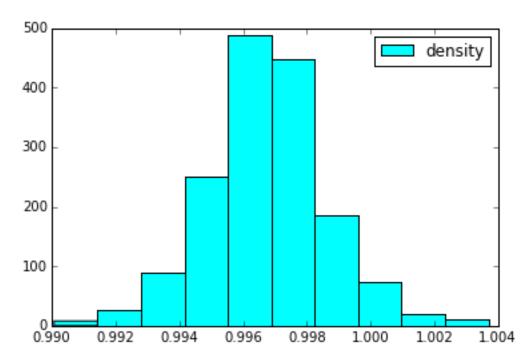


Out[194]: <matplotlib.legend.Legend at 0xe032c18>

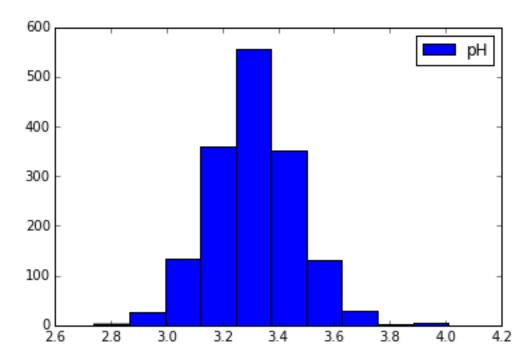




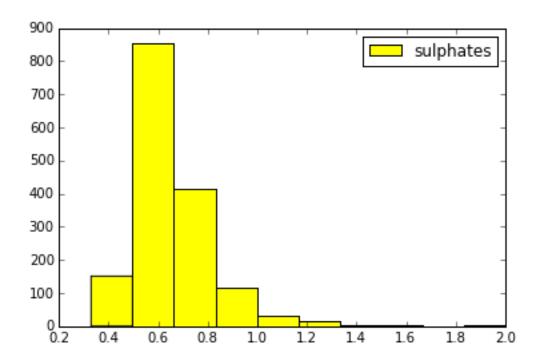
Out[196]: <matplotlib.legend.Legend at 0x141e22b0>



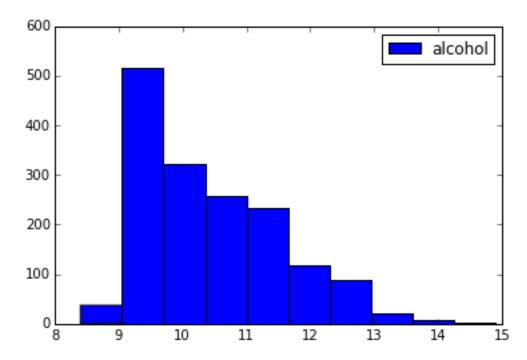
Out[197]: <matplotlib.legend.Legend at 0x13e16f60>



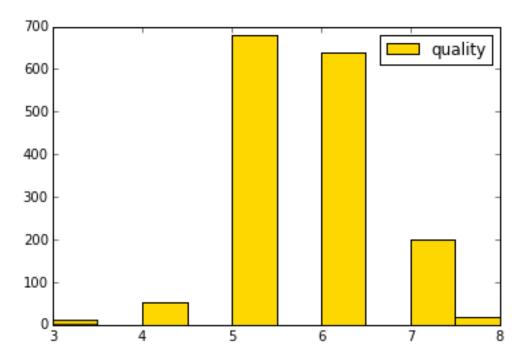
It is interesting to observe the pH values are distributed normally across the data points.



Out[199]: <matplotlib.legend.Legend at 0x13e161d0>



Out[200]: <matplotlib.legend.Legend at 0x16626cf8>



1.4.2 Statistial & Inferential Analysis

```
In [201]: #find out STD DEV of each of attributes - unbiased Std Dev
    red_wine_std_ds = pandas.Series(red_wine_df.std(), name=['Original Data'])
    red_wine_std_ds.sort()

#Join the individual filtered attribute series
    quartile_filtered_red_wine_df = pandas.concat([density_df, chlorides_df, pH_df, sulphates_df,
    #find STD DEV of filtered datasets attributes - unbiased Std Dev
    filtered_red_wine_std_ds = pandas.Series(quartile_filtered_red_wine_df.std(), name=['Filtered
    filtered_red_wine_std_ds.sort()

cmp_std_red_wine_df = DataFrame(data = {'Original STD DEV':red_wine_std_ds, 'Filtered STD DEV
    print "\t\tUnbiased Std Dev\n"
    print cmp_std_red_wine_df
```

Unbiased Std Dev

	Filtered STD DEV	Original STD DEV
density	0.001667	0.001887
chlorides	0.014865	0.047065
sulphates	0.120963	0.169507
рН	0.140498	0.154386
volatile acidity	0.166581	0.179060
citric acid	0.194006	0.194801
residual sugar	0.449141	1.409928
quality	0.745227	0.807569
alcohol	1.021412	1.065668
fixed acidity	1.513582	1.741096
free sulfur dioxide	9.226586	10.460157
total sulfur dioxide	27.214797	32.895324

We filter the outliers by finding the lower and upper bound of the sorted individual attributes. It can be observed from the **Filtered STD DEV** table that it gives a slimmer standard deviation for :

- density
- chlorides

and increases for other attributes.

This can make for finding correlation between density vs quality and chlorides vs quality or doing a multiregression among density vs chlorides and quality, we still need to investigate further.

Let us take the filtered dataset and perform:

keys = df.columns

attr_permutations = permutations(keys, 2)

- Univariate analysis;
- Bivariate analysis;

Let us take the quartile filtered data and find the Coefficient of Determination using Pearson's R for all possible combinations for the 11 input attributes as Dataset df.

First, let us perform the univariate analysis by finding descriptive statistics variables.

```
In [202]: import math
          from itertools import permutations
          from scipy.stats import pearsonr
          #from linear_regression import r_squared, line_fitting
          #from py_variance_std import critical_t
          red_wine_dof = len(quartile_filtered_red_wine_df) - 2
          #critical_t_val = critical_t(95, red_wine_dof, 0)
          critical_t_per = 0.05
          #Drop all NaN rows
          quartile_filtered_red_wine_df.dropna(inplace=True)
          #Drop all null or nan rows and drop the Quality Column
          quartile_filtered_red_wine_df = quartile_filtered_red_wine_df[quartile_filtered_red_wine_df.n
          [(quartile_filtered_red_wine_df != math.isnan) & (quartile_filtered_red_wine_df != np.NaN)].
          drop(['quality'], axis=1)
          df = quartile_filtered_red_wine_df
          #get all permutations of column pairs
```

```
coeff_r = {}
         [coeff_r.setdefault(each_comb[0], {}).update({each_comb[1]:pearsonr(df[each_comb[0]],\
                                                                         df[each_comb[1]])[0]}) \
          for each_comb in attr_permutations]
         df = DataFrame(data=coeff_r, columns=keys, index=keys).fillna(1)
         #correlation table
         print df
density chlorides
                        pH sulphates \
density
                    1.000000 0.411902 -0.227471
                                                  0.081691
chlorides
                    0.411902
                              1.000000 -0.175758 -0.076853
                   -0.227471 -0.175758 1.000000 0.013972
                   0.081691 -0.076853 0.013972 1.000000
sulphates
volatile acidity
                  citric acid
                   alcohol
                   -0.538901 -0.300750 0.126747
                                                  0.260783
residual sugar
                  0.394732 0.232752 -0.054684
                                                  0.040172
fixed acidity
                    0.610125
                              0.197774 -0.684378
                                                  0.165367
free sulfur dioxide -0.021505
                              0.012326 0.149126
                                                  0.107455
total sulfur dioxide 0.149847
                              0.176938 0.010031 -0.049655
                    volatile acidity citric acid alcohol residual sugar \
density
                                        0.305458 -0.538901
                                                                0.394732
                            0.044174
chlorides
                            0.117805
                                        0.073031 -0.300750
                                                                0.232752
рΗ
                           0.220702
                                       -0.470286 0.126747
                                                               -0.054684
                           -0.317346
                                       0.256747 0.260783
                                                                0.040172
sulphates
volatile acidity
                           1.000000
                                       -0.627194 -0.220600
                                                                0.035215
citric acid
                          -0.627194
                                       1.000000 0.137762
                                                                0.149494
alcohol
                          -0.220600
                                    0.137762 1.000000
                                                                0.098175
                                                                1.000000
residual sugar
                          0.035215
                                     0.149494 0.098175
fixed acidity
                           -0.271010
                                        0.659397 -0.037999
                                                                0.229653
free sulfur dioxide
                          -0.016718
                                       -0.068852 -0.022415
                                                                0.088405
total sulfur dioxide
                           0.097487
                                        0.004660 -0.245125
                                                                0.199534
                    fixed acidity free sulfur dioxide total sulfur dioxide
                         0.610125
                                           -0.021505
density
                                                                 0.149847
chlorides
                         0.197774
                                            0.012326
                                                                 0.176938
рΗ
                        -0.684378
                                            0.149126
                                                                 0.010031
sulphates
                         0.165367
                                            0.107455
                                                                -0.049655
volatile acidity
                        -0.271010
                                           -0.016718
                                                                 0.097487
citric acid
                        0.659397
                                           -0.068852
                                                                 0.004660
alcohol
                        -0.037999
                                            -0.022415
                                                                -0.245125
residual sugar
                         0.229653
                                            0.088405
                                                                 0.199534
fixed acidity
                         1.000000
                                           -0.150845
                                                                -0.087083
free sulfur dioxide
                        -0.150845
                                            1.000000
                                                                 0.619675
total sulfur dioxide
                        -0.087083
                                            0.619675
                                                                 1.000000
```

Now that we have correlation dataset df, let us summarize the descriptive analysis in a table.

mean_tbl = quartile_filtered_red_wine_df[['citric acid', 'total sulfur dioxide', 'free sulfur

```
min_tbl = quartile_filtered_red_wine_df[['citric acid', 'total sulfur dioxide', 'free sulfur
                     max_tbl = quartile_filtered_red_wine_df[['citric acid', 'total sulfur dioxide', 'free sulfu
                     #get unbiased std deviation of quartile filtered dataset
                     std_tbl = (quartile_filtered_red_wine_df[['citric acid', 'total sulfur dioxide', 'free sulfur
                     median_tbl = quartile_filtered_red_wine_df[['citric acid', 'total sulfur dioxide', 'free sulf
                     q1_tbl = red_wine_df[['citric acid','total sulfur dioxide','free sulfur dioxide','fixed acidi
                     q3_tbl = red_wine_df[['citric acid','total sulfur dioxide','free sulfur dioxide','fixed acidi
                     #calculate std err in a dict and create its dataframe
                     std_err_dct = {index:se(sd, len(df[index])) \
                                                                                    for sd,index in izip(std_tbl, \
                                                                                                                                 list(std_tbl.index))}
                     std_err_tbl = DataFrame(data=std_err_dct, index = ['std err']).transpose()
                     #create a DF of all tables and join std_err_tbl
                     tbl = DataFrame(data=[mean_tbl, min_tbl, max_tbl, std_tbl, median_tbl, q1_tbl, q3_tbl], index
                     #calculate range b/w max and min values
                     data_range = DataFrame(data = tbl['max'] - tbl['min'], columns=['range'])
                     #calculate Quartile range between Q3 and Q1
                     iqr = DataFrame(data = tbl['Q3'] - tbl['Q1'], columns=['iqr'])
                     #join tbl with range and Quartile data
                     tbl = tbl.join([data_range, iqr])
                     print tbl.transpose()
citric acid total sulfur dioxide free sulfur dioxide fixed acidity
mean
                        0.246760
                                                                     42.268024
                                                                                                                  15.020356
                                                                                                                                                    8.162002
min
                         0.000000
                                                                        6.000000
                                                                                                                    1.000000
                                                                                                                                                    5.100000
                         0.730000
                                                                   122.000000
                                                                                                                  42.000000
                                                                                                                                                  12.300000
max
std
                         0.179441
                                                                     26.106438
                                                                                                                    8.792916
                                                                                                                                                    1.458270
                         0.240000
                                                                     36.000000
                                                                                                                  13.000000
                                                                                                                                                    7.800000
median
                                                                                                                    7.000000
Q1
                         0.090000
                                                                      22.000000
                                                                                                                                                    7.100000
QЗ
                         0.420000
                                                                     62.000000
                                                                                                                  21.000000
                                                                                                                                                    9.200000
std err
                         0.054103
                                                                       7.871387
                                                                                                                    2.651164
                                                                                                                                                    0.439685
                                                                   116.000000
                                                                                                                  41.000000
                                                                                                                                                    7.200000
range
                         0.730000
                         0.330000
                                                                     40.000000
                                                                                                                  14.000000
                                                                                                                                                    2.100000
iqr
```

We observe that:

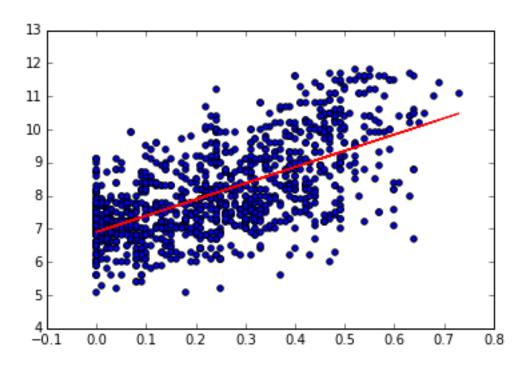
- We see that **range** is *greater* than the **IQR**;
- Overall since unbiased Std Dev of Citric acid is smallest under analysis, it has lowest overall score across all parameters;
- Median is greater than the mean;

We conclude that since range is greater than iqr even after filtering out the outliers, the quartile range is lesser than the range of extreme data points which means that we need to reduce the range less than iqr. This implies that we still need to clean the outliers.

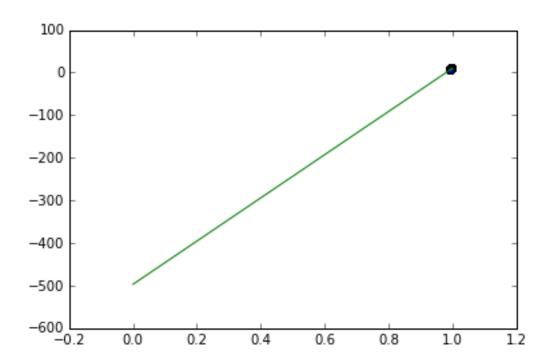
Now lets look at the high correlation value r, in the range $0.40 \ll r \ll 1$ and see which attributes share these values.

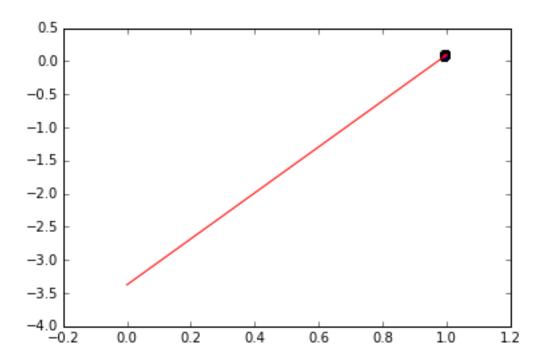
```
col, attr = each
              #condition to negate nan/null
              if limit_df[col][attr] > 0.:
                  if attr in red_wine_correl:
                      if (col in red_wine_correl[attr]):
                           continue
                  red_wine_correl.setdefault(col, []).append(attr)
          print red_wine_correl
{'citric acid': ['fixed acidity'], 'free sulfur dioxide': ['total sulfur dioxide'], 'density': ['chloric
   We find out that there seems to be correlation between Citric acid and Fixed acidity, density and fixed
acidity and density and chlorides and between free and total sulfur dioxide.
  Here are the scatter plots for these attributes, using the filtered dataset for red wine.
In [231]: from linear_regression import trace_line
          #Generate Scatter Plots of the red_wine_correl attributes
          #scatter plot for citric acid and fixed acidity
          #filter out the outliers and recreate DF and drop all null values
          citric_fixed_acid_filter_df = DataFrame(data=[filter_outlier_df(quartile_filtered_red_wine_df
          filter_outlier_df(quartile_filtered_red_wine_df['fixed acidity'])]).transpose().dropna()
          scatter(citric_fixed_acid_filter_df['citric acid'],citric_fixed_acid_filter_df['fixed acidity
          #R value
          citric_fixed_acid_r = pearsonr(citric_fixed_acid_filter_df['citric acid'], citric_fixed_acid_f
          print citric_fixed_acid_r
          #plot line
          x,y = zip(*trace_line(citric_fixed_acid_filter_df['citric acid'],citric_fixed_acid_filter_df[
          plot(x,y, color='red')
(0.62990096553285213, 1.0407110522614968e-128)
Out[231]: [<matplotlib.lines.Line2D at 0x18f7a518>]
```

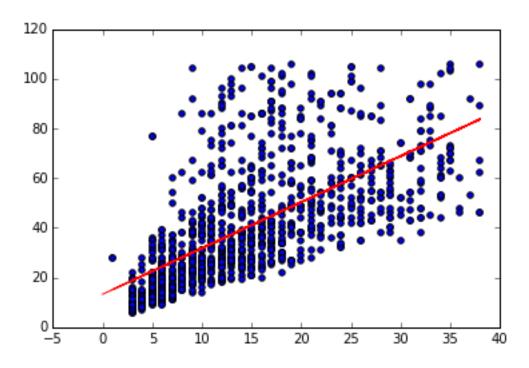
for each in permutations(keys, 2):



Out[233]: [<matplotlib.lines.Line2D at 0x18f7aba8>]





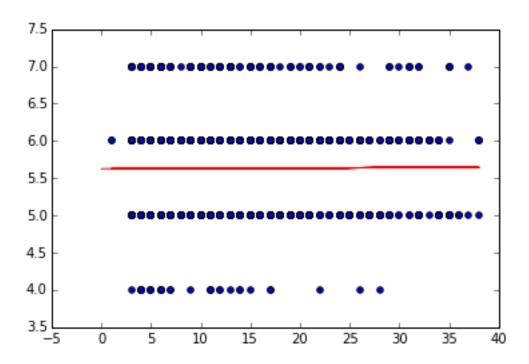


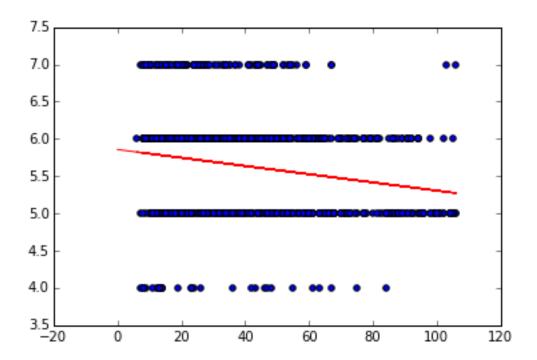
Noticeable correlations:

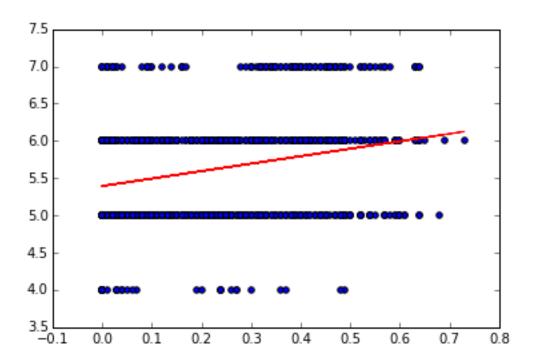
- ~63% of the relation can be described between citric and fixed acidity;
- ~65% of the relation can be described between free and total sulfur;

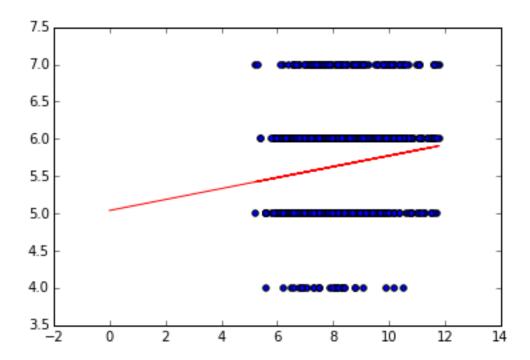
Let us test the scatterplot between:

- Quality vs Free Sulfur Dioxide;
- Quality vs Total Sulfur Dioxide;
- Quality vs Citric acid;
- Quality vs Fixed acidity;









From the Pearson R of the scatter plots we conclude there is no significant correlation between (fixed acidity, citric acid, total sulfur dioxide, free sulfur dioxide) and quality as the output variable.

We are unable to establish any significance to the positive correlation between citric vs fixed acidity and quality nor with free vs total sulfur and quality.

1.5 Conclusions

We see that density and chlorides provided minimal standard deviations so we proceed further for a univariate and bivariate analysis to test their correlations with other attributes and quality finally.

We find out the Pearson's R and summarize the descriptive analysis. We fid out the data still has outliers from the extreme range and inter-quartile range. We find out the probable lines of best fit could be among citric acid, (having the minimum standard error out of all probably correlation attributes) free and total sulfur dioxide, density, chlorides and fixed acidity.

As a result, we re run the filtering process to clear out any outliers from these attributes and run a scatter plot among each of the select physiochemical attributes against quality. But we find that the line of best fit and the scatterplot don't quite do justice and are in agreement with the Pearson's R showing no to littler significance between the correlation of the select physiochemical attributes and the quality of wine.

Therefore, we fail to reject the Null Hypothesis H0 and conclude that the dataset given is not appropriate for this test.

1.5.1 Suggestions based on Result

But for ages Sommeliers have been grading wine based on taste and taste is a side-effect of the physiochemical makeup of the wine. Which leaves us with one possibility and that is of wine-maturity and time.

Thus, a Pre- and Post- Time-period analysis is needed where we record the physiochemical data for a considerable period of time, say over 50 years and record the same attributes at the time of brewing wine and after 50 years and what changes have the physiochemical scores have gone through as well as comparing the *Quality* of wine for atleast these two given periods of time.

This way, we will have a Pre- and Post- dataset with the same number of attributes. With this kind of pair of dataset, we need to test the Null Hypothesis that the Quality of wine has remaind the same and

the mean Quality of the two datasets is the same while the Alternative Hypothesis would be that there is significant difference between the two mean Quality attributes. Since, there could be 2 or more datasets over an interval of time, a T-test would be a better measure of significance. If we negate the criteria of independent datasets, a One Way ANOVA test could also be performed over datasets over periods of intervals.

If we find there is a significant difference between the quality per dataset, then we could perform a T-test on the physiochemical makeup between the two datasets. From there, we might be able to infer some significant change in the physiochemical property that is correlated to the change in the quality of the wine over the period of time and come to a conclusion.

In []: