A Data mining approach to predict human wine taste preferences A dataset with white and red vinho verde samples is considered. The Feature vector: 1. fixed acidity 2. volatile acidity 3. citric acid 4. residual suggar 5. chlorides 6. free sulfur dioxide 7. total sulfur dioxide 8. density 9. pH 10. sulphates 11. alcohol **Final Prediction:** 1. Quality The original paper uses MR(multiple regression), SVN (Support Vector Machines) and NN (Neural Networks) for data mining. Categorization of the problem: By Input: We have labeled data, which means we will do supervised learning • By Output: We want to predict a class, which means we will do classification Here, wee will utilize Random Forests for classification. We achieve an accuracy of 96.22% without any model improvement. **Game Plan** The ML Pipeline: 1. Question and the required data 2. Acquire the data 3. Data Analysis 4. Prepare the data for the ML model 5. Train the Model 6. Test the Model 7. Evaluate the Model 8. Interpret the Model and report results visually and numerically 9. Adjust the Model if necessary In [1]: import pandas as pd import numpy as np import random import collections import matplotlib.pyplot as plt import seaborn as sns import time from pprint import pprint from sklearn.model\_selection import train\_test\_split, RandomizedSearchCV, GridSearchCV from sklearn.ensemble import RandomForestClassifier from sklearn.metrics import confusion matrix, accuracy score # Can be used to export a decision tree in DOT format from sklearn.tree import export graphviz import pydot # Visualizing decision trees from IPython.display import Image sns.set() **Data Analysis: Cleaning & Preparing** Data analysis usually occupies 80% of the time of any Data Scientist and Machine Learning Engineer. Without this crucial phase all the state-of-the-art models offered by sklearn would be completely in vain. 1. Tidy Data 2. Missing Data 3. Outliers 4. Class Imbalance Problem 5. Feature Correlation features = pd.read csv("data/winequality-white.csv", sep=";") In [2]: features.head() Out [2]: fixed volatile citric residual free sulfur total sulfur chlorides pH sulphates alcohol quality density acidity dioxide dioxide acidity acid sugar 0 7.0 0.27 0.36 20.7 0.045 45.0 170.0 1.0010 3.00 0.45 8.8 6 0.9940 3.30 1 6.3 0.30 0.34 0.049 14.0 0.49 6 1.6 132.0 9.5 2 8.1 0.28 0.40 6.9 0.050 30.0 97.0 0.9951 3.26 0.44 10.1 6 3 7.2 0.23 0.058 6 0.32 8.5 47.0 186.0 0.9956 3.19 0.40 9.9 8.5 0.058 7.2 0.23 0.32 47.0 186.0 0.9956 3.19 0.40 9.9 6 Tidy Data Data is <u>tidy</u> Identifying anomalies/missing data Missing Data: Impute or drop the values altogether. Generally speaking, if an observation should have been made but it was not made, then you do not drop the sample. If it could not be made (e.g. pregnant males) then you drop it. Outliers: Can be dropped if few One way to spot different annomalies as well as missing data is to compute a summary statistics. The following will give us a descriptive statistics In [3]: features.describe() Out[3]: volatile residual free sulfur total sulfur fixed acidity citric acid chlorides sulphate density dioxide acidity sugar dioxide count 4898.000000 4898.00000 4898.000000 4898.000000 4898.000000 4898.000000 4898.000000 4898.000000 4898.000000 4898.000000 6.854788 0.278241 0.334192 6.391415 0.045772 35.308085 138.360657 0.994027 3.188267 0.48984mean 0.843868 0.100795 0.121020 5.072058 0.021848 17.007137 42.498065 0.002991 0.151001 0.11412 std 3.800000 0.080000 0.000000 0.600000 0.009000 2.000000 9.000000 0.987110 2.720000 0.22000 0.991723 3.090000 6.300000 0.210000 0.270000 0.41000 25% 1.700000 0.036000 23.000000 108.000000 50% 5.200000 0.043000 75% 7.300000 0.320000 0.390000 9.900000 0.050000 167.000000 0.996100 3.280000 0.55000 46.000000 14.200000 1.100000 1.660000 65.800000 0.346000 289.000000 440.000000 1.038980 3.820000 1.08000 max The dataset seems to contain no missing values. However, it looks like we might have some outliers. total sulfur dioxide for example as a std of 42, mean value of 138 and a possible outlier (max value) of 440. Let's visualize the data so that we can better tell this. In [4]: # Set the style plt.style.use('fivethirtyeight') # Plotting layout fig, (ax1, ax2, ax3) = plt.subplots(nrows=1, ncols=3, figsize=(15,5))# residual sugar ax1.plot(features['residual sugar'], 'ro') ax1.set ylabel("Measure"); ax1.set xlabel("Count") ax1.set title("Residual Sugar") # free sulfur dioxide ax2.plot(features['free sulfur dioxide'], 'ro') ax2.set\_ylabel(""); ax2.set\_xlabel("Count") ax2.set title("Free Sulfur Dioxide") # total sulfur dioxide ax3.plot(features['total sulfur dioxide'], 'ro') ax3.set ylabel(""); ax3.set xlabel("Count") ax3.set title("Total Sulfur Dioxide") plt.show() Free Sulfur Dioxide Total Sulfur Dioxide Residual Sugar 300 400 250 50 200 300 150 30 200 100 100 50 10 1000 2000 3000 4000 5000 1000 2000 3000 4000 5000 1000 2000 3000 5000 Count Count Count We can certainly see outliers for these attributes. One way to deal with outliers is to remove and if we don't have many we can do so. The outlier in the first figure belongs to quality 6.0 for which we do have plenty of samples. However, the two other outliers belong to 3.0 for which we do not have too many samples. Dropping them means dropping 10% of the data for that kind of quality. Lets set a threshold of 125 for outliers in Free Sulfur Dioxide and 300 for outliers in Total Sulfur Dioxide in order to further investigate this. In [5]: features[features['total sulfur dioxide']>300] Out[5]: free sulfur fixed volatile citric residual total sulfur chlorides density sulphates alcohol quality acidity dioxide acidity dioxide acid sugar 325 7.5 0.31 0.057 131.0 0.27 5.80 313.0 0.99460 3.18 0.59 10.5 0.55 3 1417 8.6 0.35 15.55 0.057 35.5 366.5 1.00010 3.04 0.63 11.0 1931 0.49 0.22 2.00 0.047 146.5 307.5 0.99240 3.24 0.37 11.0 7.1 2127 9.1 0.33 0.38 1.70 0.062 50.5 344.0 0.99580 3.10 0.70 9.5 5 2654 6.9 0.40 0.22 5.95 0.081 76.0 303.0 0.99705 0.57 9.4 4745 0.26 289.0 440.0 0.99314 3.44 0.64 3 6.1 0.25 2.90 0.047 10.5 features[features['free sulfur dioxide']>125] In [6]: Out[6]: volatile citric free sulfur total sulfur fixed residual chlorides density pH sulphates alcohol quality dioxide acidity acidity acid sugar dioxide 325 7.5 0.270 0.31 5.8 0.057 131.0 313.0 0.99460 3.18 0.59 10.5 5 1931 7.1 0.490 0.22 2.0 0.047 146.5 307.5 0.99240 3.24 0.37 11.0 3 2334 7.5 0.230 0.35 17.8 0.058 128.0 212.0 1.00241 0.43 3050 6.2 0.255 0.24 0.039 138.5 272.0 0.99452 3.53 0.53 4 1.7 9.6 4745 6.1 0.260 0.25 2.9 0.047 289.0 440.0 0.99314 3.44 0.64 10.5 3 We can see that it that *quality=3* seems to have more outliers in both of these attributes and since we don't have much data of it (20 samples) it does not make sense to drop the outliers for these two features. Actually it seems to be the case that these are the values that those attributes take that make up for a quality of 3. In the greater context of the dataset, however they are called as outliers. So we will stick with dropping a single outlier for the feature Residual Sugar. features = features.drop(index=features[features['residual sugar']>40].index, axis=0) Class-Imbalance Problem Class Imbalance problem is a really nasty issue which is often difficult to tackle. Therefore a thumb up rule here is: data, and some more data. When we have made sure that the phenomenon comes as a result of nature itself (from the way things are) and not from low amount of data we can proceed with investigating it. In [8]: print("Classes are indeed imbalanced") print(round(100\*(features['quality'].value counts()/features.shape[0])), 2) Classes are indeed imbalanced 45.0 5 30.0 7 18.0 8 4.0 4 3.0 3 0.0 9 0.0 Name: quality, dtype: float64 2 We can visualize this In [9]: sns.countplot(x='quality', data=features, palette='hls'); plt.show() 2000 1500 1000 500 6 quality We can see that a whooping 75% of the data belong to only two classes! However, if our classes are nicely separated then the class-imbalance is not really a problem. Although there are tools and techniques to check this, here we will just visualize for a couple of attributes and classes at a time. In [10]: def get rand class(): """Get 3 random classes from a total of 6. """ rand = []while True: **if** len(rand) == 3: return rand r = random.randint(0,6)if r not in rand: rand.append(r) In [11]: fig, ((ax1, ax2), (ax3, ax4), (ax5, ax6)) = plt.subplots(nrows=3, ncols=2, figsize=(15,12)) # Feature: residual sugar rs = list(features['residual sugar'].groupby(features['quality'])) # Randomly pick 3 classes to display c1, c2, c3 = get rand class()ax1.plot(rs[c1][1], 'g^', label=rs[c1][0]) ax1.plot(rs[c2][1], 'ro', label=rs[c2][0]) ax1.plot(rs[c3][1], 'v', label=rs[c3][0]) ax1.set xlabel(""); ax1.set\_ylabel("Count"); ax1.set\_title("Residual Sugar") ax1.legend() # Feature: Fixed acidity fa = list(features['fixed acidity'].groupby(features['quality'])) # Randomly pick 3 classes to display c1, c2, c3 = get rand class()ax2.plot(fa[c1][1], 'g^', label=fa[c1][0]) ax2.plot(fa[c2][1], 'ro', label=fa[c2][0])
ax2.plot(fa[c3][1], 'v', label=fa[c3][0]) ax2.set\_xlabel(""); ax2.set\_ylabel(""); ax2.set\_title("Fixed acidity") ax2.legend() # Feature: citric axid ca = list(features['citric acid'].groupby(features['quality'])) c1, c2, c3 = get rand class()ax3.plot(ca[c1][1], 'g^', label=ca[c1][0]) ax3.plot(ca[c2][1], 'ro', label=ca[c2][0]) ax3.plot(ca[c3][1], 'v', label=ca[c3][0]) ax3.set xlabel(""); ax3.set ylabel("Count"); ax3.set title("Citric Acid") ax3.legend() # Feature: total sulfur dioxide tsd = list(features['total sulfur dioxide'].groupby(features['quality'])) c1, c2,  $c3 = get_rand class()$ ax4.plot(tsd[c1][1], 'g^', label=tsd[c1][0]) ax4.plot(tsd[c2][1], 'ro', label=tsd[c2][0]) ax4.plot(tsd[c3][1], 'v', label=tsd[c3][0]) ax4.set xlabel(""); ax4.set ylabel(""); ax4.set title("Total Sulfur Dioxide") ax4.legend() # Feature: residual sugar rs2 = list(features['residual sugar'].groupby(features['quality'])) c1, c2,  $c3 = get_rand_class()$ ax5.plot(rs2[c1][1], 'g^', label=rs2[c1][0]) ax5.plot(tsd[c2][1], 'ro', label=rs2[c2][0]) ax5.plot(tsd[c3][1], 'v', label=rs2[c3][0]) ax5.set\_xlabel("Measure"); ax5.set\_ylabel("Count"); ax5.set\_title("Residual Sugar") ax5.legend() # Feature: pH ph = list(features['pH'].groupby(features['quality'])) c1, c2, c3 = get rand class() $ax6.plot(ph[c1][1], 'g^{'}, label=ph[c1][0])$ ax6.plot(ph[c2][1], 'ro', label=ph[c2][0]) ax6.plot(ph[c3][1], 'v', label=ph[c3][0]) ax6.set xlabel("Measure"); ax5.set ylabel(""); ax6.set title("pH") ax6.legend() plt.tight layout(pad=2) Residual Sugar Fixed acidity 25 Count 3000 5000 1000 2000 4000 5000 Citric Acid Total Sulfur Dioxide 1.50 300 1.25 1.00 Count 200 0.75 150 0.50 0.25 0.00 4000 5000 Residual Sugar 350 300 250 3.2 3.0 2.8 4000 4000 Measure Measure We can tell from this plots that the features are not at all separated (some exceptions are there but they do not change the rule). This means that the class-imbalance problem for this dataset is real! Among the options that we are left with is undersampling or oversampling but for now we will just stick with the data as is and see how our model fares. We basically do nothing regarding this. Feature correlation A high correlation between features is almost always not feasible for the ML algorithms. Therefore we always aim to feature engineer correlated features. Correlation with the quality variable Lets see important variables in predicting the quality by checking the feature's correlation with it. In [12]: # Drop the quality and plot with pandas features.drop("quality", axis=1).corrwith(features['quality']).plot.bar(figsize=(10,5), title='Correlation with the class variable', rot=45, fontsize=1 plt.show() Correlation with the class variable 0.4 0.3 0.2 0.1 0.0 -0.1-0.2-0.3residual sugar dhorides (ree suffur dioxide suffur dioxide pensity) So, taking the correlation into acount, we can see that alcohol is the most important feature in our feature vector for predicting the quality of the wine. Note that even variables that are negatively correlated with it (like density) are indeed because in this case they could simply be contributors of a lower quality. Citric acid and free sulfur dioxide seem to have the lowest correlation. alcohol and density seem to have the highest correlation. We can also check features' importances using panda's groupby In [13]: quality\_group = features.groupby('quality') print(quality\_group.agg(np.mean)) fixed acidity volatile acidity citric acid residual sugar \ quality 3 7.600000 0.333250 0.336000 6.392500 4 7.129448 0.381227 0.304233 4.628221 5 0.302011 0.337653 6.933974 7.334969 0.337906 6 6.837233 0.260244 6.414588 0.325625 6.734716 7 0.262767 5.186477 0.277400 0.326514 8 6.657143 5.671429 0.386000 9 7.420000 0.298000 4.120000 chlorides free sulfur dioxide total sulfur dioxide density \ quality 3 0.054300 53.325000 170.600000 0.994884 0.050098 125.279141 0.994277 4 23.358896 36.432052 150.904598 0.995263 5 0.051546 0.045204 6 35.663177 137.036868 0.993941 7 0.038191 34.125568 125.114773 0.992452 0.038314 36.720000 126.165714 0.992236 0.027400 9 33.400000 116.000000 0.991460 pH sulphates alcohol quality 3 3.187500 0.474500 10.345000 3.182883 0.476135 10.152454 4 3.168833 0.482203 9.808840 5 3.188507 0.491015 10.574860 3.213898 0.503102 11.367936 7 3.218686 0.486229 11.636000 3.308000 0.466000 12.180000 Here we see that alcohol doesn't have the importance that the correlation plot showed us because the mean of it among the classes does not clearly separate them. correlation != causality Correlation Matrix: Correlation of features with each-other. Variables to utilize when using sns.heatmap • vmax: Achoring the color map to values. If not specified, it will infer from the data linewidths: The widths of the lines dividing the cells cbar\_kws: in the below case we specify the height of the stripe showing the values • annot: allow annotations inside the boxes fmt: formatting the annotations In [14]: sns.set(style='white', font scale=1.5) # Compute the correlation matrix # The correlation matrix is an array where the main diagonal separetes two identical triangles corrMatrix = features.corr() # Create a mask for the upper triangle so that we can ignore it later when building the heatmap # When we pass this mask to the heatmap function, it will generate no data for the upper triangle mask = np.zeros\_like(corrMatrix, dtype=np.bool) # Get the indices of the upper-triangle of the array mask[np.triu indices from(mask)] = True # Generate a custom diverging colormap # Colormap for the different values of the correlation matrix cmap = sns.diverging palette(220, 10, as cmap=True) plt.figure(figsize=(9, 7)) plt.title("Correlation Matrix of Features") # Draw the heatmap sns.heatmap(corrMatrix, square=True, mask=mask, cmap=cmap, center=0, linewidths=2.0, cbar kws={"shrink" : 0.8}) plt.show() Correlation Matrix of Features fixed acidity - 0.8 volatile acidity citric acid - 0.6 residual sugar - 0.4 chlorides -0.2 free sulfur dioxide -0.0total sulfur dioxide - -0.2 density - -0.4 pН sulphates alcohol quality alcohol citric acid total sulfur dioxide density volatile acidity residual sugar chlorides free sulfur dioxide quality sulphates fixed acidity The features seem to be somewhat correlated with each-other. alcohol and density are negatively correlated to a rather significant amount. density and residual sugar are positively correlated to a significant amount as well desity and alcohol are also highly correlated with the quality. An increase of alcohol increases the quality but an increase in density decreases it. Therefore it doesn't seem such a good idea to merge them in one single feature. Prepare the data for the machine learning model 1. One-Hot Encoding 2. Class and Features 3. Train/Test 4. Scaling/Standardisation if needed One-Hot encoding: We need not perform this for our current dataset Features and classes In [15]: labels = features.pop('quality') print(features.shape) print(labels.shape) (4897, 11) (4897,)Train & Test Data We use stratify because our classes are not balanced. With stratify we can preserve the class imbalance into the train, test sets. In [16]: train\_features, test\_features, train\_labels, test\_labels = train\_test\_split(features, labels, test size = 0.2, random state = 3, stra tify=labels) print("Shape of our train and test samples") print("Shape of train features:", train features.shape) print("Shape of train labels:", train labels.shape) print("Shape of test features:", test\_features.shape) print("Shape of test labels:", test\_labels.shape) Shape of our train and test samples Shape of train features: (3917, 11) Shape of train labels: (3917,) Shape of test features: (980, 11) Shape of test labels: (980,) Train the Model Yes! With the state-of-the-art scikit-learn algorithm, training our model looks this the following! In [17]: # Instantiate Model # Set a random state in order to get consistent results rf = RandomForestClassifier(n estimators=100, random state=3) # Train the model rf.fit(train\_features, train\_labels); Make Predictions on Test Data One way to do this is using the confusion matrix and then calculating the Micro-Precision. We use Micro- and not Macro- precission because Macro-Precision is not flexible to class-imbalance problem which we do have in this case.  $MicroP = rac{TP}{(TP+FP)}$ In [18]: predictions = rf.predict(test features) confusion mat = confusion matrix(test labels, predictions) microP = sum(np.diag(confusion mat) / sum(sum(confusion mat))) print("Micro precision {}%".format(round(microP\*100, 2))) # Calculate with library print("Precision {}%".format(round(100\*accuracy\_score(test\_labels, predictions), 2))) Micro precision 68.06% Precision 68.06% Evaluate the Model Visualize the confusion matrix In [19]: plt.figure(figsize=(9,5)) xticklabels=np.append(3.0, np.unique(predictions)) xticklabels=np.append(xticklabels, 9.0) yticklabels=np.unique(np.array(test labels)) sns.heatmap(confusion mat, square=False, annot=True, fmt='d', cbar=True, xticklabels=xticklabels, yticklabels=yticklabels) plt.xlabel("Predicted") plt.ylabel("Truth") plt.show() 350 0 0 0 3 - 300 5 15 13 0 0 4 - 250 3 210 77 1 0 0 200 64 352 23 0 0 - 150 0 5 81 88 2 0 - 100 0 0 12 11 12 0  $\infty$ 3.0 4.0 5.0 6.0 7.0 8.0 9.0 Predicted In [20]: # We get get a dic of the values as keys and the count as the values of the dic print("Number of samples per class, real data", collections.Counter(np.array(test\_labels))) print("Number of samples per class, predicted data", collections. Counter(predictions)) Number of samples per class, real data Counter({6: 440, 5: 291, 7: 176, 8: 35, 4: 33, 3: 4, 9: 1}) Number of samples per class, predicted data Counter({6: 538, 5: 296, 7: 123, 8: 14, 4: 9}) It looks like our model is not doing such a good job since its accuracy is 68.08%. It completely misses out on classes with quality 9 and 3. This makes sense because we do not have so many samples for both of them. For class 9 specifically we had 4 training and 1 testing samples, which is terrible. It also misclassifies some values from the other classes. As already investigated a little bit another reason for this this might be due the class-imbalance problem. However, the paper reports that, when admitting only the correct classifed classes, the overal accuracy was 62.4%. So already our model is faring better than the SVN and NN version's of the paper. The performance is then substantionally increased when they set a tolerance of accepting responses that are correct within the one of the two nearest classes, obtaining an accuracy of 89.0%. Let us calculate this kind of tolerance accuracy as described by the paper and observe the results of our model. Indicentally, this is the reason why we also manually calculated the micro precision using the confusion matrix earlier. In [21]: def evaluate\_model(model, test\_features, test\_labels): """ Evaluate the model using the test features and test labels and then calculate tolerance precision as defined on the paper. Arguments: model: the model to evaluate test features: the test features test labels: the test labels 11 11 11 # Test the model predictions = model.predict(test\_features) # Evaluate the model confusion\_mat = confusion\_matrix(test\_labels, predictions) # Calculate tolerance micro precision sum tp = 0sum\_tp\_fp = sum(sum(confusion\_mat)) for i in range(len(confusion\_mat)): for j in range(len(confusion\_mat)): # element in main diagonal **if** (i == j): sum\_tp += confusion\_mat[i][j] # element around main diagonal **elif** (j == i+1) & (i<5): sum\_tp += confusion\_mat[i][j] **elif** (j == i-1) & (i>0): sum\_tp += confusion\_mat[i][j] micro\_p = sum\_tp/sum\_tp\_fp print("Tolerance precision:", round(100\*micro\_p, 2)) evaluate\_model(rf, test\_features, test\_labels) Tolerance precision: 96.22 So, if we set a tolerance of accepting responses that are correct within the one of the two nearest classes, we obtain an accuracy of 96.22% which is pretty good and even better than the original paper's results (although the paper is from 2009)! Interpreting Model Results Visualizing a Single Decision Tree In [23]: # Pull out one random tree from the forest tree = rf.estimators\_[int(random.random()\*10)] # Export the image to a dot file # This function generates a GraphViz representation of the decision tree, which is then written into ou export\_graphviz(tree, out\_file='images/tree.dot', feature\_names=features.columns, rounded=True, precisi on=2) # Use dot file to create a graph (graph, ) = pydot.graph\_from\_dot\_file('images/tree.dot') # Write graph to a png file graph.write\_png('images/tree.png') In [24]: print("The depth of the tree is", tree.tree\_.max\_depth) The depth of the tree is 31 Visualizing a smaller decision Tree In [25]: mini\_rf = RandomForestClassifier(n\_estimators=100, max\_depth=3, random\_state=3) mini\_rf.fit(train\_features, train\_labels) predictions2 = mini\_rf.predict(test\_features) print("The accuracy of the mini tree is {}%".format(round(100\*accuracy\_score(test\_labels, predictions2 ), 2))) The accuracy of the mini tree is 53.67% Understandibly the precision is decreasing. Let's visualize the tree so that we can better understand what's going on Incidentally decision trees have the advantage of being readily interpretable at a time when many ML algorithms appear to be black boxes. In [26]: | mini\_tree = mini\_rf.estimators\_[1] export\_graphviz(mini\_tree, out\_file='images/mini\_tree.dot', feature\_names=features.columns, rounded=Tru precisi on=1) (graph, ) = pydot.graph\_from\_dot\_file('images/mini\_tree.dot') graph.write\_png('images/mini\_tree.png') Visualize the tree

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