

# sommelieR

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# Introduction

- ▶ Wine tasting can range from a casual pastime to a lucrative profession
- ▶ For professional sommeliers, considerable time and training is required to adequately rate wine quality
- ▶ Intuitively, we might expect expert ratings to reflect the underlying chemical composition of the wines
- ▶ We decided to more formally investigate this idea

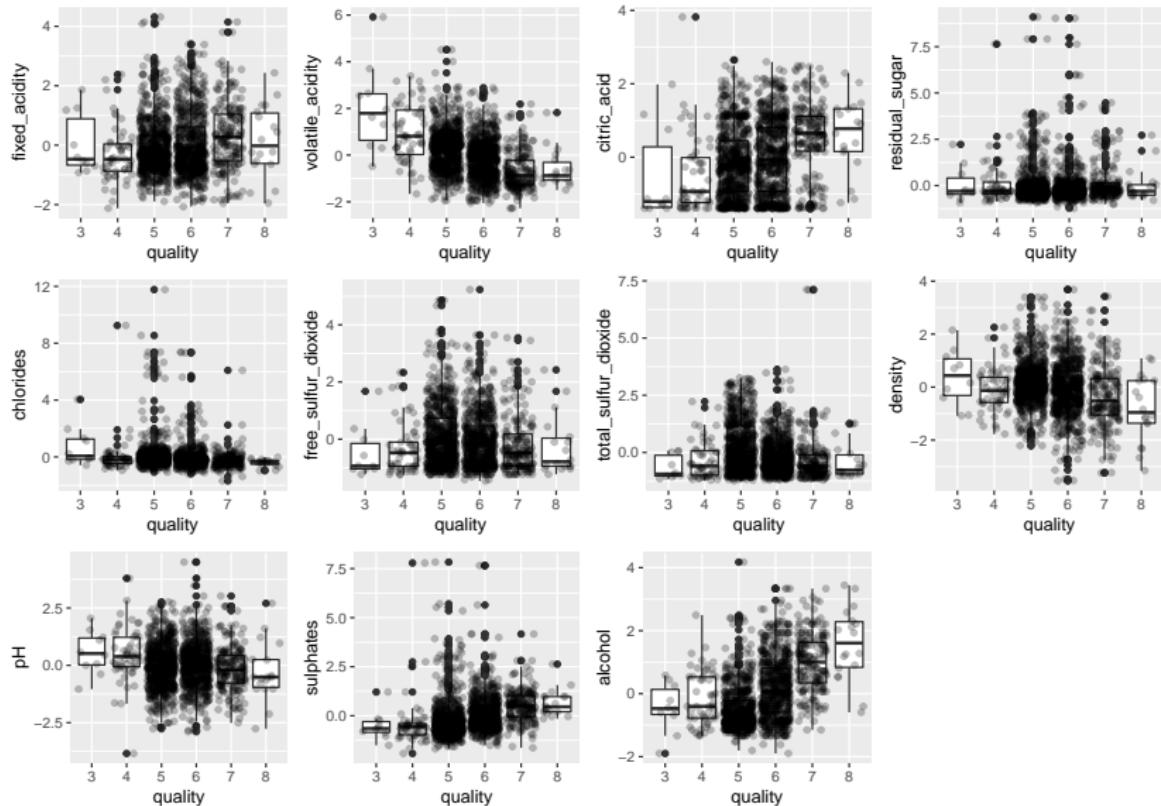
# Project Aim

To determine how accurately expert wine quality ratings can be predicted using a set of easily measured chemical components.

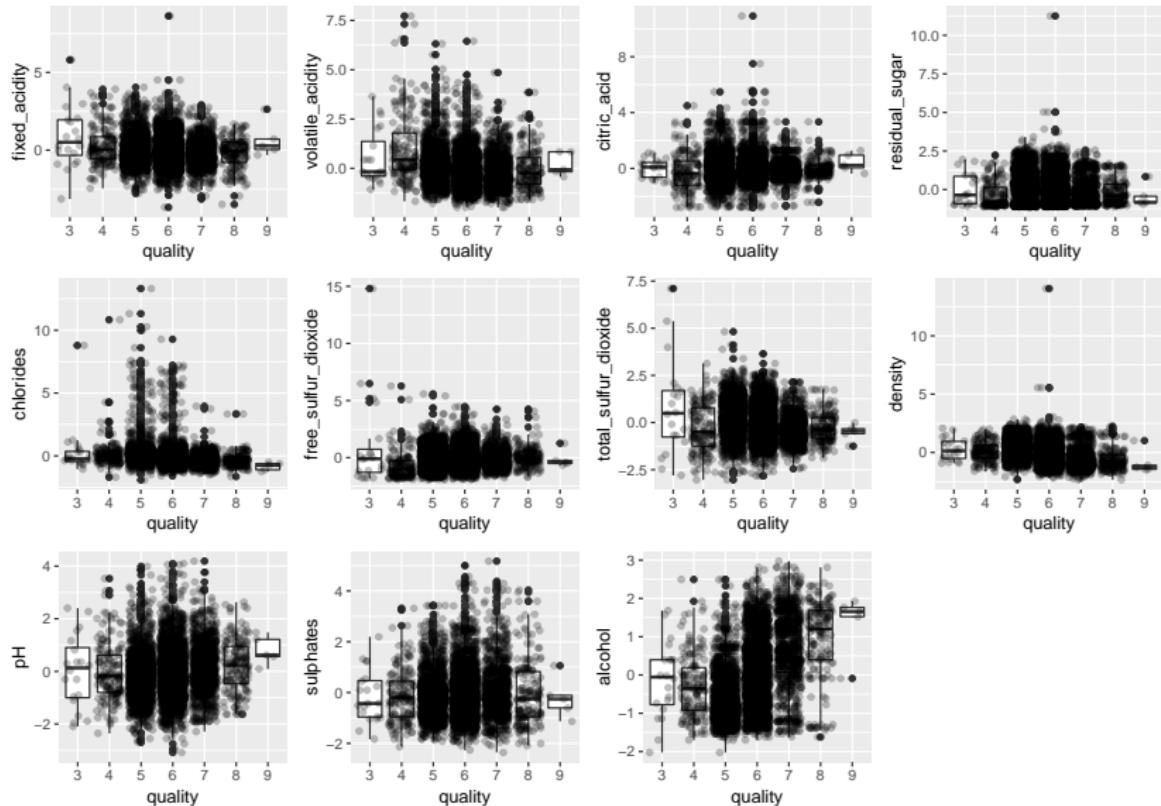
# Data

- ▶ 2 datasets of expert quality ratings of red and white Vinho Verde wines
  - ▶ source: <http://archive.ics.uci.edu/ml/datasets/wine+quality>
  - ▶ 1599 red wines
  - ▶ 4898 white wines
- ▶ Outcome variable: wine quality
  - ▶ ordinal variable theoretically ranging from 0-10
    - ▶ Observed ratings range from 3-9
  - ▶ 0 is poor, 10 is excellent
  - ▶ classes are unbalanced
- ▶ Predictor variables: 11 physiochemical wine components:
  - ▶ fixed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, alcohol

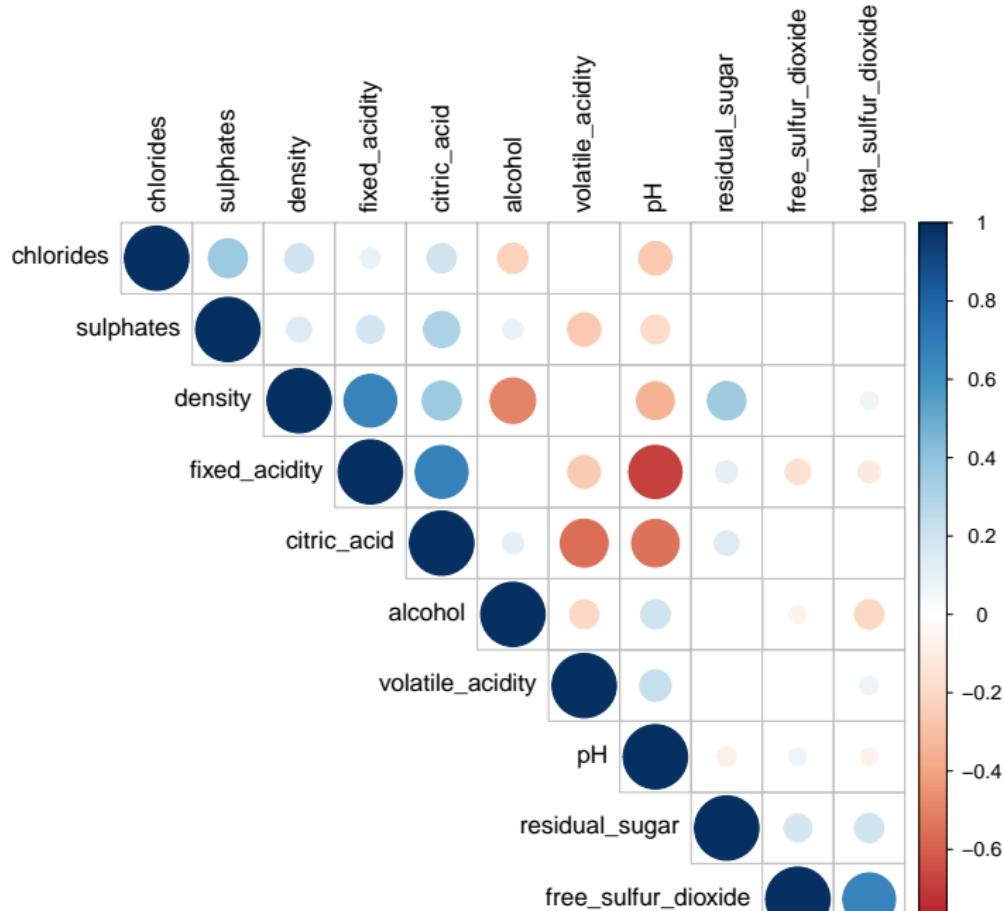
# Looking At the Red Wine Data



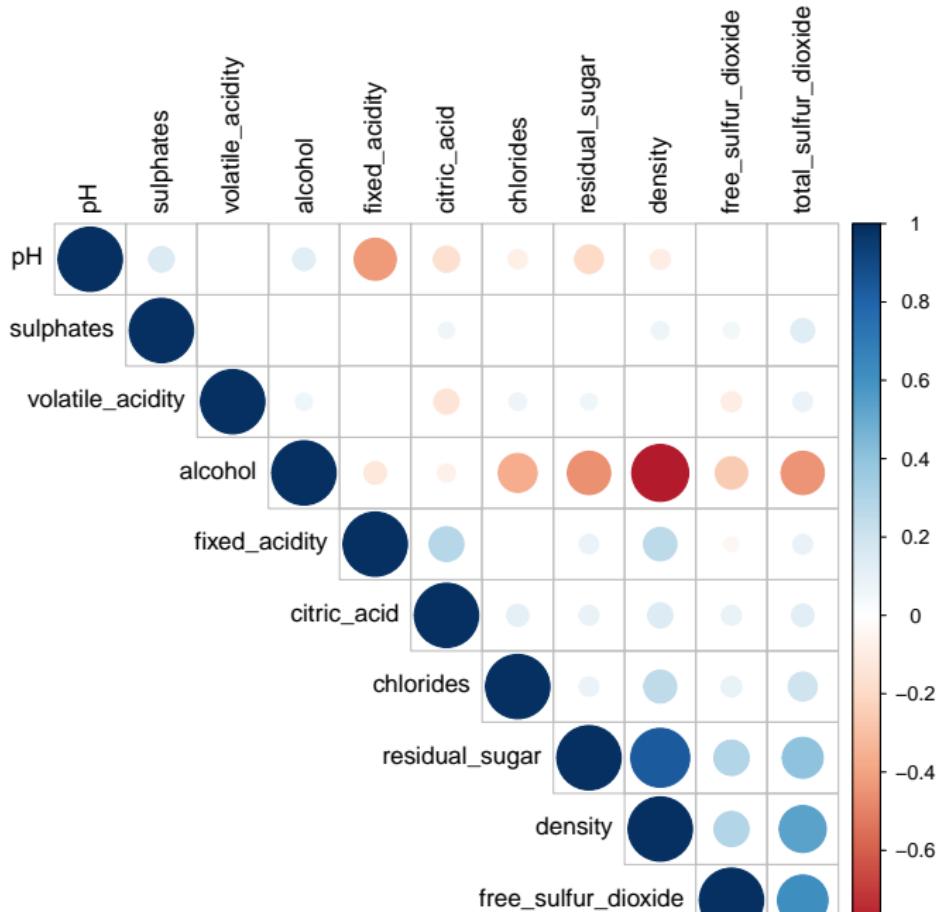
# Looking At the White Wine Data



## Correlations- Red Wine



## Correlations- White Wine



# Methods

- ▶ The red and white wine datasets were split into training and testing sets
  - ▶ 80% of available data sampled for training models
  - ▶ Remaining 20% used to evaluate accuracy
  - ▶ Relative frequencies of quality ratings in full dataset were preserved in training and testing data
- ▶ Modeling Approach
  - ▶ Machine learning
    - ▶ Random forest classification of quality ratings
  - ▶ Likelihood based
    - ▶ linear regression
    - ▶ partial proportional odds model
    - ▶ multinomial model

## Methods: Linear Regression

- ▶  $Z = X^T \beta + \epsilon$ , where  $\epsilon \sim N(0, \sigma^2 I)$
- ▶  $\hat{\beta} = (X^T X)^{-1} X^T Z$
- ▶ Predicted classification: The nearest integer to the predicted mean rating

## Methods: Partial Proportional Odds Models

Three different approaches were considered:

- ▶ Non-proportional odds:  $\text{logit}(P(Z \leq j|x)) = \alpha_j + x^T \beta_j$
- ▶ Proportional odds:  $\text{logit}(P(Z \leq j|x)) = \alpha_j + x^T \beta$
- ▶ Partial proportional odds:  
$$\text{logit}(P(Z \leq j|x)) = \alpha_j + x_*^T \beta + x_{**}^T \beta_j$$
- ▶  $\alpha_j > \alpha_i$  for  $j > i$
- ▶ Log likelihood maximized using BFGS (default) or any available method in package optimx
- ▶ Predicted classification: the rating with the highest predicted probability

## Methods: Multinomial Regression

- ▶ Response takes values in K classes
- ▶ Model:  $\log \frac{Pr(G=k|X=x)}{P(G=K|X=x)} = X\beta_k$  for  $k = 1, \dots, (K - 1)$
- ▶ Predictions:  
$$P(G = k|X = x) = \frac{\exp(X\beta_k)}{1 + \sum_{l=1}^{K-1} \exp(X\beta_l)}, k = 1, \dots, K - 1$$
- ▶ Considered 3 Models: All Predictors with Linear Terms, Reduced Model with Linear Terms, and Reduced Model with All Second Order Terms
- ▶ Computational Efficiency Challenges

## Methods: Random Forest

- ▶ Ensembles of decision trees which are built by bootstrapping the observations
- ▶ Final prediction is made by a majority vote of the ensemble of trees

# Variable Selection

- ▶ Random Forest: all physiochemical variables included
- ▶ Likelihood based models:
  - ▶ We examined the correlations between predictors and considered best subsets found in R based on linear regression.
  - ▶ The final predictor variables selected were:
    - ▶ red wine: volatile acidity, total sulfur dioxide, pH, alcohol, sulphates
    - ▶ white wine: pH, volatile\_acidity, residual\_sugar, alcohol

# Model Evaluation

Models were compared on the following metrics:

- ▶ Accuracy
  - ▶ Correct Classifications/Total
- ▶ Kappa
- ▶ Weighted Kappa - used to select the final model
  - ▶ A more useful version of Kappa for data with inherent ordering that penalizes misclassifications proportional to the distance from the true category.
  - ▶ For instance, when the true quality rating is 4, a prediction of 7 will be penalized more severely than a prediction of 5.

# Results: Linear Model

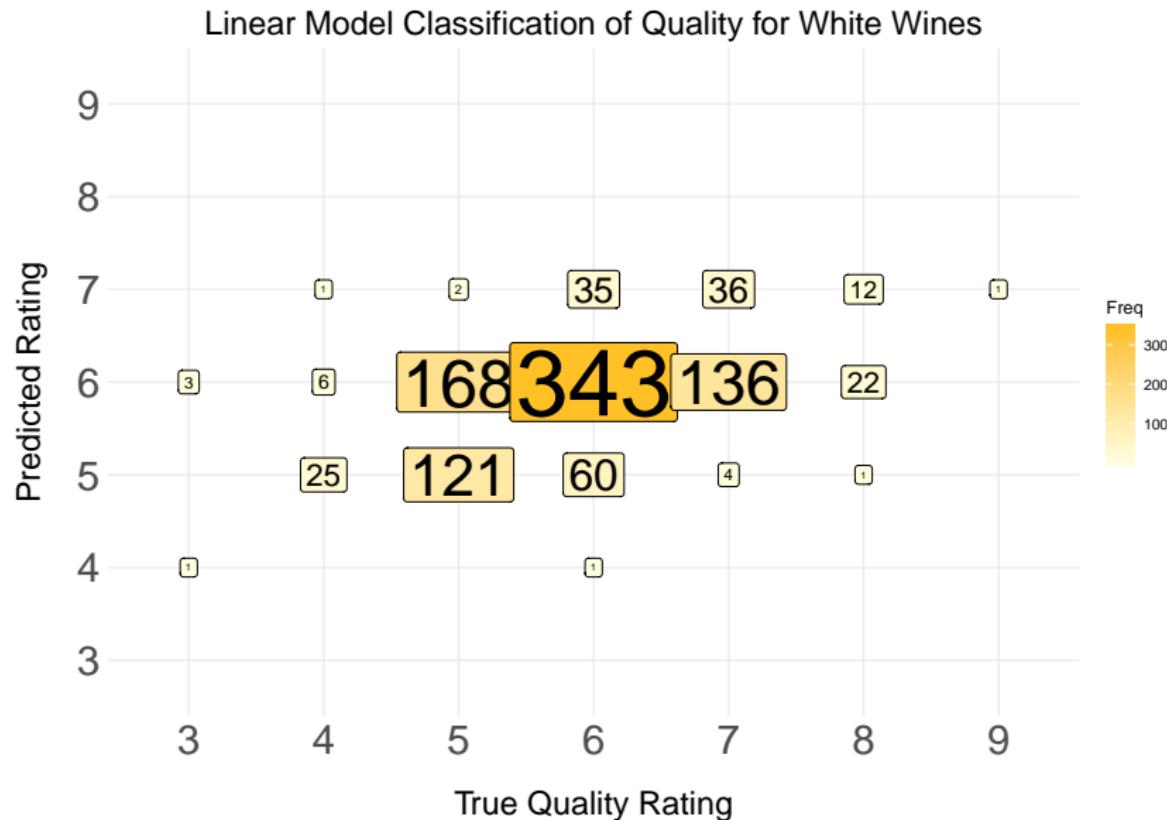
Table 1: Comparison of Full and Reduced Linear Regression Models for Red and White Wine Quality

	Overall Results			Percent Correct by Category						
	Accuracy	Kappa	Weighted Kappa	3	4	5	6	7	8	9
Full (Red)	57.73	0.2998	0.4996	0	0	67.65	64.57	23.08	0	NA
Reduced (Red)	56.15	0.2728	0.4545	0	0	65.44	63.78	20.51	0	NA
Full (White)	52.61	0.2162	0.4211	0	0	39.86	81.78	22.16	0	0
Reduced (White)	51.12	0.1969	0.4067	0	0	41.58	78.13	20.45	0	0

# Results: Linear Model (Red Wine)



# Results: Linear Model (White Wine)

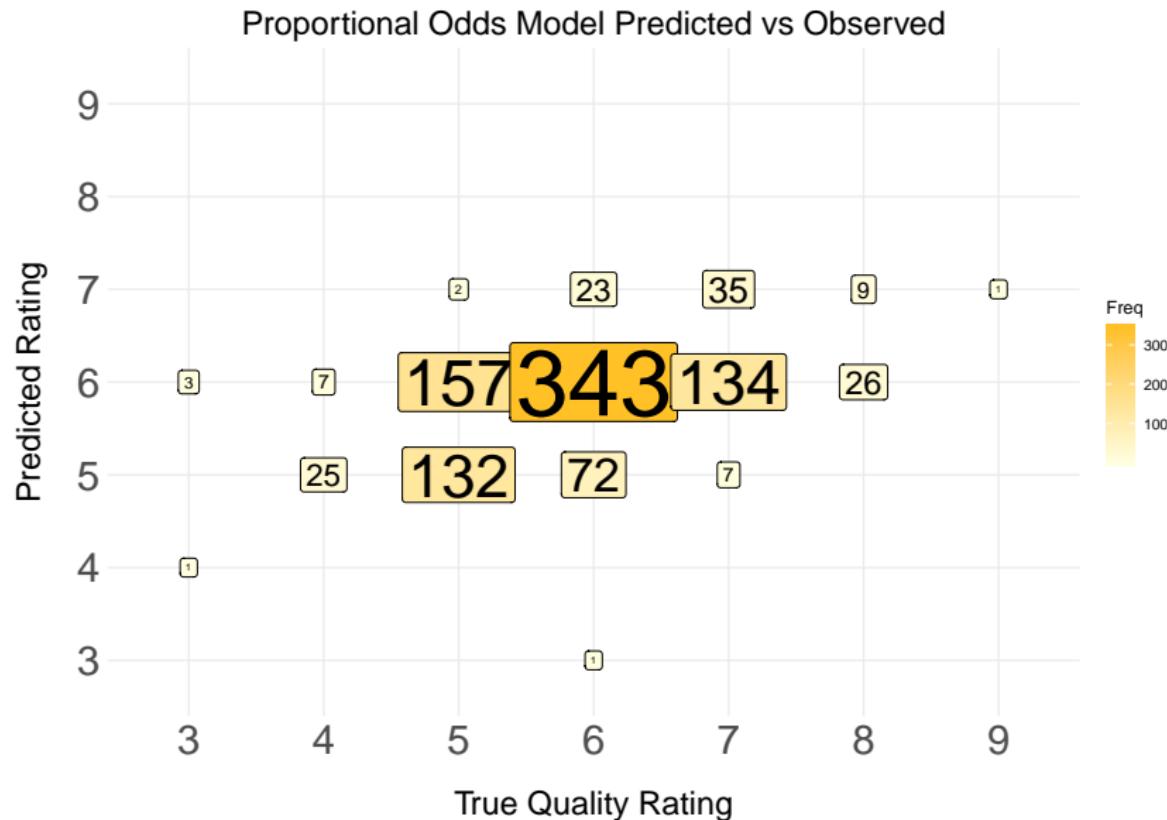


# Results: Partial Proportional Odds Model (White Wine)

Table 2: Comparison of White Wine Proportional Odds Model Results

	Overall Results			Percent Correct by Category						
	Prediction Accuracy	Kappa	Weighted Kappa	3	4	5	6	7	8	9
Proportional Odds (F)	52.1472	0.2126	0.4053	0	0	45.3608	78.1321	19.8864	0	0
Proportional Odds (R)	51.7382	0.2108	0.3993	0	0	51.2027	74.9431	15.9091	0	0

# Results: Proportional Odds Model (White Wine, Full)



## Results: Partial Proportional Odds Model (Red Wine)

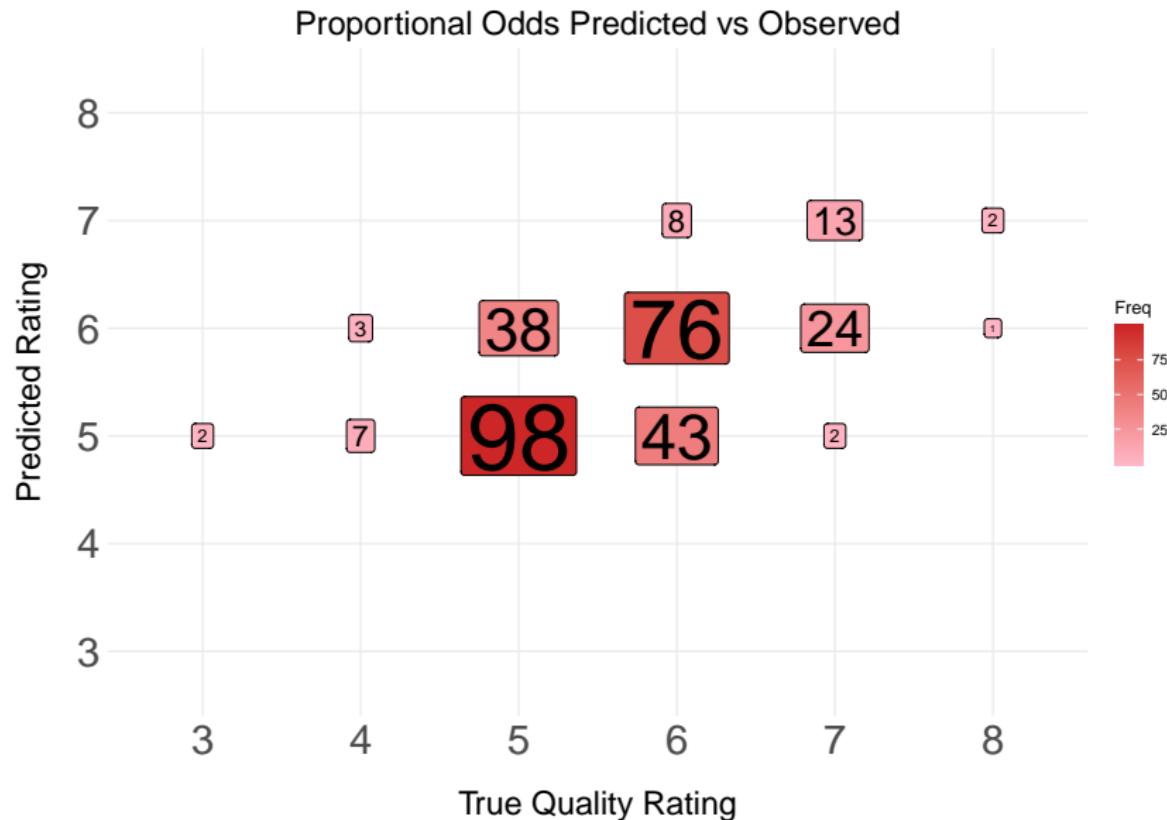
- ▶ Proportional, partial proportional models converged
- ▶ Results presented for partial proportional model with coefficient for total sulfur dioxide allowed to vary with the level of wine quality

# Results: Comparison of Partial Proportional Odds Models (Red Wine)

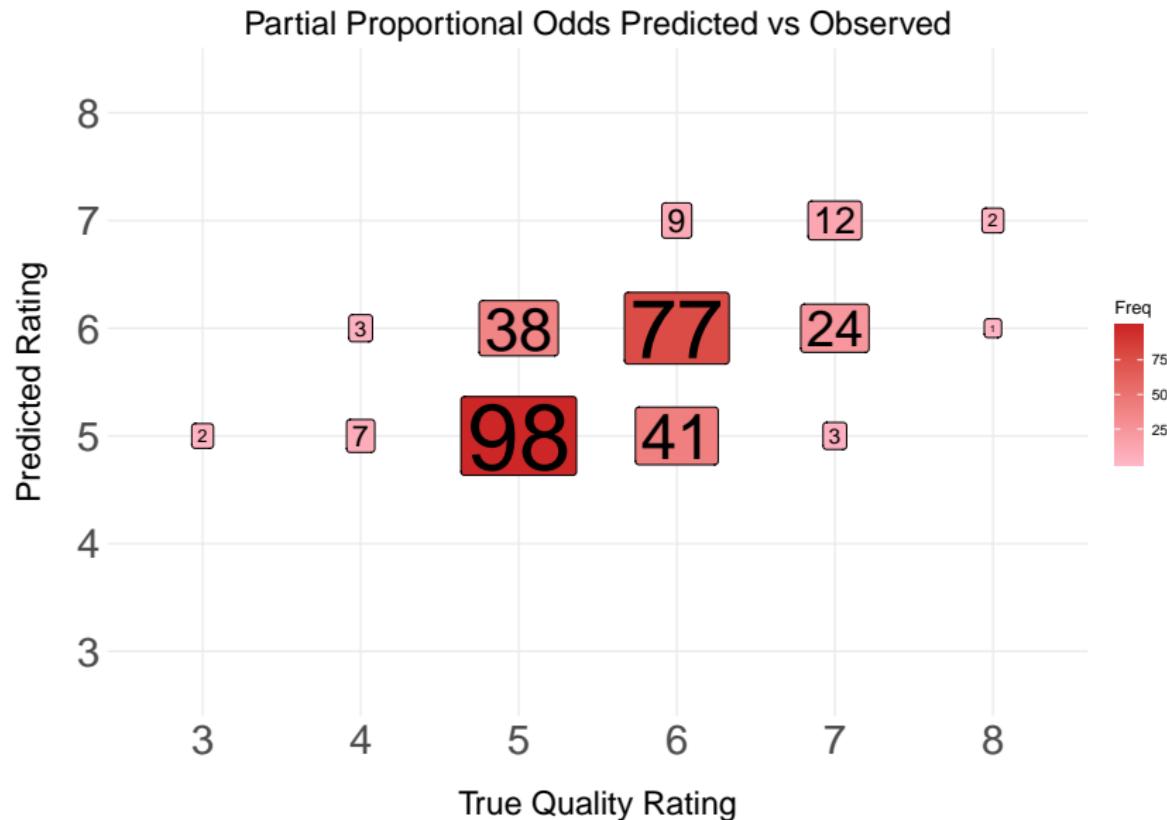
Table 3: Comparison of Red Wine Proportional Odds Model Results

	Overall Results			Percent Correct by Category						
	Prediction Accuracy	Kappa	Weighted Kappa	3	4	5	6	7	8	
Proportional Odds (F)	58.9905	0.3232	0.5258	0	0	72.0588	59.8425	33.3333	0	
Proportional Odds (R)	58.0442	0.3065	0.4707	0	0	72.0588	59.8425	25.6410	0	
Partial Proportional Odds (F)	58.9905	0.3233	0.5162	0	0	72.0588	60.6299	30.7692	0	
Partial Proportional Odds (R)	58.3596	0.3117	0.4742	0	0	72.0588	59.8425	28.2051	0	

# Results: Proportional Odds Model (Red Wine, Full)



# Results: Partial Proportional Odds Model (Red Wine, Full)

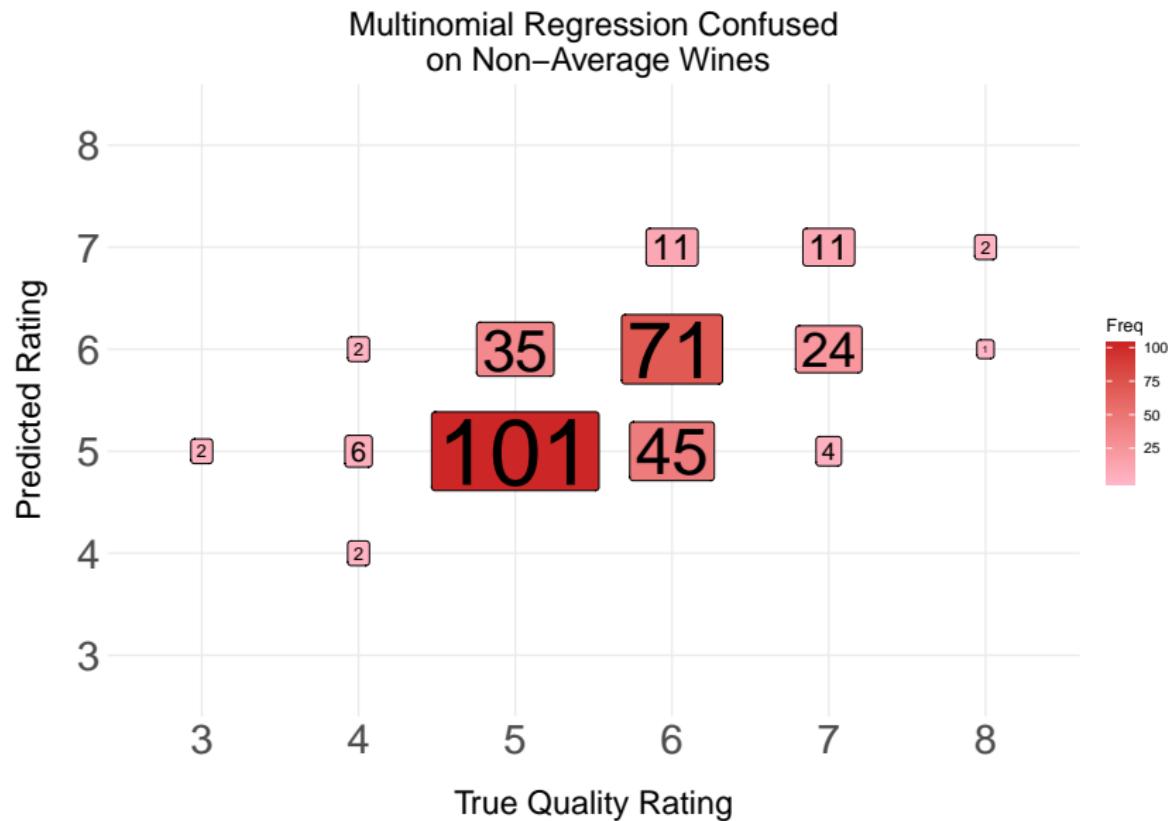


# Results: Multinomial Regression (Red Wine Quality Classification)

Table 4: Comparison of Multinomial Regression Models for Red Wine Quality

Model	Accuracy	Kappa	Weighted Kappa	3	4	5	6	7	8
Full Model (Linear Terms)	58.3596	0.3158	0.5227	0	20	74.2647	55.9055	28.2051	0
Reduced Model (Linear Terms)	58.3596	0.3193	0.4952	0	10	72.7941	56.6929	33.3333	0
Reduced Model (Second Order Terms)	55.2050	0.2702	0.4789	0	0	67.6471	55.1181	33.3333	0

# Results: Multinomial Regression - Full Model Confusion Matrix (Red Wine)

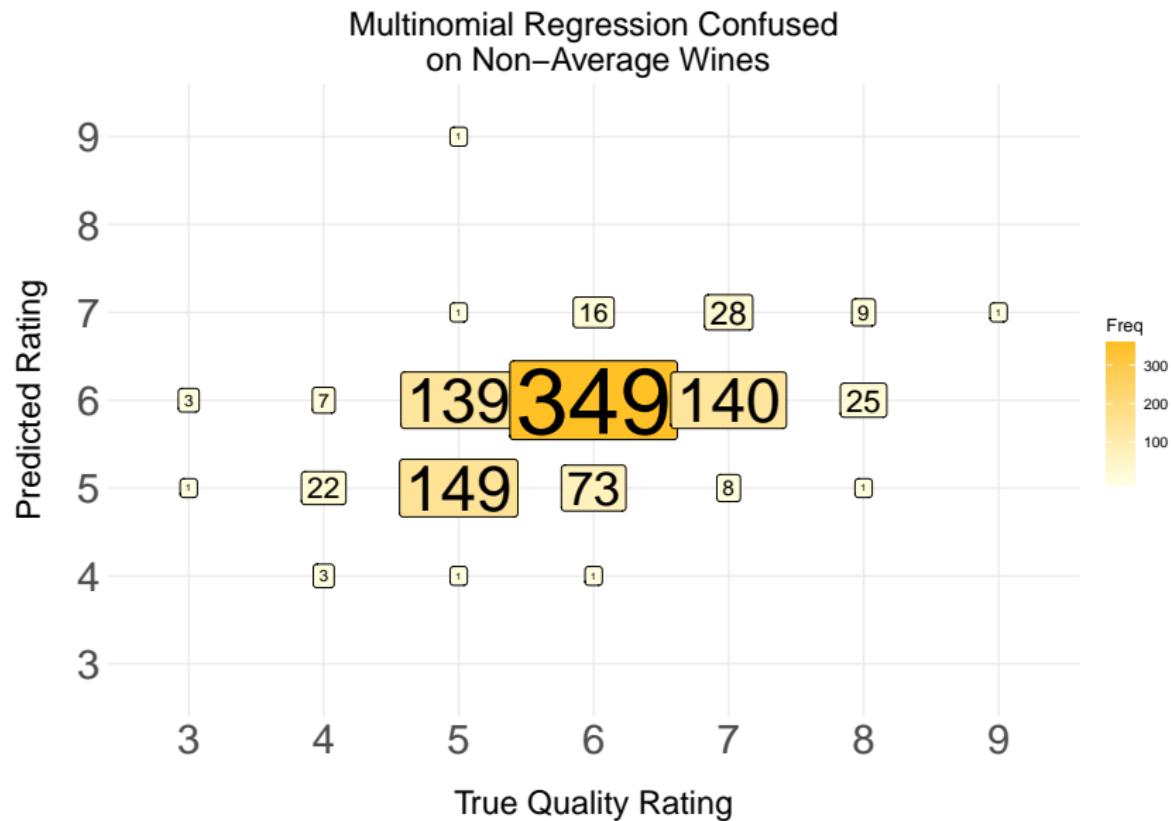


# Results: Multinomial Regression (White Wine Quality Classification)

Table 5: Comparison of Multinomial Regression Models for Red Wine Quality

Model	Accuracy	Kappa	Weighted Kappa	3	4	5	6	7	8	9
Full Model (Linear Terms)	54.0900	0.2451	0.4121	0	9.375	51.2027	79.4989	15.9091	0	0
Reduced Model (Linear Terms)	51.9427	0.2201	0.4093	0	3.125	54.6392	72.6651	16.4773	0	0
Reduced Model (Second Order Terms)	53.2720	0.2396	0.4010	0	3.125	54.2955	74.4875	19.8864	0	0

# Results: Multinomial Regression - Full Model Confusion Matrix (White Wine)

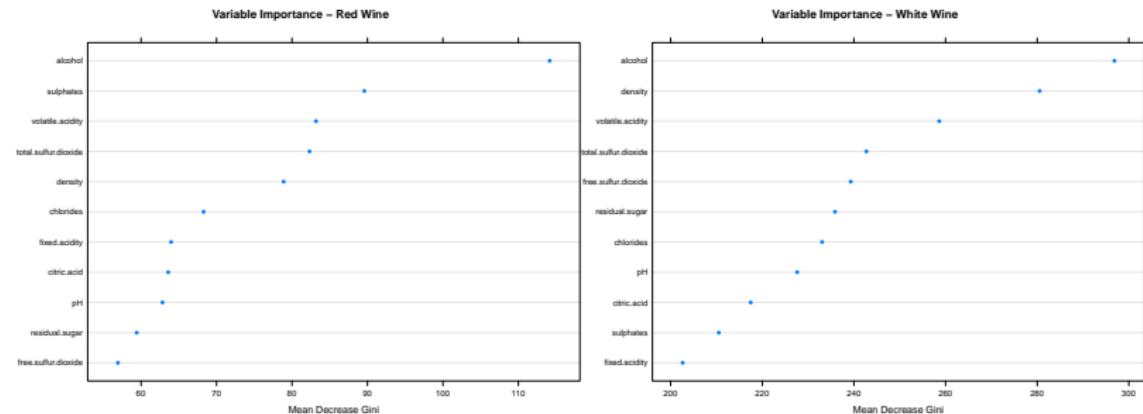


# Results: Random Forest

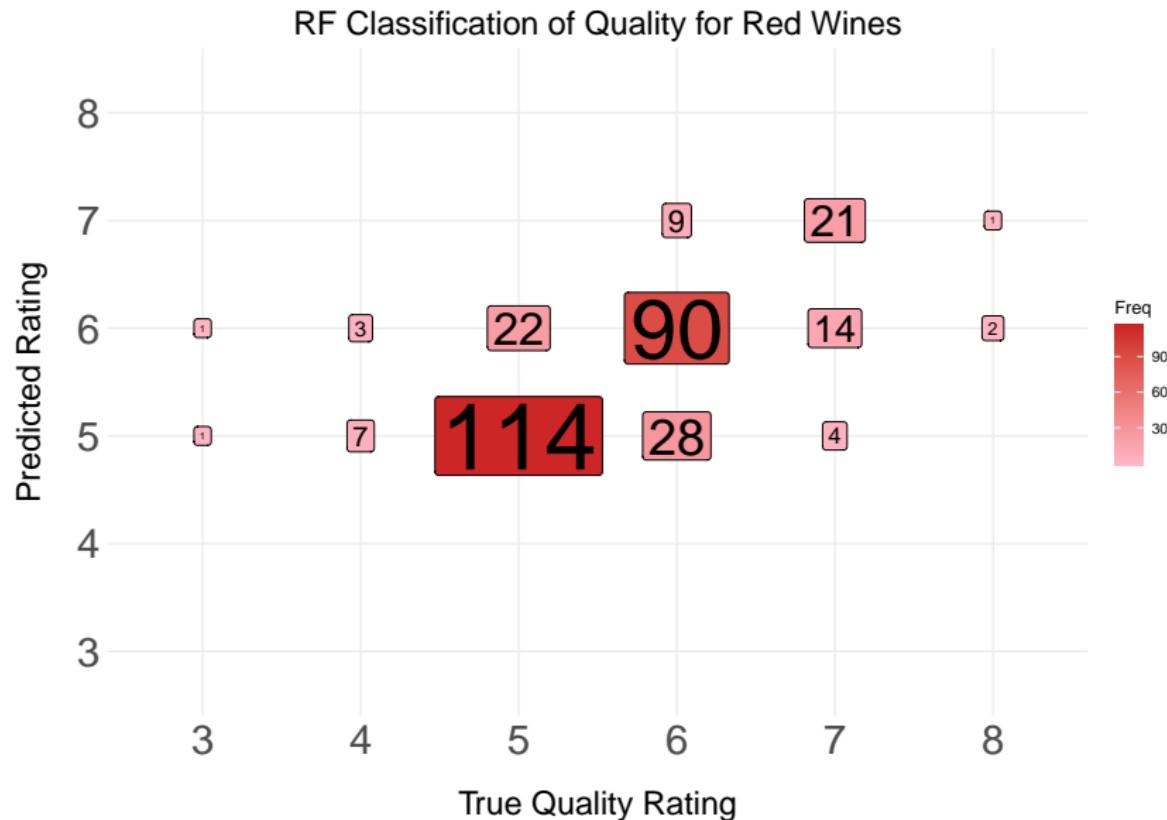
Table 6: Random Forest Results for Red and White Wine

	Overall Results			Percent Correct by Category							
	Prediction Accuracy	Kappa	Weighted Kappa	3	4	5	6	7	8	9	
Red Wine	70.98	0.5263	0.6168	0	0	83.82	70.87	53.85	0.00	NA	
White Wine	67.28	0.4862	0.6542	0	25	67.35	80.87	47.73	42.86	0	

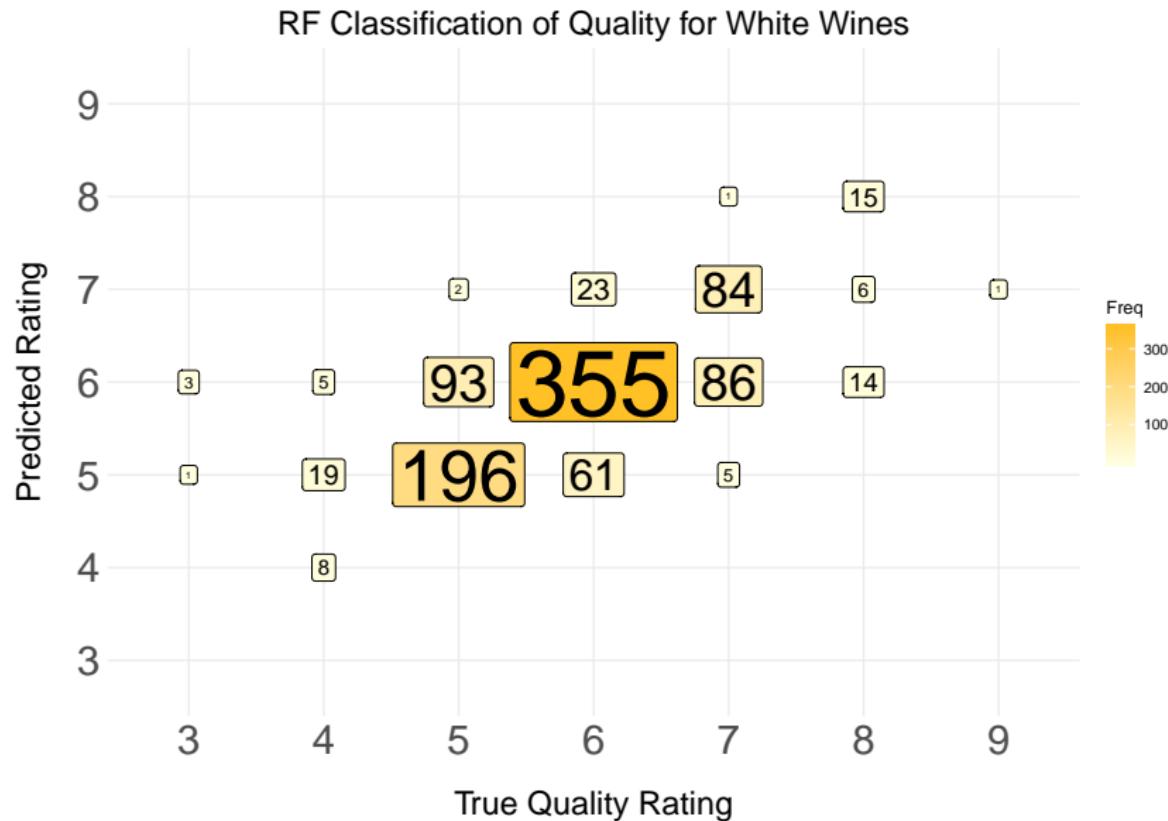
# Results: Random Forest (Variable Importance)



# Results: Random Forest (Red Wine)



# Results: Random Forest (White Wine)



# Comparison of Results: Red Wine

Table 7: Comparison of Results for Red Wine

	Overall Results			Percent Correct by Category					
	Prediction Accuracy	Kappa	Weighted Kappa	3	4	5	6	7	8
Random Forest	70.9800	0.5263	0.6168	0	0	83.8200	70.8700	53.8500	0
Proportional Odds	58.9905	0.3232	0.5258	0	0	72.0588	59.8425	33.3333	0
Partial Proportional Odds	58.9905	0.3233	0.5162	0	0	72.0588	60.6299	30.7692	0
Multinomial	58.3596	0.3158	0.5227	0	20	74.2647	55.9055	28.2051	0
Linear Regression	56.1500	0.2728	0.4545	0	0	65.4400	63.7800	20.5100	0

# Comparison of Results: White Wine

Table 8: Comparison of Results for White Wine

	Overall Results			Percent Correct by Category							
	Prediction	Accuracy	Kappa	Weighted Kappa	3	4	5	6	7	8	9
Random Forest		67.2800	0.4862	0.6542	0	25.000	67.3500	80.8700	47.7300	42.86	0
Proportional Odds		52.1472	0.2126	0.4053	0	0.000	45.3608	78.1321	19.8864	0.00	0
Multinomial		54.0900	0.2451	0.4121	0	9.375	51.2027	79.4989	15.9091	0.00	0
Linear Regression		51.1200	0.1969	0.4067	0	0.000	41.5800	78.1300	20.4500	0.00	0

## Discussion: Random Forest

- ▶ Using random forests, we were able to predict expert wine quality ratings fairly accurately using measurements of a small number of chemical components of wine
  - ▶ White wine
    - ▶ Accuracy: 67.28%
    - ▶ Weighted Kappa: 0.6542
  - ▶ Red wine
    - ▶ Accuracy: 70.98%
    - ▶ Weighted Kappa: 0.6168
- ▶ Using the proposed cutoffs from Landis and Koch, these weighted Kappa values suggest moderate to substantial agreement with the expert ratings

## Discussion: Likelihood Based Approaches

- ▶ The likelihood based approaches performed more poorly, with accuracies 10-15% lower than random forest and weighted kappas 0.1 to 0.2 lower
- ▶ Even so, the weighted kappas all suggested moderate agreement with the expert ratings and were clearly better than random guessing
- ▶ There was not a clear winner among the likelihood based approaches, accuracies and kappas were very similar across multinomial, ordinal, and linear regression models
  - ▶ However, linear model showed a tendency to predict as a mean value, which resulted in poor prediction other than the middle quality categories
  - ▶ Accounting for the ordered nature of the ratings did not make a difference in predictions
  - ▶ In some cases, doing so actually resulted in (slightly) worse predictive performance

## Discussion: Limitations and Future Directions

- ▶ We only had data on a small number of reasonably easy to measure chemicals, we speculate some misclassification was due to failure to measure other important chemicals.
- ▶ Our goal was simply to predict quality ratings, in the future, it would be interesting characterize how individual chemicals relate to wine quality.
- ▶ There were only a small number of truly excellent wines (rating of 8 or higher) making it particularly difficult to predict these ratings. It would be worthwhile to examine whether various outlier detection algorithms are more suited to characterizing these wines than the approaches we took.

## Bottom Line

Expert wine quality ratings can be predicted reasonably well using chemical components, but true wine connoisseurs are still better off consulting a sommelier.

## References

Landis JR, Koch GG. The measurement of observer agreement for categorical data. Biometrics. 1977 Mar;33(1):159-74.