Predicting Wine Quality: A Conundrum

Would you like some cheese with that?

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Popping the Cork

Task

Predict the blind taster quality score of a wine based on chemical tests.

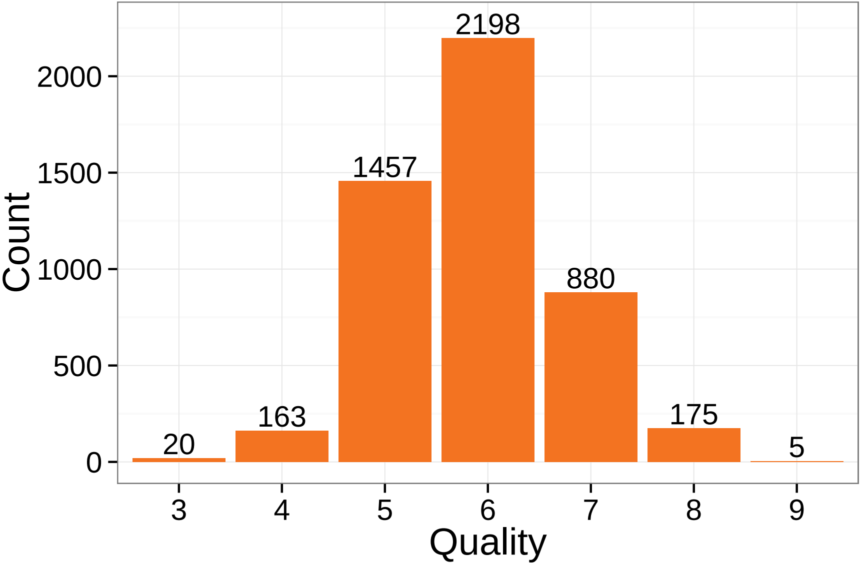
Data

- Two Datasets: Red & White vinho verde wine samples from northern Portugal
- 1599 & 4898 rows, respectively
- Concentrated on White Wine, due to more data

Data

- 11 Explanatory variables: measurements from various phytochemicals in wine
- Response variable "quality" is discrete variable on ordered scale from 0 (worst) to 10 (best)
- Nothing graded as 0, 1, 2, or 10

White Wine Quality Scores



Learning about Wine

Training and Testing Sets

- Training and Testing sets constructed through stratified sampling.
- Quality variable was the strata
- Why: Ensure representation of all quality categories in both Training & Testing datasets.
- How: 37.5% of items (rounded up) in strata were randomly selected to be in the testing set. Remaining 62.5% were the training set.
- Regression and Random method used these training sets, Classification used different set.

Methods

- With "prediction" as the goal, we think regression.
- Forward, Backward and Subset Model Selection done, all resulted in same model.
- Classification Method can also be used to predict.

K-Nearest Neighbor Regression

- Using some measure of distance, find nearest neighbors in dataset
- Order examples by increasing distance
- Find a "optimal" number k of nearest neighbors
- Calculate an inverse distance weighted average with the k-nearest multivariate neighbors
- Used `fit` function from `rminer` package in R. Offers many regression types

Ordinal Regression

Also "Ordered Logistic" Regression

- Estimate seperate binary regression models for all of: $P(score \leq j)/P(score > j)$, for all j
- To get the probability of the score being j: $P(Score = j) = P(score \leq j) - P(score < j)$
- So we can get the probability of each category.

Multiclass Classification

One-vs-All (or One-vs-Rest) Algorithm

- Split problem into n binary classification problems, where n is number of classes.
- Treat class i as "positive" class, everything else as "negative" class
- Train logistic regression classifier $h_\theta^i(x)$ for each class i to predict the probability that $y = i$
- On new input x, evaluate $\max_i h_\theta^i(x)$, so whichever class has the highest probability based on our input, we then predict $\hat{y}$ to be in that class

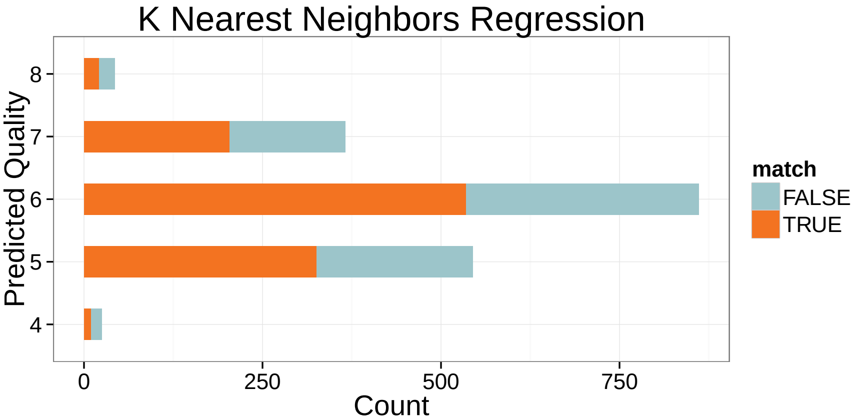
Random Randomness is Random

- 75% of Quality ratings were either 5 or 6.
- Is randomly assigning 5 or 6 to everything as good as, or better than, our other methods?
- Using `rbinom(1,1,0.6014)`, 1s were predicted as quality 6, 0s as quality 5
- Probability of 60.14% because from Training Set, considering only 5s and 6s, 6s were 60.14% of total observations
- Our base line success rate to compare other methods.

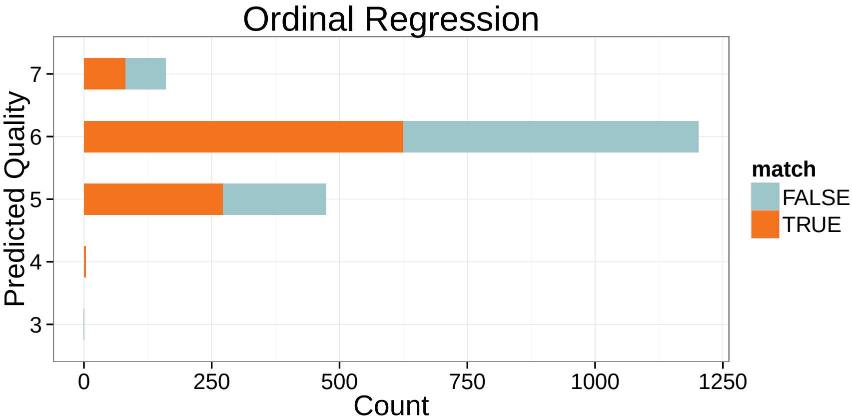
Results


pale yellow core
rich gold core
primary colors
primary colors

K Nearest Neighbors Regression: 59.6% Success Rate



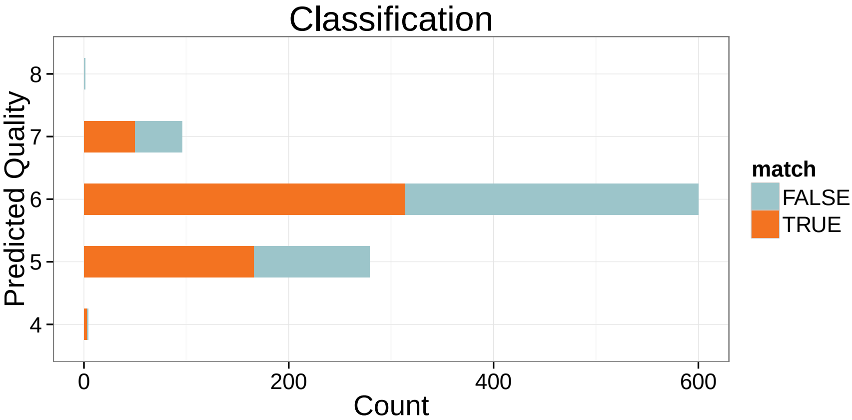
Ordinal Regression: 53.3% Success Rate



Regression Summary

- K Nearest Neighbors
  - Overall 59.6% success rate.
  - No properly allocated 3s or 9s
- Ordinal Regression
  - Overall 53.3% success rate
  - No properly allocated 3s, 8s or 9s.

Classification: 54.4% Success Rate



Classification Summary

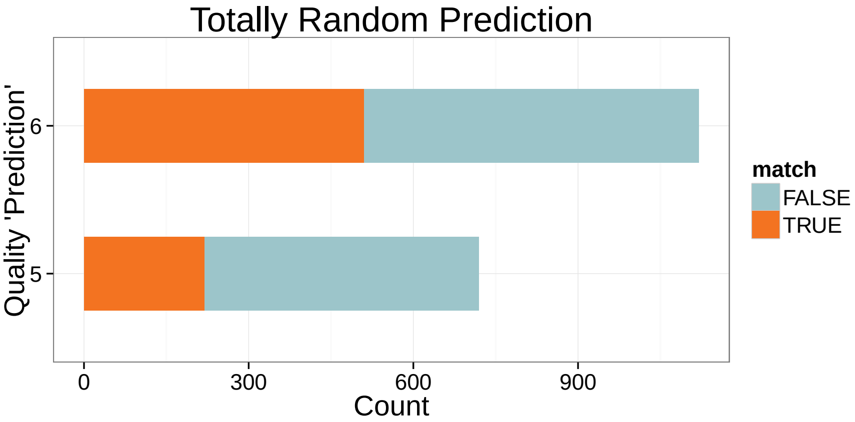
- 54.4% success rate
- No properly allocated 3s or 9s

Comparison: Success by Quality Predicted

	KNN		Ordinal		Classification	
Prediction	% Match	% Fail	% Match	% Fail	% Match	% Fail
3	n/a	n/a	0%	100%	n/a	n/a
4	40.0%	60.0%	100%	0%	75.0%	25.0%
5	59.8%	40.2%	57.4%	42.6%	59.5%	40.5%
6	62.1%	37.9%	52.0%	48.0%	52.3%	47.7%
7	55.7%	44.3%	50.6%	49.4%	52.1%	47.9%
8	48.8%	51.2%	n/a	n/a	0%	100%
9	n/a	n/a	n/a	n/a	n/a	n/a

'N/A' means nothing predicted at that quality.

Random 'Prediction': 39.67% Success Rate



Turns out, that's not really a great 'prediction' method. Who knew?

Discussion


ELKI
LAS MORAS
TORRONTES
2017
LE CHANAY
Hubert Lamy
BOURGOGNE
2009
Finest
2009
MORA

One-vs-All Classification: Assumptions

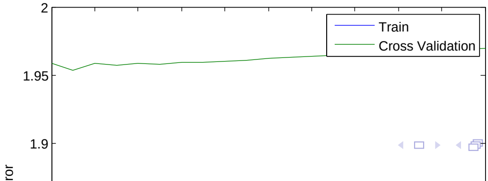
- Need 3 data sets if doing Model Selection.
- Assumes that the the individual log reg are indepent–meaning that the probability of all categories do not sum to one.
- Approach assumes that the category with higher prob is more likely to occur that other categories

One-vs-All Classification: Limitations

- When two or more categories have the same probability of success, then the approach will just pick one.
- The algorithm is computationally expensive. Ran in about 3 mins for this data set.
- Scalability is an issue for the algorithm, larger data sets could cause issues.

Cross-Validation

Lambda is tuning parameter for model. Want to pick the cross validation set with the lowest cross-validation.



Regression: Assumptions

- Multicollinearity is not an issue with prediction. It blows up SE, which is bad for estimation, not so bad with prediction.
- K-Neighbors: Options available for the "search method" for KNN algorithm were not explored. This changes how the hyper-parameters of the algorithm are tuned.
- Cross validation was not explored.

Ordinal Regression Assumptions

Also "Ordered Logistic" Regression

- Because it is likelihood based, need to have "enough" data for modeling.
- Proportional odds - coefficients stay the same, and the intercept value changes. Need to verify. Did not do it.
- To verify, would run each category independently, verifying slopes are the same.
- All explanatory variables have the same weight for all categories. Puts them in possible categories, picks the one with the highest probability.

Regression:Limitations and Scaling

- K-Neighbors: if category distribution is skewed, larger categories can dominate, which is what we see in our results.
- Regression does not always scale well, adding covariates can bog down the number of comparisons, especially with model selection
- Random or stratified sampling of data to get a reasonable set size and model selection to cut down number of covariates could help.

Questions