VinoMetrics

Mission: Build a model that predicts the quality of wine

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Background

Dataset

WINE DATASET	Input variable	Explained variable
Count	11	1
Index	['fixed acidity', 'volatile acidity', 'citric acid', 'residual sugar', 'chlorides', 'free sulfur dioxide', 'total sulfur dioxide', 'density','pH', 'sulphates', 'alcohol']	[‘quality’]
Dtype	float	int
Null values	0	
Instances red (of which duplicates)	1599 (240 = 15%)	
Instances white (of which duplicates)	4898 (937 = 19%)	

Variable Overview

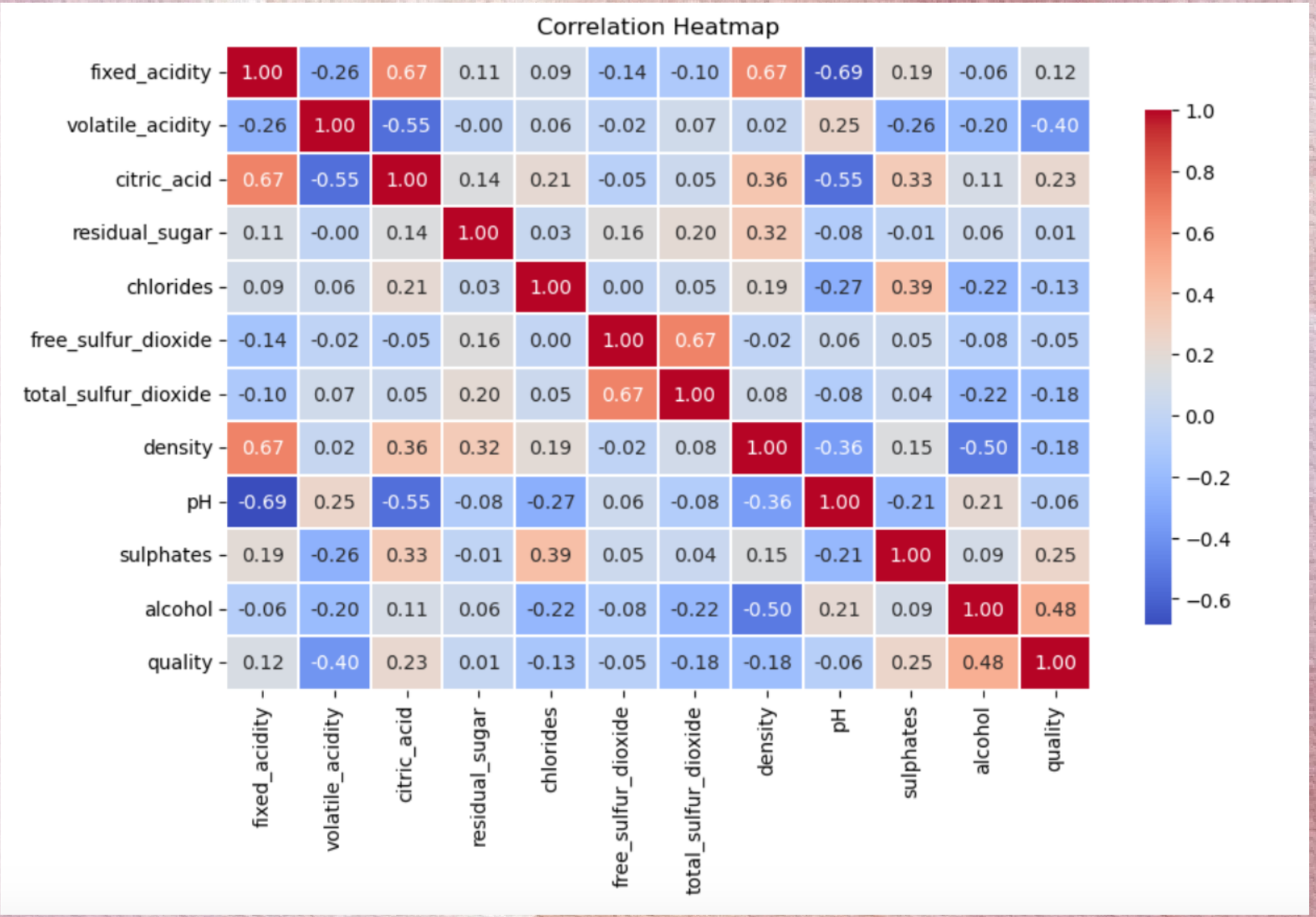
Input Variables	Effect	Controlled by producer
fixed acidity	more or less robust	yes
volatile acidity	tanginess or sharpness	yes
citric acid	notes of lemon or lime	yes
residual sugar	sweetness	yes
chlorides	saltiness	yes
free sulfur dioxide	preservative	yes
total sulfur dioxide	stability and longevity	yes
density	richness (high = 'full-bodied	yes
pH	acidity	yes
sulphates	maintains freshness	yes
alcohol	strength (high = warm, full-bodied)	yes

Output variable: quality

Explanation: Three experts rated each wine, and the quality score for each wine is calculated as the average of these three ratings.

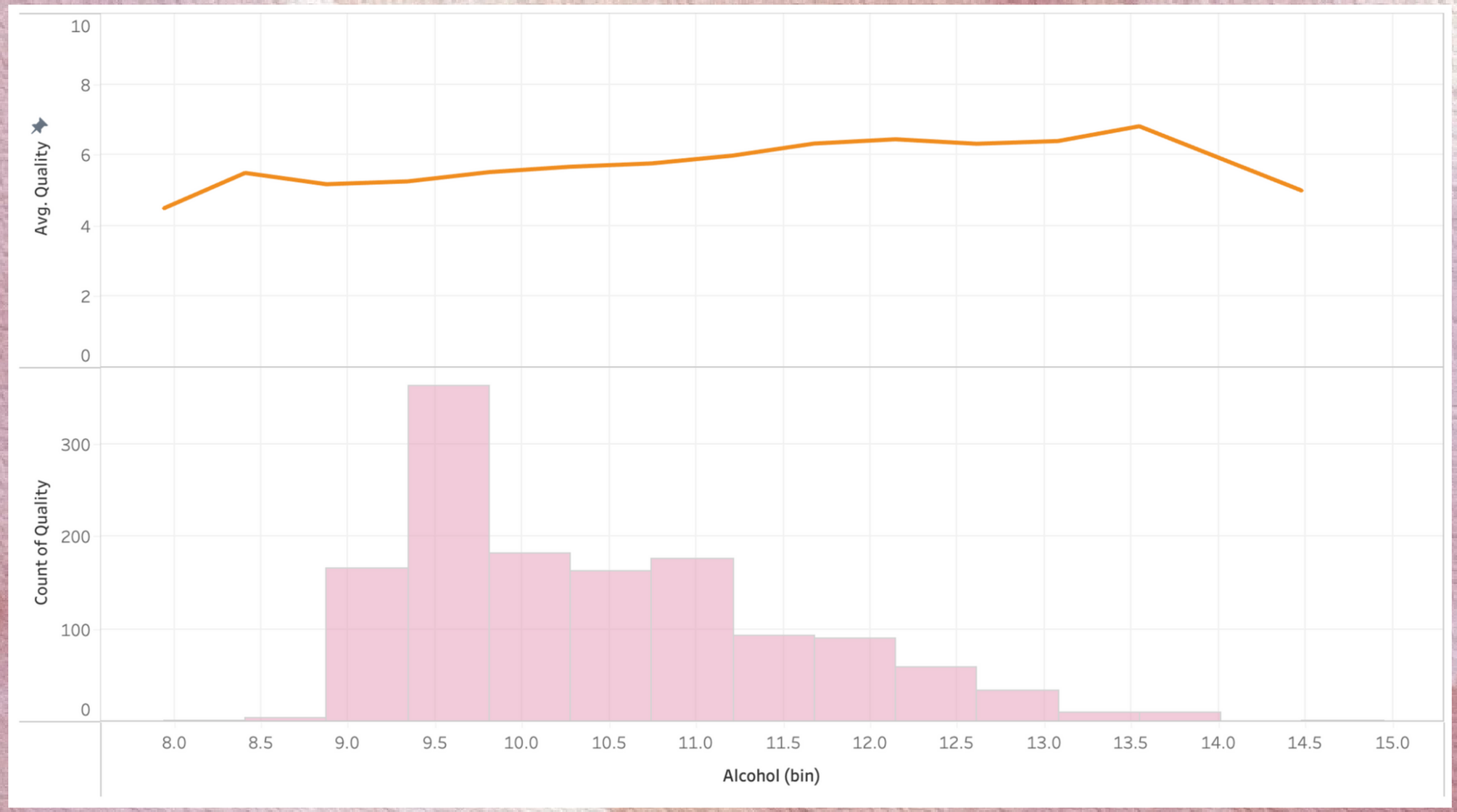
Range: 0-10

Correlation heatmap - red wine



Alcohol vs Wine Quality

Strongest correlated variable combination (alcohol x quality) – example of 'piecewise linear trend''



Linear Regression - before optimization

Linear Regression Model

In [9]:
```
# Linear regression
lm = LinearRegression()
model = lm.fit(X_train, y_train)
print(f'model coefficients:\n {model.coef_}\n')
print(f'model intercept:\n {model.intercept_}\n')

# Applying model to X test
y_pred = model.predict(X_test)
#y_pred = pd.DataFrame(scaler_s_y.inverse_transform(y_pred)) # inversing y
y_pred = pd.DataFrame(y_pred)

y_pred = y_pred.rename(columns = {0:"y_pred"})

y_test = y_test.reset_index(drop=True)
y_test = y_test.rename(columns = {"quality":"y_test"})

residuals_df = pd.concat([y_test,y_pred], axis = 1)
residuals_df["residual"] = residuals_df["y_test"] - residuals_df["y_pred"]


# Root mean squared error
rmse = mse(y_test, residuals_df["y_pred"], squared=False)
print(f'Root mean squared error: {rmse} \n')

# R^2
r2 = r2_score(y_test, residuals_df["y_pred"])
print(f'R2: {r2} \n')

# Calculating adjusted R^2
n = X_train.shape[0]  # Number of observations in the training set
p = X_train.shape[1]  # Number of features used for training
adjusted_r2 = 1 - (1 - r2) * (n - 1) / (n - p - 1)
print(f'Adjusted R2: {adjusted_r2} \n')

residuals_df
```

```
model coefficients:
 [[-4.14972197e-02 -9.94118538e-01 -2.30359318e-02 -2.34947735e-03
  -2.04381921e+00  5.60218000e-03 -3.96020465e-03  2.31453631e+01
  -8.73151979e-01  9.07091584e-01  3.04300621e-01]]

model intercept:
 [-17.15994201]

Root mean squared error: 0.6377068568203348

R2: 0.39830469246210143

Adjusted R2: 0.3917320525585096
```

OLS Regression Results - before model optimization

In [16]:
```
X_train = sm.add_constant(X_train)
model = sm.OLS(y_train,X_train).fit()
model.summary()
```

Out[16]:

OLS Regression Results

Dep. Variable:	quality	**R-squared:**	0.347
Model:	OLS	**Adj. R-squared:**	0.340
Method:	Least Squares	**F-statistic:**	48.71
Date:	Thu, 08 Feb 2024	**Prob (F-statistic):**	1.27e-85
Time:	11:29:31	**Log-Likelihood:**	-1030.6
No. Observations:	1019	**AIC:**	2085.
Df Residuals:	1007	**BIC:**	2144.
Df Model:	11		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
const	-17.1599	27.713	-0.619	0.536	-71.542	37.222
fixed_acidity	-0.0415	0.035	-1.201	0.230	-0.109	0.026
volatile_acidity	-0.9941	0.157	-6.320	0.000	-1.303	-0.685
citric_acid	-0.0230	0.189	-0.122	0.903	-0.394	0.348
residual_sugar	-0.0023	0.020	-0.115	0.909	-0.042	0.038
chlorides	-2.0438	0.513	-3.982	0.000	-3.051	-1.037
free_sulfur_dioxide	0.0056	0.003	1.950	0.051	-3.53e-05	0.011
total_sulfur_dioxide	-0.0040	0.001	-4.148	0.000	-0.006	-0.002
density	23.1454	28.311	0.818	0.414	-32.410	78.700
pH	-0.8732	0.261	-3.341	0.001	-1.386	-0.360
sulphates	0.9071	0.148	6.115	0.000	0.616	1.198
alcohol	0.3043	0.034	8.840	0.000	0.237	0.372

Omnibus:	14.137	**Durbin-Watson:**	1.974
Prob(Omnibus):	0.001	**Jarque-Bera (JB):**	17.934
Skew:	-0.177	**Prob(JB):**	0.000128
Kurtosis:	3.545	**Cond. No.**	1.15e+05

Hypothesis testing

H0 : β 1 = β 2 = β 3 = β 4 = β 5 = β 6 = β 7 = β 8 = β 9 = β 10 = β 11 = 0

REJECTED

Null hypothesis: The coefficients of all input variables are equal to 0.
None of our wine properties predict wine quality.

H1 : β 1 = β 2 = β 3 = β 4 = β 5 = β 6 = β 7 = β 8 = β 9 = β 10 = β 11 != 0

Alternative hypothesis: Significant linear relationship between at least one of the 11 input variables and the explained variable.
At least one of our wine properties predicts wine quality.

R-squared:	0.347
Adj. R-squared:	0.340
F-statistic:	48.71
Prob (F-statistic):	1.27e-85

Linear Regression

Optimisation

Outliers:

- IQR method (**Applied**)
- **Action:** Converted outliers to 0.25/0.75 percentile

Feature selection:

- Recursive Feature Elimination (RFE) (**Tested, not applied**)
- **Action:** dropped 'free_sulfur_dioxide'

Scalers/Transformers (Applied)

- **Action:** Standard Scaler on *X*, no scaler on *y*

Impact

RMSE:
Before: 0.67
After: **0.63**

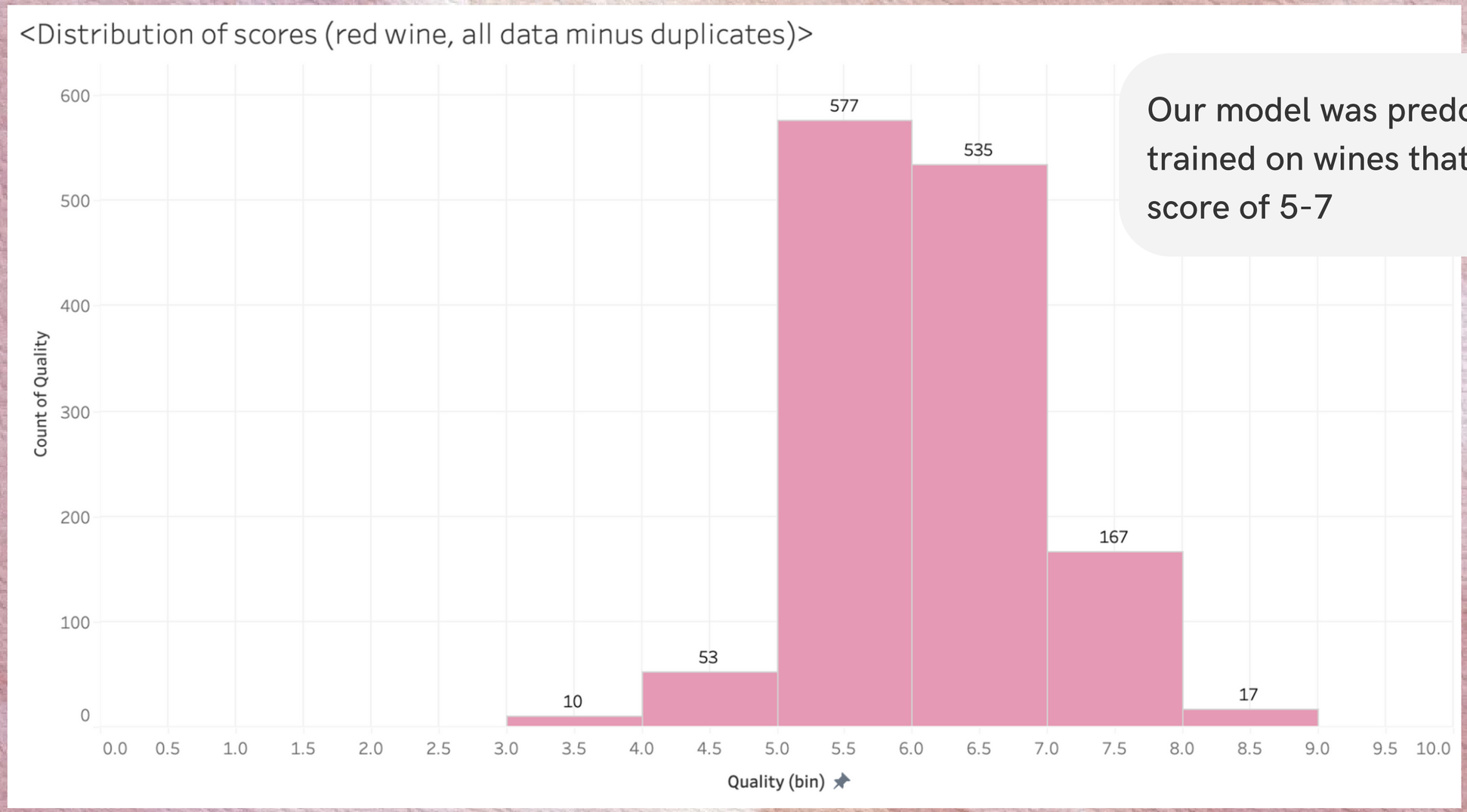
R2:
Before: 0.35
After: **0.41**

R2 adjusted:
Before: 0.34
After: **0.40**

Outcome:

- our predictions are on average within 0.6 for wines scores
- approx **40%** of variability in quality can be accounted for by the input variables

Model Evaluation



Our model was predominantly trained on wines that received a score of 5-7

Model Evaluation

The model is a much stronger predictor (lower residuals) for wines in the 5-7 quality groups.

Constraints of model

- **data availability:** lack of accessible data to further train model
  - wine producers dont publish physiochemical properties
  - very limited data on high scoring and low scoring wines
- **Human bias:** quality score is somewhat subjective
- **Other variables :** no data on effect of grape, location etc

Conclusion

- While not perfect our model has some degree of explanatory power in predicting wine quality. On a scale of 0-10 points, we can predict score to within 0.6 points of accuracy
- In a commercial setting, our model would fulfil a business need of enabling wine producers to increase their likelihood of producing high-quality wine
- With access to more data we could refine our model further and improve its accuracy

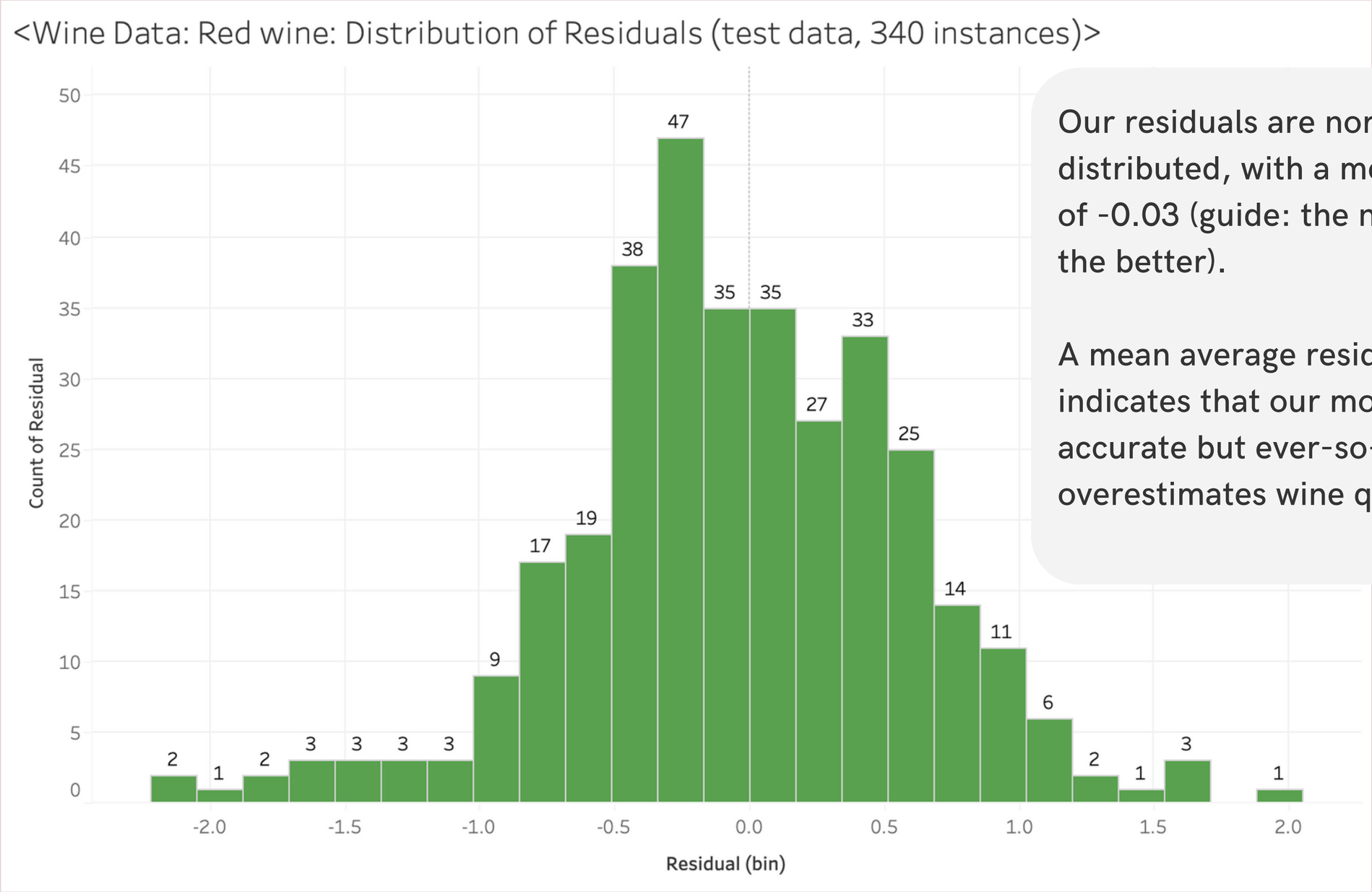
Introducing…

VinoMetrics

VINOMETRICS WINE QUALITY PREDICTOR ©

Cheers!

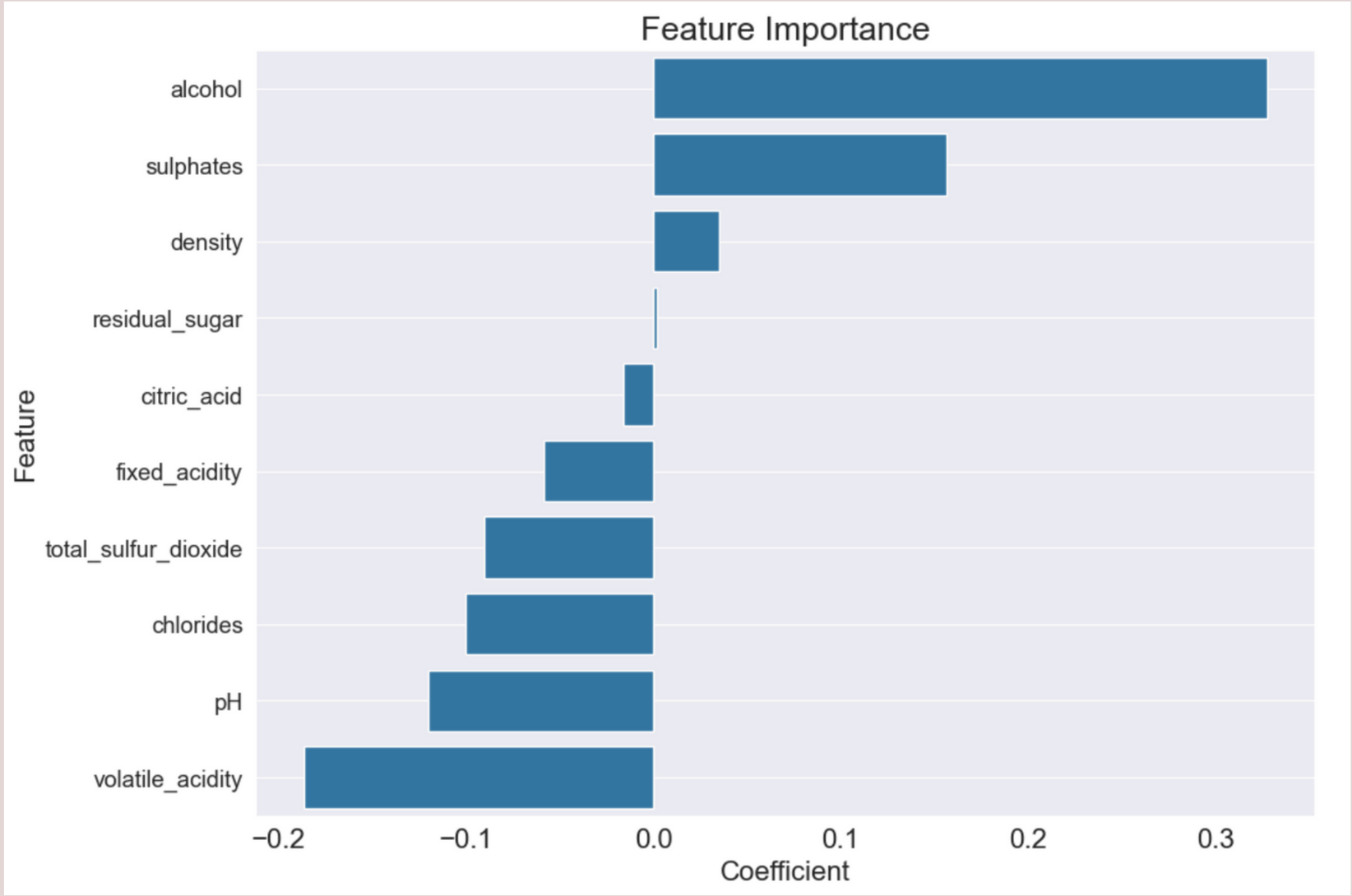
Model Evaluation



Our residuals are normally distributed, with a mean average of -0.03 (guide: the nearer to 0, the better).

A mean average residual of -0.03 indicates that our model is accurate but ever-so-slightly overestimates wine quality.

Linear regression - feature importance



Linear Regression

Stated mission:

- Build a model that predicts the quality of wine

Outcome:

- 40% of the variability in wine quality can be accounted for by the input variables
- 60% of the variability in wine quality is unexplained by the input variables