Assignment 8

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Contents

Homework 7, Part 1

Read in the data set

Since we have a comma-separated file, we can read in our training data using the function `read_csv()`.

```
# Read in CSV train file, subset data
wineTrainingData <- as_tibble(read.csv(file = "./wineQualityTrain.csv"))
names(wineTrainingData)
```

```
##  [1] "fixed.acidity"        "volatile.acidity"     "citric.acid"
##  [4] "residual.sugar"       "chlorides"            "free.sulfur.dioxide"
##  [7] "total.sulfur.dioxide" "density"              "pH"
## [10] "sulphates"            "alcohol"              "quality"
## [13] "type"
```

Plan our models

When planning our initial models, we can either start with the single best variable and add more or consider all variables and remove ones which are the least significant. When considering a subset, we can remove certain predictors if they are colinear (highly correlated within the same model).

In this case, we can start with a model that incorporates all terms.

```
# Create model with all terms
linearModel1 <- lm(quality ~ ., data = wineTrainingData)
summary(linearModel1)
```

```
##
## Call:
## lm(formula = quality ~ ., data = wineTrainingData)
##
```

```
## Residuals:
##     Min      1Q  Median      3Q     Max 
## -3.3559 -0.4734 -0.0486  0.4474  2.7786 
## 
## Coefficients:
##                        Estimate Std. Error t value Pr(>|t|)    
## (Intercept)           1.511e+02  3.733e+01   4.048 5.47e-05 ***
## fixed.acidity         1.010e-01  3.855e-02   2.620 0.008909 ** 
## volatile.acidity     -1.529e+00  1.849e-01  -8.267 3.40e-16 ***
## citric.acid           7.198e-02  1.888e-01   0.381 0.703133    
## residual.sugar        8.246e-02  1.475e-02   5.592 2.74e-08 ***
## chlorides            -1.375e+00  8.027e-01  -1.713 0.087039 .  
## free.sulfur.dioxide   3.337e-03  1.626e-03   2.053 0.040320 *  
## total.sulfur.dioxide -1.538e-03  7.115e-04  -2.161 0.030867 *  
## density              -1.494e+02  3.780e+01  -3.953 8.15e-05 ***
## pH                    2.889e-01  2.105e-01   1.373 0.170142    
## sulphates             7.750e-01  1.804e-01   4.296 1.87e-05 ***
## alcohol               1.749e-01  4.796e-02   3.648 0.000275 ***
## typeWhite            -5.307e-01  1.332e-01  -3.985 7.13e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## 
## Residual standard error: 0.7499 on 1287 degrees of freedom
## Multiple R-squared:  0.3089, Adjusted R-squared:  0.3025 
## F-statistic: 47.95 on 12 and 1287 DF,  p-value: < 2.2e-16
```

We can then see which predictor variable we may want to delete.

```r
# Compute AIC values to drop the lowest one(s)
drop1(linearModel1)
```

```
## Single term deletions
## 
## Model:
## quality ~ fixed.acidity + volatile.acidity + citric.acid + residual.sugar + 
##     chlorides + free.sulfur.dioxide + total.sulfur.dioxide + 
##     density + pH + sulphates + alcohol + type
##                      Df Sum of Sq    RSS     AIC
## <none>                            723.81 -735.27
## fixed.acidity         1     3.859 727.67 -730.36
## volatile.acidity      1    38.433 762.24 -670.01
## citric.acid           1     0.082 723.89 -737.12
## residual.sugar        1    17.588 741.40 -706.06
## chlorides             1     1.649 725.46 -734.31
## free.sulfur.dioxide   1     2.369 726.18 -733.02
## total.sulfur.dioxide  1     2.627 726.44 -732.56
## density               1     8.787 732.60 -721.58
## pH                    1     1.059 724.87 -735.37
## sulphates             1    10.378 734.19 -718.76
## alcohol               1     7.484 731.29 -723.90
## type                  1     8.930 732.74 -721.33
```

Here, the Akaike information criterion (AIC) is lowest for `citric.acid` (-737.12), so we remove this term from our model.

```r
# Get model formula
formula(linearModel1)
```

```
## quality ~ fixed.acidity + volatile.acidity + citric.acid + residual.sugar +
##     chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
##     density + pH + sulphates + alcohol + type
```

```r
# Create model without citric.acid
linearModel2 <- lm(quality ~ fixed.acidity + volatile.acidity + residual.sugar +
    chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
    density + pH + sulphates + alcohol + type, data = wineTrainingData)
summary(linearModel2)
```

```
##
## Call:
## lm(formula = quality ~ fixed.acidity + volatile.acidity + residual.sugar +
##     chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
##     density + pH + sulphates + alcohol + type, data = wineTrainingData)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -3.3462 -0.4735 -0.0507  0.4449  2.7738
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)           1.501e+02  3.723e+01   4.033 5.83e-05 ***
## fixed.acidity         1.038e-01  3.784e-02   2.742 0.006195 **
## volatile.acidity     -1.556e+00  1.708e-01  -9.105  < 2e-16 ***
## residual.sugar        8.223e-02  1.473e-02   5.583 2.88e-08 ***
## chlorides            -1.339e+00  7.970e-01  -1.680 0.093180 .
## free.sulfur.dioxide   3.314e-03  1.624e-03   2.040 0.041538 *
## total.sulfur.dioxide -1.500e-03  7.044e-04  -2.130 0.033394 *
## density              -1.484e+02  3.770e+01  -3.937 8.69e-05 ***
## pH                    2.807e-01  2.093e-01   1.341 0.180202
## sulphates             7.760e-01  1.803e-01   4.303 1.81e-05 ***
## alcohol               1.777e-01  4.741e-02   3.748 0.000186 ***
## typeWhite            -5.276e-01  1.329e-01  -3.970 7.58e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7497 on 1288 degrees of freedom
## Multiple R-squared:  0.3089, Adjusted R-squared:  0.303
## F-statistic: 52.33 on 11 and 1288 DF,  p-value: < 2.2e-16
```

We can then see which predictor variable we may want to delete next.

```r
# Compute AIC values to drop the lowest one(s)
drop1(linearModel2)
```

```
## Single term deletions
##
## Model:
## quality ~ fixed.acidity + volatile.acidity + residual.sugar +
##     chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
##     density + pH + sulphates + alcohol + type
##                      Df Sum of Sq    RSS     AIC
## <none>                            723.89 -737.12
## fixed.acidity         1     4.225 728.12 -731.56
## volatile.acidity      1    46.588 770.48 -658.04
## residual.sugar        1    17.519 741.41 -708.04
## chlorides             1     1.586 725.48 -736.28
## free.sulfur.dioxide   1     2.339 726.23 -734.93
## total.sulfur.dioxide  1     2.549 726.44 -734.55
## density               1     8.712 732.60 -723.57
## pH                    1     1.010 724.90 -737.31
## sulphates             1    10.408 734.30 -720.56
## alcohol               1     7.894 731.79 -725.02
## type                  1     8.859 732.75 -723.31
```

Here, the AIC is lowest for `pH` (-737.31), so we remove this term from our model.

```
# Create model without citric.acid, pH
linearModel3 <- lm(quality ~ fixed.acidity + volatile.acidity + residual.sugar +
    chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
    density + sulphates + alcohol + type, data = wineTrainingData)
summary(linearModel3)
```

```
##
## Call:
## lm(formula = quality ~ fixed.acidity + volatile.acidity + residual.sugar +
##     chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
##     density + sulphates + alcohol + type, data = wineTrainingData)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -3.3398 -0.4771 -0.0360  0.4510  2.7295
##
## Coefficients:
##                        Estimate Std. Error t value Pr(>|t|)
## (Intercept)           1.186e+02  2.888e+01   4.107 4.26e-05 ***
## fixed.acidity         6.542e-02  2.480e-02   2.638  0.00843 **
## volatile.acidity     -1.569e+00  1.706e-01  -9.197  < 2e-16 ***
## residual.sugar        6.975e-02  1.142e-02   6.109 1.32e-09 ***
## chlorides            -1.458e+00  7.922e-01  -1.841  0.06591 .
## free.sulfur.dioxide   3.446e-03  1.622e-03   2.125  0.03379 *
## total.sulfur.dioxide -1.584e-03  7.018e-04  -2.257  0.02417 *
## density              -1.159e+02  2.885e+01  -4.016 6.26e-05 ***
## sulphates             7.400e-01  1.784e-01   4.148 3.57e-05 ***
## alcohol               2.149e-01  3.845e-02   5.589 2.79e-08 ***
## typeWhite            -4.947e-01  1.307e-01  -3.787  0.00016 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7499 on 1289 degrees of freedom
## Multiple R-squared:  0.3079, Adjusted R-squared:  0.3025
## F-statistic: 57.35 on 10 and 1289 DF,  p-value: < 2.2e-16
```

We repeat this process several more times.

```
# Compute AIC values to drop the lowest one(s)
drop1(linearModel3)
```

```
## Single term deletions
##
## Model:
## quality ~ fixed.acidity + volatile.acidity + residual.sugar +
##     chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
##     density + sulphates + alcohol + type
##                       Df Sum of Sq    RSS     AIC
## <none>                              724.90 -737.31
## fixed.acidity          1     3.914 728.82 -732.31
## volatile.acidity       1    47.567 772.47 -656.69
## residual.sugar         1    20.989 745.89 -702.20
## chlorides              1     1.905 726.81 -735.90
## free.sulfur.dioxide    1     2.539 727.44 -734.76
## total.sulfur.dioxide   1     2.865 727.77 -734.18
## density                1     9.071 733.97 -723.14
## sulphates              1     9.678 734.58 -722.07
## alcohol                1    17.565 742.47 -708.18
## type                   1     8.064 732.97 -724.93
```

```
# Create model without citric.acid, pH, chlorides
linearModel4 <- lm(quality ~ fixed.acidity + volatile.acidity + residual.sugar +
                     free.sulfur.dioxide + total.sulfur.dioxide +
                     density + sulphates + alcohol + type, data = wineTrainingData)
summary(linearModel4)
```

```
##
## Call:
## lm(formula = quality ~ fixed.acidity + volatile.acidity + residual.sugar +
##     free.sulfur.dioxide + total.sulfur.dioxide + density + sulphates +
##     alcohol + type, data = wineTrainingData)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -3.3249 -0.4731 -0.0409  0.4464  2.7390
##
## Coefficients:
##                        Estimate Std. Error t value Pr(>|t|)
## (Intercept)           1.213e+02  2.887e+01   4.200 2.85e-05 ***
## fixed.acidity         6.485e-02  2.482e-02   2.613  0.00907 **
## volatile.acidity     -1.600e+00  1.699e-01  -9.416  < 2e-16 ***
## residual.sugar        7.178e-02  1.137e-02   6.311 3.82e-10 ***
## free.sulfur.dioxide   3.299e-03  1.621e-03   2.035  0.04210 *
## total.sulfur.dioxide -1.546e-03  7.022e-04  -2.202  0.02785 *
## density              -1.187e+02  2.884e+01  -4.117 4.09e-05 ***
## sulphates             7.180e-01  1.781e-01   4.031 5.89e-05 ***
## alcohol               2.237e-01  3.818e-02   5.860 5.87e-09 ***
## typeWhite            -4.679e-01  1.300e-01  -3.600  0.00033 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7506 on 1290 degrees of freedom
## Multiple R-squared:  0.3061, Adjusted R-squared:  0.3012
## F-statistic: 63.22 on 9 and 1290 DF,  p-value: < 2.2e-16
```

```
# Compute AIC values to drop the lowest one(s)
drop1(linearModel4)
```

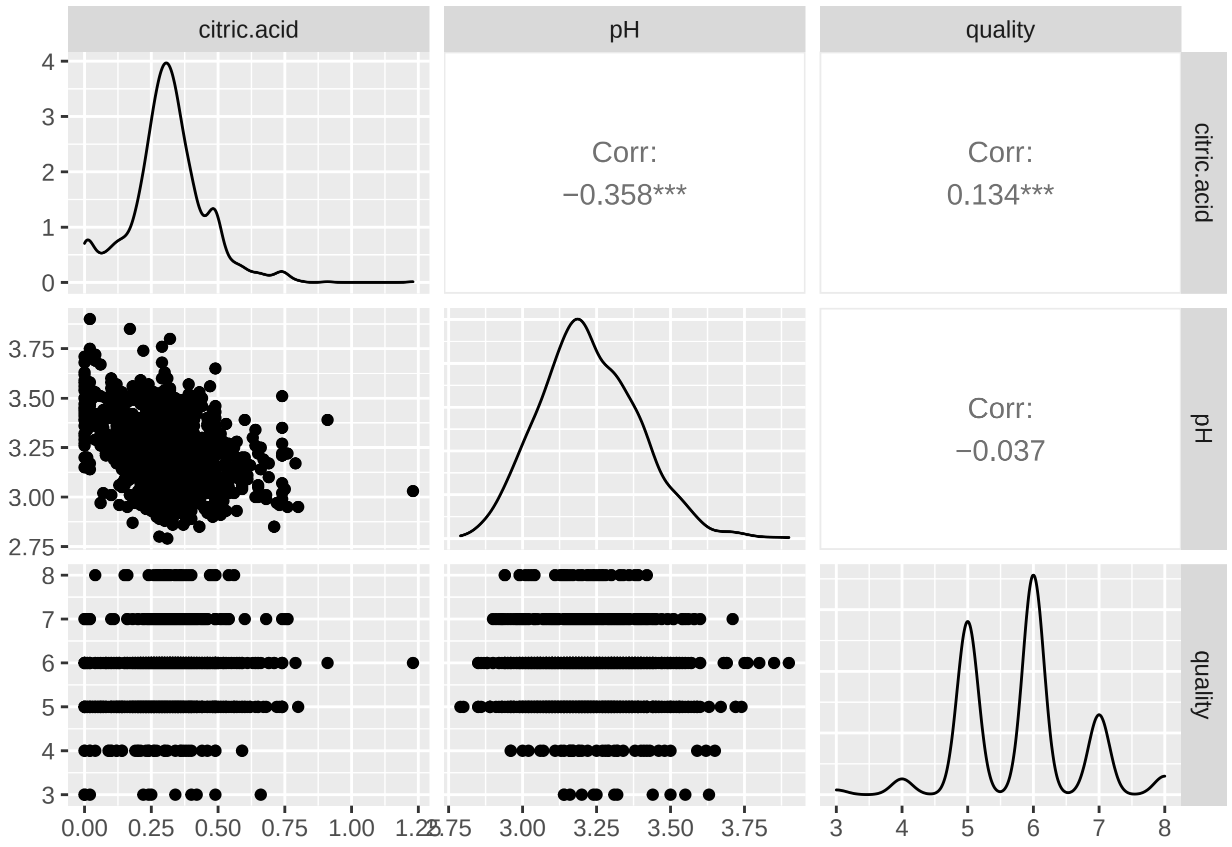
```
## Single term deletions
##
## Model:
## quality ~ fixed.acidity + volatile.acidity + residual.sugar +
##     free.sulfur.dioxide + total.sulfur.dioxide + density + sulphates +
##     alcohol + type
##                      Df Sum of Sq    RSS     AIC
## <none>                            726.81 -735.90
## fixed.acidity         1     3.848 730.65 -731.03
## volatile.acidity      1    49.958 776.77 -651.48
## residual.sugar        1    22.437 749.24 -698.37
## free.sulfur.dioxide   1     2.332 729.14 -733.73
## total.sulfur.dioxide  1     2.732 729.54 -733.02
## density               1     9.548 736.35 -720.93
## sulphates             1     9.154 735.96 -721.63
## alcohol               1    19.348 746.15 -703.74
## type                  1     7.304 734.11 -724.90
```

```
# Create model without citric.acid, pH, chlorides, free.sulfur.dioxide
linearModel5 <- lm(quality ~ fixed.acidity + volatile.acidity + residual.sugar +
                     total.sulfur.dioxide + density + sulphates + alcohol +
                      type, data = wineTrainingData)
summary(linearModel5)
```

```
##
## Call:
## lm(formula = quality ~ fixed.acidity + volatile.acidity + residual.sugar +
##     total.sulfur.dioxide + density + sulphates + alcohol + type,
##     data = wineTrainingData)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -3.3197 -0.4834 -0.0477  0.4459  2.7752
##
## Coefficients:
##                        Estimate Std. Error t value Pr(>|t|)
## (Intercept)           1.274e+02  2.875e+01   4.429 1.03e-05 ***
## fixed.acidity         6.348e-02  2.484e-02   2.556   0.0107 *
## volatile.acidity     -1.645e+00  1.687e-01  -9.752  < 2e-16 ***
## residual.sugar        7.497e-02  1.128e-02   6.647 4.41e-11 ***
## total.sulfur.dioxide -6.991e-04  5.661e-04  -1.235   0.2171
## density              -1.248e+02  2.872e+01  -4.344 1.51e-05 ***
## sulphates             7.353e-01  1.782e-01   4.127 3.90e-05 ***
## alcohol               2.210e-01  3.820e-02   5.785 9.06e-09 ***
## typeWhite            -5.212e-01  1.274e-01  -4.090 4.59e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7515 on 1291 degrees of freedom
## Multiple R-squared:  0.3039, Adjusted R-squared:  0.2995
## F-statistic: 70.44 on 8 and 1291 DF,  p-value: < 2.2e-16
```

By this point, our multiple R-squared values are decreasing and we may wish to stop. Since there was little difference in models using all predictors and models without `citric.acid` and `pH`, we may wish to check if these two variables are colinear.

```
# Visualizations to look at relationships
# income is our response
varAnalysis <- wineTrainingData %>% select(citric.acid, pH, quality)
GGally::ggpairs(varAnalysis)
```



There appears to be a weak relationship between the two. Therefore, we may wish to consider a model that excludes `citric.acid` and `pH`.

Using the caret package

The `preProcess()` function in the `caret` package ensures that, when we center and scale our training data, the set's mean and standard deviation values are saved and applied to the test data to validate our predictions.

```
# Standardize all numeric columns,
# save mean and standard deviation from train set for
# future application to test set
preProcValues <- preProcess(wineTrainingData, method = c("center", "scale"))
trainTransformed <- predict(preProcValues, wineTrainingData)
```

Train our models

We can use the `trainControl()` function in the `caret` package to specify how we will fit our model to the training set. In this case, we specify ten-fold cross-validation, which splits our training set into ten unique partitions and uses nine as the "training" data. The tenth partition then behaves as the "test" data. This partitioning is repeated for all possible iterations and the errors are averaged to help estimate performance.

```
# Example of out-of-band trainControl use
trainControl(method = "cv", number = 10)
```

If we wish, we may also perform the steps above in one sequence.

```
# Set seed for repeatability
set.seed(11)

# Fit a linear model
fit1 <- train(quality ~ ., data = wineTrainingData,
              method = "lm",
              preProcess = c("center", "scale"),
              trControl = trainControl(method = "cv", number = 10))
```

The returned linear regression fit specifies a root mean squared error (RMSE) of ~0.755 on the training set.

```
# View RMSE
fit1
```

```
## Linear Regression
##
## 1300 samples
##   12 predictor
##
## Pre-processing: centered (12), scaled (12)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1169, 1170, 1170, 1171, 1170, 1170, ...
## Resampling results:
##
##   RMSE       Rsquared   MAE
##   0.7547436  0.2955158  0.5795928
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

We can fit four additional models for comparison.

```
set.seed(11)

# Fit a model with quadratics
fit2 <- train(quality ~ .^2, data = wineTrainingData,
              method = "lm",
              preProcess = c("center", "scale"),
              trControl = trainControl(method = "cv", number = 10))

# View RMSE
fit2
```

```
## Linear Regression
##
## 1300 samples
##   12 predictor
##
## Pre-processing: centered (78), scaled (78)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1169, 1170, 1170, 1171, 1170, 1170, ...
## Resampling results:
##
```

```
##   RMSE       Rsquared   MAE
##   0.7694926  0.3047192  0.5812276
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

```
set.seed(11)

# Exclude citric.acid and pH as discussed in the planning section
fit3 <- train(quality ~ fixed.acidity + volatile.acidity + residual.sugar +
    chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
    density + sulphates + alcohol + type, data = wineTrainingData,
             method = "lm",
             preProcess = c("center", "scale"),
             trControl = trainControl(method = "cv", number = 10))

# View RMSE
fit3
```

```
## Linear Regression
##
## 1300 samples
##   10 predictor
##
## Pre-processing: centered (10), scaled (10)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1169, 1170, 1170, 1171, 1170, 1170, ...
## Resampling results:
##
##   RMSE       Rsquared   MAE
##   0.7542811  0.2961162  0.5806917
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

We can look at all interactions by wine type.

```
set.seed(11)

# Consider interactions of all variables with type
fit4 <- train(quality ~ (fixed.acidity + volatile.acidity + residual.sugar +
    chlorides + free.sulfur.dioxide + total.sulfur.dioxide +
    density + sulphates + alcohol):type, data = wineTrainingData,
             method = "lm",
             preProcess = c("center", "scale"),
             trControl = trainControl(method = "cv", number = 10))

# View RMSE
fit4
```

```
## Linear Regression
##
## 1300 samples
##   10 predictor
##
## Pre-processing: centered (18), scaled (18)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1169, 1170, 1170, 1171, 1170, 1170, ...
## Resampling results:
##
##   RMSE       Rsquared   MAE
##   0.7529892  0.2992554  0.5776987
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

```
set.seed(11)

# Consider all possible combinations with type
fit5 <- train(quality ~ (fixed.acidity*volatile.acidity + residual.sugar*alcohol +
    chlorides + free.sulfur.dioxide*total.sulfur.dioxide +
    density + sulphates + type), data = wineTrainingData,
             method = "lm",
             preProcess = c("center", "scale"),
             trControl = trainControl(method = "cv", number = 10))

# View RMSE
fit5
```

```
## Linear Regression
##
## 1300 samples
##   10 predictor
##
## Pre-processing: centered (13), scaled (13)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1169, 1170, 1170, 1171, 1170, 1170, ...
## Resampling results:
##
##   RMSE       Rsquared   MAE
##   0.7414448  0.3184701  0.5749434
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

We can compare the results for all five models.

```
# Side-by-side comparison of results
data.frame(t(fit1$results), t(fit2$results), t(fit3$results), t(fit4$results), t(fit5$results))
```

```
##                     X1       X1.1       X1.2       X1.3       X1.4
## intercept  1.00000000 1.00000000 1.00000000 1.00000000 1.00000000
## RMSE       0.75474358 0.76949258 0.75428113 0.75298920 0.74144484
## Rsquared   0.29551581 0.30471919 0.29611619 0.29925537 0.31847012
## MAE        0.57959276 0.58122760 0.58069169 0.57769866 0.57494342
## RMSESD     0.05773285 0.07854383 0.05786779 0.05212590 0.04822564
## RsquaredSD 0.05538567 0.04513442 0.05429469 0.05147422 0.03752897
## MAESD      0.03510706 0.03499465 0.03642084 0.03288621 0.03551370
```

Now that we have fitted our models, we wish to do predictions. We can use the `predict()` function on the `fit` object that was returned by the `caret` package above and view useful metrics using the `postResample()` function.

```
set.seed(11)

# Do predictions using fit object
pred1 <- predict(fit1, newdata = wineTrainingData)
```

```
pred4 <- predict(fit4, newdata = wineTrainingData)

# View useful metrics on these predictions
postResample(pred1, obs = wineTrainingData$quality)
```

```
##      RMSE  Rsquared       MAE
## 0.7461747 0.3089458 0.5728856
```

```
postResample(pred4, obs = wineTrainingData$quality)
```

```
##      RMSE  Rsquared       MAE
## 0.7400542 0.3202360 0.5677883
```

Apply models to test set

Now, we can use our selected model to perform predictions on the test set.

```
# Read in CSV test file, subset data
wineTest <- tbl_df(read.csv(file = "./wineQualityTest.csv"))
```

```
## Warning: `tbl_df()` was deprecated in dplyr 1.0.0.
## Please use `tibble::as_tibble()` instead.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was generated.
```

```
set.seed(11)

# Apply final model to test set
pred1 <- predict(fit1, newdata = wineTest)
pred5 <- predict(fit5, newdata = wineTest)

postResample(pred1, obs = wineTest$quality)
```

```
##      RMSE  Rsquared       MAE
## 0.7335588 0.2860098 0.5719915
```

```
postResample(pred5, obs = wineTest$quality)
```

```
##      RMSE  Rsquared       MAE
## 0.7316239 0.2899658 0.5726234
```

The best model had an RMSE of 0.732. The best model was one which removed two variables with mild correlation (citric.acid and pH) after gauging their Akaike information criterion (AIC). The model also included all possible interactions between `fixed.acidity` and `volatile.acidity`, `residual.sugar and alcohol`, and `free.sulfur.dioxide` and `total.sulfur.dioxide`. These interactions were selected as an educated guess (acidities and sulfur dioxides are generally to one another and sugar is a key component of fermentation) and all five RMSE values were relatively similar, suggesting that our models do a relatively poor job of predicting quality.

Homework 7, Part 2

In this section, we will consider the logistic regression model, which applies to a boolean response (such as a "success" or a "failure").

Create a new output variable

We can add an additional variable, `superior`, to our training data to indicate whether the quality of wine is 6 or higher.

```
# Add "superior" variable to indicate if quality of wine is 6 or higher
newWineTraining <- wineTrainingData %>% mutate(superior = NA)
names(newWineTraining)
```

```
##  [1] "fixed.acidity"        "volatile.acidity"     "citric.acid"
##  [4] "residual.sugar"       "chlorides"            "free.sulfur.dioxide"
##  [7] "total.sulfur.dioxide" "density"              "pH"
## [10] "sulphates"            "alcohol"              "quality"
## [13] "type"                 "superior"
```

```
# Populate "superior" variable
for (i in 1:length(newWineTraining$quality)){
  if (wineTrainingData$quality[i] >= 6) {
    newWineTraining$superior[i] = 1
  } else {
    newWineTraining$superior[i] = 0
  }
}

names(newWineTraining)
```

```
##  [1] "fixed.acidity"        "volatile.acidity"     "citric.acid"
##  [4] "residual.sugar"       "chlorides"            "free.sulfur.dioxide"
##  [7] "total.sulfur.dioxide" "density"              "pH"
## [10] "sulphates"            "alcohol"              "quality"
## [13] "type"                 "superior"
```

We can now identify correlations between `superior` and other variables.

```
# Display correlations to "superior"
# Remove type (char), convert superior (factor) to superior (int)
noType <- newWineTraining %>% select(-type)
noType$superior <- as.integer(noType$superior)
cor(noType$superior, noType)
```

```
##      fixed.acidity volatile.acidity citric.acid residual.sugar  chlorides
## [1,]    -0.0873774       -0.2862673   0.1338821    -0.03899322 -0.2359268
##      free.sulfur.dioxide total.sulfur.dioxide    density            pH
## [1,]          0.04798056          -0.05010813 -0.3192483 -0.0001220397
##       sulphates   alcohol   quality superior
## [1,] 0.02073574 0.4146408 0.8092307        1
```

`alcohol` has the highest correlation to the `superior` variable (0.41). We can create a plot, weighed by the number of data points, for the relationship between alcohol content and wines with a quality rating of 6 and above.

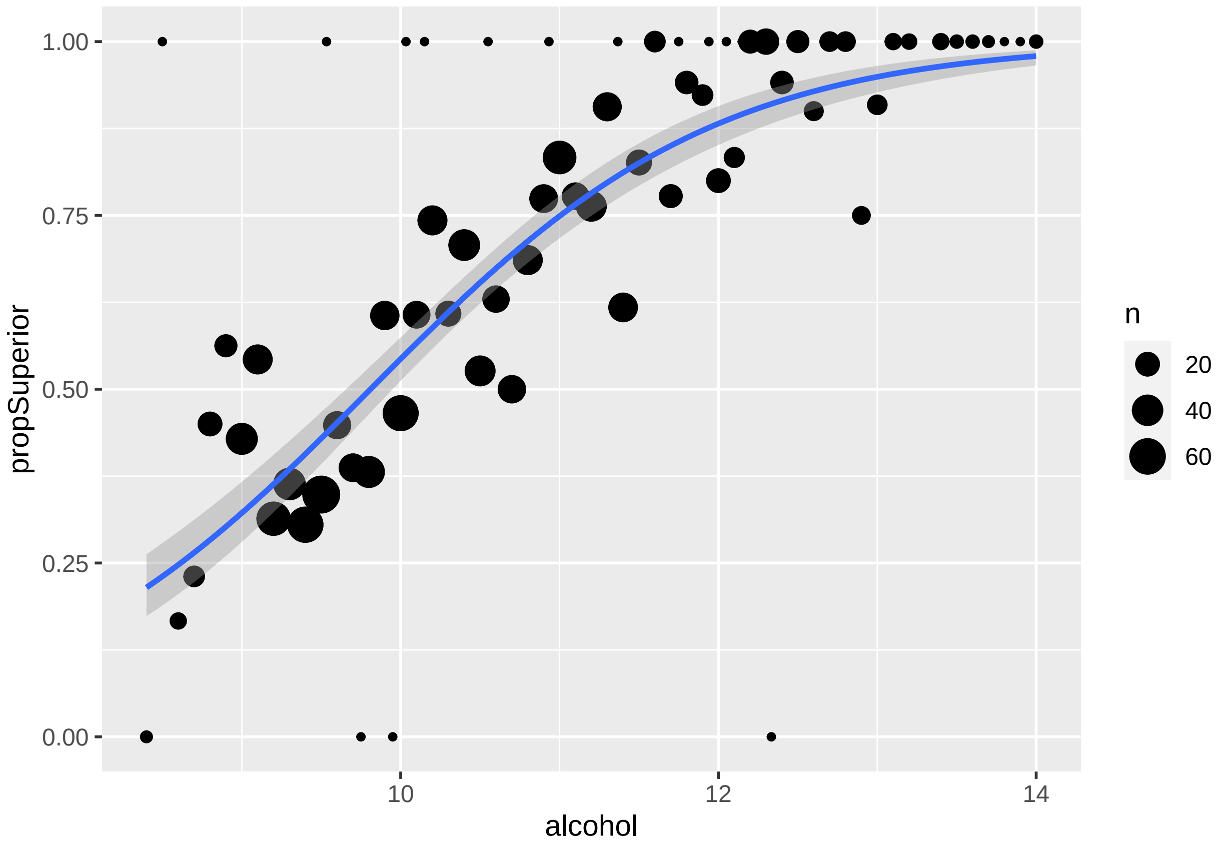
```
# Binomial plot
alcSum <- newWineTraining %>% group_by(alcohol) %>% summarize(propSuperior = mean(superior), n = n())

alcSum
```

```
## # A tibble: 69 x 3
##    alcohol propSuperior     n
##      <dbl>        <dbl> <int>
## 1      8.4        0          2
## 2      8.5        1          1
## 3      8.6        0.167      6
## 4      8.7        0.231     13
## 5      8.8        0.45      20
## 6      8.9        0.562     16
## 7      9          0.429     42
## 8      9.1        0.543     35
## 9      9.2        0.314     51
## 10     9.3        0.364     44
## # ... with 59 more rows
```

```
ggplot(alcSum, aes(x = alcohol, y = propSuperior)) +
  geom_point(stat = "identity", aes(size = n)) +
  stat_smooth(data = newWineTraining, aes(x = alcohol, y = superior), method = "glm",
              method.args = list(family = "binomial"))
```

```
## `geom_smooth()` using formula 'y ~ x'
```



Behind `alcohol`, there are also mild correlations between the variables `superior` and `density` (-0.32), `volatile.acidity` (-0.29), and `chlorides` (-0.24). From the analysis of these coefficients, it appears that three are statistically significant (`alcohol`, `density`, and `volatile.acidity`). The fourth, `chlorides`, is not and we will remove it from subsequent models.

```
lgModel <- glm(superior ~ alcohol + density + volatile.acidity + chlorides, data = newWineTraining, fam
summary(lgModel)
```

```
##
## Call:
```

```
## glm(formula = superior ~ alcohol + density + volatile.acidity +
##     chlorides, family = "binomial", data = newWineTraining)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -2.3359  -0.9240   0.4476   0.8229   2.1760
##
## Coefficients:
##                     Estimate Std. Error z value Pr(>|z|)
## (Intercept)      -123.96739   36.10479  -3.434 0.000596 ***
## alcohol             1.12544    0.09697  11.606  < 2e-16 ***
## density           115.00099   35.66312   3.225 0.001261 **
## volatile.acidity   -4.24049    0.48341  -8.772  < 2e-16 ***
## chlorides          -2.10932    2.29600  -0.919 0.358256
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 1724.6  on 1299  degrees of freedom
## Residual deviance: 1359.1  on 1295  degrees of freedom
## AIC: 1369.1
##
## Number of Fisher Scoring iterations: 4
```

Create models

We can produce models using the `caret` package. The first model includes all variables except for "quality" and wields an accuracy of ~74.6%. Accuracy tells us how many of the training set observations we correctly predicted.

```r
# Set seed for repeatability
set.seed(11)

# Convert response to factor to avoid
# "use a 2 level factor as your outcome column" error
newWineTraining$superior <- as.factor(newWineTraining$superior)

# Fit linear regression model
glmFit1 <- train(superior ~ fixed.acidity + volatile.acidity + citric.acid +
                   residual.sugar + chlorides + free.sulfur.dioxide +
                   total.sulfur.dioxide + density + pH + sulphates + alcohol + type,
                 data = newWineTraining,
                 method = "glm",
                 family = "binomial",
                 preProcess = c("center", "scale"),
                 trControl = trainControl(method = "cv", number = 10))

# View accuracy
glmFit1
```

```
## Generalized Linear Model
##
## 1300 samples
##   12 predictor
##    2 classes: '0', '1'
##
## Pre-processing: centered (12), scaled (12)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1170, 1171, 1170, 1170, 1170, 1169, ...
## Resampling results:
##
##   Accuracy   Kappa
##   0.7461181  0.4507696
```

We can also use the `confusionMatrix()` function to see which predictions were made correctly and incorrectly.

```
# View number of correct and incorrect predictions
confusionMatrix(data = newWineTraining$superior, reference = predict(glmFit1, newdata = newWineTraining
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 309 183
##          1 138 670
##
##                Accuracy : 0.7531
##                  95% CI : (0.7287, 0.7763)
##     No Information Rate : 0.6562
##     P-Value [Acc > NIR] : 2.593e-14
##
##                   Kappa : 0.4656
##
##  Mcnemar's Test P-Value : 0.01406
##
##             Sensitivity : 0.6913
##             Specificity : 0.7855
##          Pos Pred Value : 0.6280
##          Neg Pred Value : 0.8292
##              Prevalence : 0.3438
##          Detection Rate : 0.2377
##    Detection Prevalence : 0.3785
##       Balanced Accuracy : 0.7384
##
##        'Positive' Class : 0
##
```

We see that our model incorrectly predicted 138 values. We can create four more models and compare their accuracy.

```
# Set seed for repeatability
set.seed(11)

# Include only alcohol, density, and volatile.acidity based on highest correlations
glmFit2 <- train(superior ~ alcohol + density + volatile.acidity, data = newWineTraining,
                 method = "glm",
                 family = "binomial",
                 preProcess = c("center", "scale"),
                 trControl = trainControl(method = "cv", number = 10))
```

```r
# View accuracy
glmFit2
```

```
## Generalized Linear Model
##
## 1300 samples
##    3 predictor
##    2 classes: '0', '1'
##
## Pre-processing: centered (3), scaled (3)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1170, 1171, 1170, 1170, 1170, 1169, ...
## Resampling results:
##
##   Accuracy   Kappa
##   0.7345853  0.4238213
```

```r
# Set seed for repeatability
set.seed(11)

# Look at interactions with "type"
glmFit3 <- train(superior ~ (fixed.acidity + volatile.acidity + citric.acid +
                   residual.sugar + chlorides + free.sulfur.dioxide +
                   total.sulfur.dioxide + density + pH + sulphates + alcohol):type, data = newWineTrain
                 method = "glm",
                 family = "binomial",
                 preProcess = c("center", "scale"),
                 trControl = trainControl(method = "cv", number = 10))

# View accuracy
glmFit3
```

```
## Generalized Linear Model
##
## 1300 samples
##   12 predictor
##    2 classes: '0', '1'
##
## Pre-processing: centered (22), scaled (22)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1170, 1171, 1170, 1170, 1170, 1169, ...
## Resampling results:
##
##   Accuracy  Kappa
##   0.754609  0.4663261
```

```r
# Set seed for repeatability
set.seed(11)

# Fit linear regression model
glmFit4 <- train(superior ~ (fixed.acidity + volatile.acidity + citric.acid +
                   residual.sugar + chlorides + free.sulfur.dioxide +
                   total.sulfur.dioxide + density + pH + sulphates + alcohol)*type, data = newWineTrain
                 method = "glm",
                 family = "binomial",
                 preProcess = c("center", "scale"),
                 trControl = trainControl(method = "cv", number = 10))

# View accuracy
glmFit4
```

```
## Generalized Linear Model
##
## 1300 samples
##   12 predictor
##    2 classes: '0', '1'
##
## Pre-processing: centered (23), scaled (23)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1170, 1171, 1170, 1170, 1170, 1169, ...
## Resampling results:
##
##   Accuracy   Kappa
##   0.7538635  0.4640027
```

```
# Set seed for repeatability
set.seed(11)

# Quadratic model
glmFit5 <- train(superior ~ (fixed.acidity + volatile.acidity + citric.acid +
                   residual.sugar + free.sulfur.dioxide +
                   total.sulfur.dioxide + density + sulphates + alcohol)^2, data = newWineTraining,
                 method = "glm",
                 family = "binomial",
                 preProcess = c("center", "scale"),
                 trControl = trainControl(method = "cv", number = 10))

# View accuracy
glmFit5
```

```
## Generalized Linear Model
##
## 1300 samples
##    9 predictor
##    2 classes: '0', '1'
##
## Pre-processing: centered (45), scaled (45)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1170, 1171, 1170, 1170, 1170, 1169, ...
## Resampling results:
##
##   Accuracy   Kappa
##   0.7537929  0.4630133
```

Based on the accuracy data frame below, we will compare the performance of the __ model again our data.

```
data.frame(t(glmFit1$results[2]), t(glmFit2$results[2]), glmFit3$results[2], glmFit4$results[2], glmFit
```

```
##                 X1      X1.1 Accuracy Accuracy.1 Accuracy.2
## Accuracy 0.7461181 0.7345853 0.754609  0.7538635  0.7537929
```

Apply logistic regression models to test data

```r
# Add "superior" variable to indicate if quality of wine is 6 or higher
newWineTest <- wineTest %>% mutate(superior = NA)

# Populate "superior" variable
for (i in 1:length(newWineTest$quality)){
  if (wineTest$quality[i] >= 6) {
    newWineTest$superior[i] = 1
  } else {
    newWineTest$superior[i] = 0
  }
}

newWineTest$superior <- as.factor(newWineTest$superior)
```

We can use the `confusionMatrix()` function with our test data to see accuracy and the correct and incorrect predictions. A model with all predictors (sans `type`) has an accuracy of ~73.35%.

```r
# Accuracy of model with all predictors
confusionMatrix(data = newWineTest$superior, reference = predict(glmFit1, newdata = newWineTest))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction    0    1
##          0 1126  766
##          1  619 2686
##
##                Accuracy : 0.7335
##                  95% CI : (0.7213, 0.7455)
##     No Information Rate : 0.6642
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.4147
##
##  Mcnemar's Test P-Value : 8.742e-05
##
##             Sensitivity : 0.6453
##             Specificity : 0.7781
##          Pos Pred Value : 0.5951
##          Neg Pred Value : 0.8127
##              Prevalence : 0.3358
##          Detection Rate : 0.2167
##    Detection Prevalence : 0.3641
##       Balanced Accuracy : 0.7117
##
##        'Positive' Class : 0
##
```

Model 5, which has the quadratic formula `superior ~ (fixed.acidity + volatile.acidity + citric.acid + residual.sugar + free.sulfur.dioxide + total.sulfur.dioxide + density + sulphates + alcohol)^2`, has a slightly higher accuracy of ~74.04%, but the difference in results is negligible.

```
# View number of correct and incorrect predictions
confusionMatrix(data = newWineTest$superior, reference = predict(glmFit5, newdata = newWineTest))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction    0    1
##          0 1148  744
##          1  605 2700
##
##                Accuracy : 0.7404
##                  95% CI : (0.7283, 0.7523)
##     No Information Rate : 0.6627
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.4305
##
##  Mcnemar's Test P-Value : 0.0001718
##
##             Sensitivity : 0.6549
##             Specificity : 0.7840
##          Pos Pred Value : 0.6068
##          Neg Pred Value : 0.8169
##              Prevalence : 0.3373
##          Detection Rate : 0.2209
##    Detection Prevalence : 0.3641
##       Balanced Accuracy : 0.7194
##
##        'Positive' Class : 0
##
```