P8106_MP_xh2395

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Set random seed

```
set.seed(2020)
```

Import the data

```
wine_df = read_csv("./data/winequality_red.csv")
```

Set train data and test data

```
trRows = createDataPartition(wine_df$quality, p = .75, list = F)

train_df = wine_df[trRows,]

test_df = wine_df[-trRows,]
```

Define X, Y and control

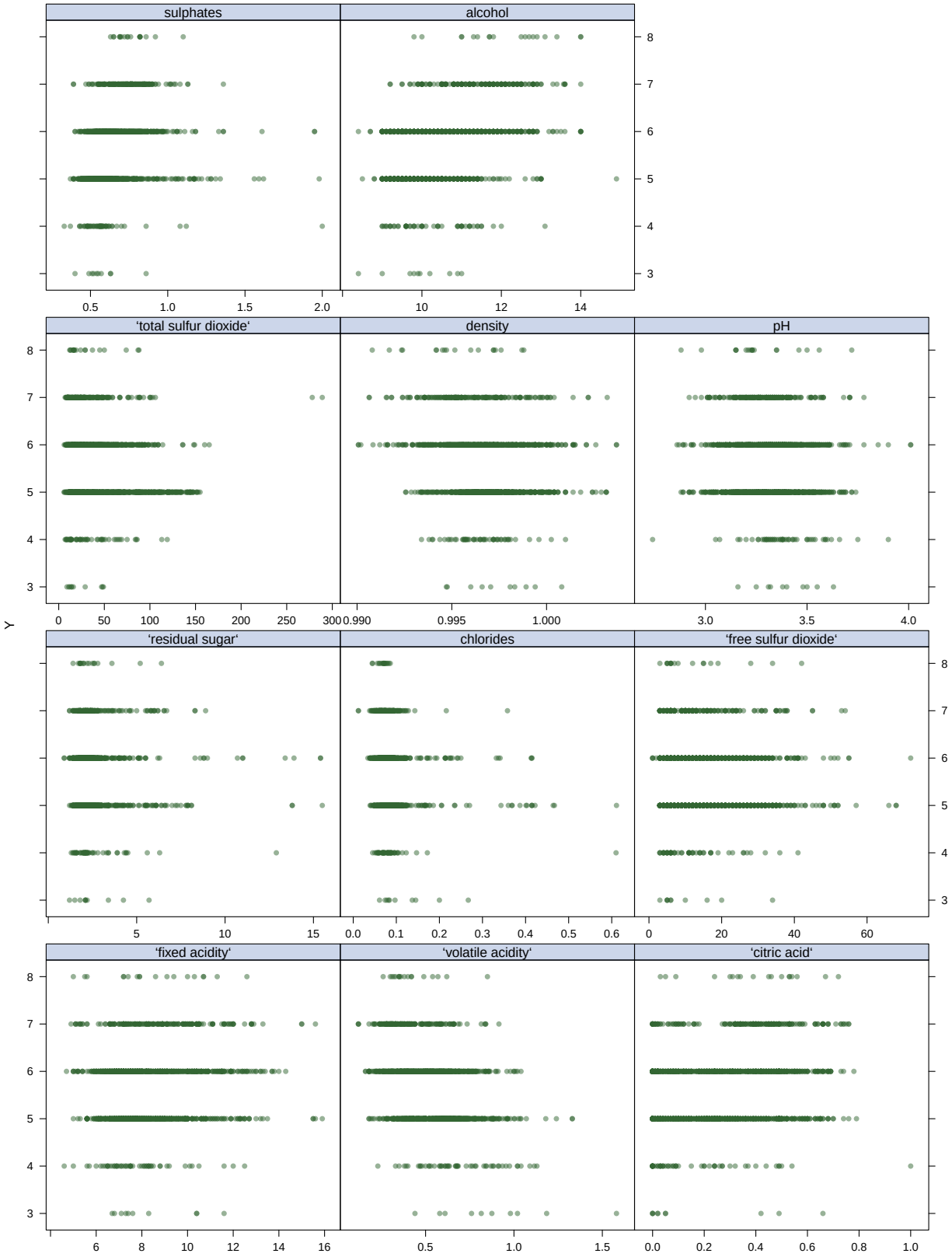
```
# full data
full_X = model.matrix(quality ~ .,wine_df)[,-1]
full_Y = wine_df$quality
# train data
train_X = model.matrix(quality ~ .,train_df)[,-1]
train_Y = train_df$quality
# test data
test_X = model.matrix(quality ~ .,test_df)[,-1]
test_Y = test_df$quality

train_control = trainControl(method = "cv",number = 10)
```

Create Scatter Plots

response vs predictors

```
featurePlot(full_X, full_Y, plot = "scatter", labels = c("","Y"), type = c("p"), layout = c(3, 4))
```


sulphates
alcohol
'total sulfur dioxide'
density
pH
'residual sugar'
chlorides
'free sulfur dioxide'
'fixed acidity'
'volatile acidity'
'citric acid'
Y

Linear model

Fit a linear model using least squares on the training data

```
lm_fit = train(
    x = train_X,
    y = train_Y,
    method = 'lm',
    trControl = train_control,
    metric = 'RMSE'
)
```

Summary

```
summary(lm_fit)
```

```
##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.70720 -0.35757 -0.04139  0.45009  2.00135
##
## Coefficients:
##                                Estimate Std. Error t value Pr(>|t|)
## (Intercept)                   1.576e+01  2.517e+01   0.626 0.531347
## `\\`fixed acidity\\``         4.446e-03  3.068e-02   0.145 0.884796
## `\\`volatile acidity\\``     -9.743e-01  1.367e-01  -7.128 1.77e-12 ***
## `\\`citric acid\\``          -2.991e-02  1.715e-01  -0.174 0.861581
## `\\`residual sugar\\``       -2.981e-03  1.849e-02  -0.161 0.871934
## chlorides                    -1.823e+00  5.240e-01  -3.479 0.000522 ***
## `\\`free sulfur dioxide\\``   6.001e-03  2.567e-03   2.338 0.019562 *
## `\\`total sulfur dioxide\\`` -3.938e-03  8.563e-04  -4.599 4.70e-06 ***
## density                      -1.132e+01  2.567e+01  -0.441 0.659388
## pH                           -5.337e-01  2.202e-01  -2.424 0.015504 *
## sulphates                     9.439e-01  1.276e-01   7.399 2.59e-13 ***
## alcohol                       2.917e-01  3.140e-02   9.287  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.6501 on 1188 degrees of freedom
## Multiple R-squared:  0.3683, Adjusted R-squared:  0.3625
## F-statistic: 62.97 on 11 and 1188 DF,  p-value: < 2.2e-16
```

R-squared: 0.3683

Calculate the mean square error using the test data

```
train_mse = mean(lm_fit$residuals^2)
train_mse
```

```
## [1] NaN
```

```
lm_predict_Y = predict.train(lm_fit, test_X)
lm_test_mse = mean((test_Y - lm_predict_Y) ^ 2)
lm_test_mse
```

```
## [1] 0.416906
```

Ridge regression model

Fit a ridge regression model on the training data, with lambda chosen by cross-validation

```
ridge_fit = train(
    x = train_X,
    y = train_Y,
    method = 'glmnet',
    tuneGrid = expand.grid(alpha = 0,lambda = exp(seq(-8, 10, length = 100))),
    trControl = train_control,
    metric = 'RMSE'
)
```

Summary

```
ridge_fit$bestTune
```

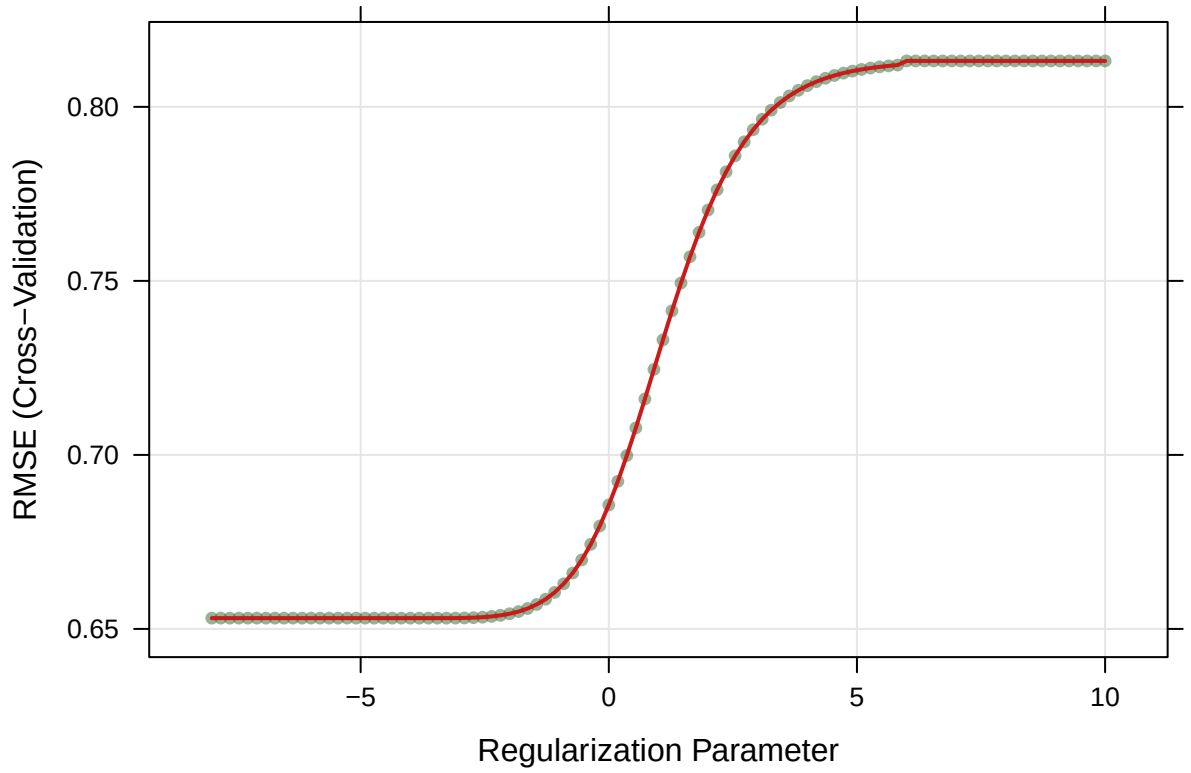
```
##    alpha     lambda
## 27     0 0.03790291
```

```
coef(ridge_fit$finalModel, ridge_fit$bestTune$lambda)
```

```
## 12 x 1 sparse Matrix of class "dgCMatrix"
##                                       1
## (Intercept)             31.187531467
## `fixed acidity`          0.018803017
## `volatile acidity`      -0.929424291
## `citric acid`            0.031242611
## `residual sugar`         0.003292101
## chlorides               -1.750103982
## `free sulfur dioxide`    0.004952667
## `total sulfur dioxide`  -0.003602773
## density                -27.161365213
## pH                      -0.388721717
## sulphates                0.927395116
## alcohol                  0.264195143
```

Plot

```
plot(ridge_fit, xTrans = function(x)log(x))
```



Report the test error

```
ridge_predict_Y = predict.train(ridge_fit, test_X)
ridge_test_mse = mean((test_Y - ridge_predict_Y)^2)

ridge_test_mse
```

```
## [1] 0.4154898
```

Lasso regression model

Fit a lasso regression model on the training data, with lambda chosen by cross-validation

```
lasso_fit = train(
    x = train_X,
    y = train_Y,
```

```
    method = 'glmnet',
    tuneGrid = expand.grid(alpha = 1,lambda = exp(seq(-8, 10, length = 100))),
    trControl = train_control
)
```

Summary

```
lasso_fit$bestTune
```

```
##    alpha      lambda
## 17     1 0.006152424
```

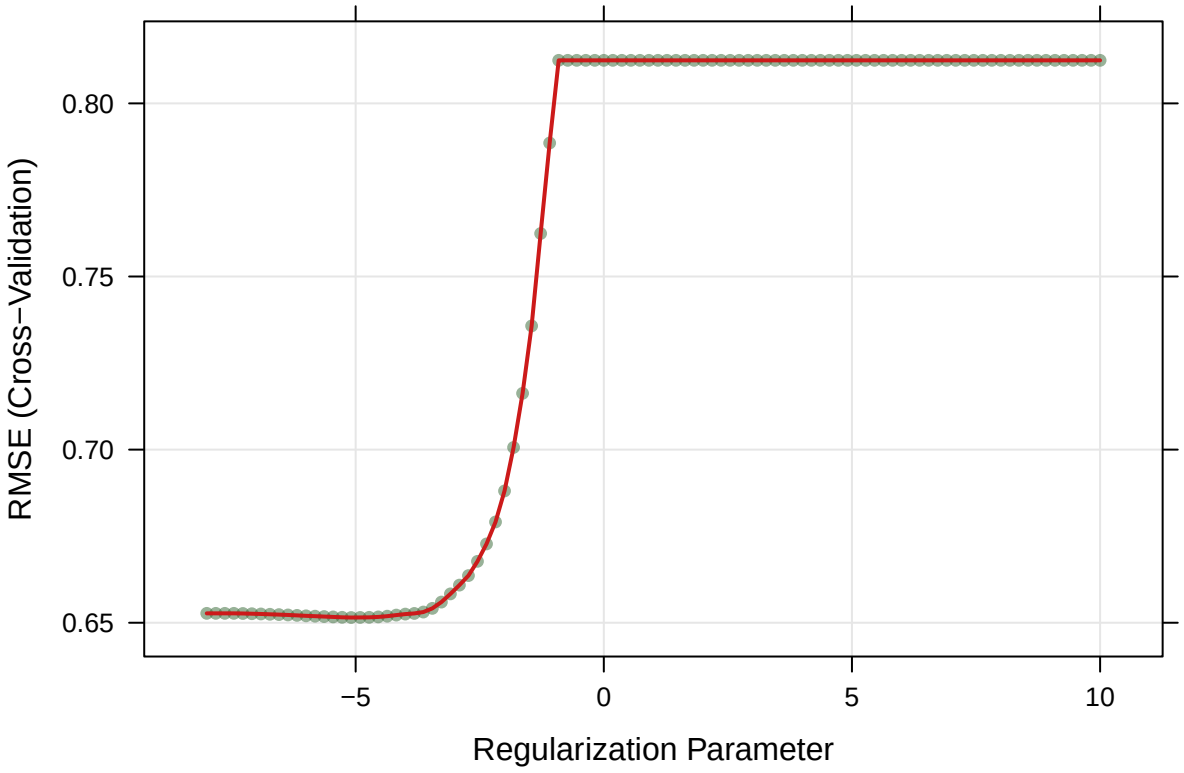
```
coef(lasso_fit$finalModel,lasso_fit$bestTune$lambda)
```

```
## 12 x 1 sparse Matrix of class "dgCMatrix"
##                                       1
## (Intercept)            10.2608767293
## `fixed acidity`         .
## `volatile acidity`     -0.9748068836
## `citric acid`           .
## `residual sugar`       -0.0006122828
## chlorides              -1.6327485797
## `free sulfur dioxide`   0.0041052968
## `total sulfur dioxide` -0.0033792702
## density                -5.9933202042
## pH                     -0.4635003403
## sulphates               0.8962790690
## alcohol                 0.2917985146
```

The number of non-zero coefficient estimates (exclude intercept) is 10.

Plot

```
plot(lasso_fit, xTrans = function(x)log(x))
```



Report the test error

```
lasso_predict_Y = predict.train(lasso_fit, test_X)
lasso_test_mse = mean((test_Y - lasso_predict_Y)^2)

lasso_test_mse
```

```
## [1] 0.4149329
```

Principle component regression model

Fit a pcr model on the training data, with M chosen by cross-validation

```
pcr_fit = train(
    x = train_X,
    y = train_Y,
    method = 'pcr',
    tuneLength = length(train_df) - 1,
    trControl = train_control,
    scale = TRUE
)
```

Summary

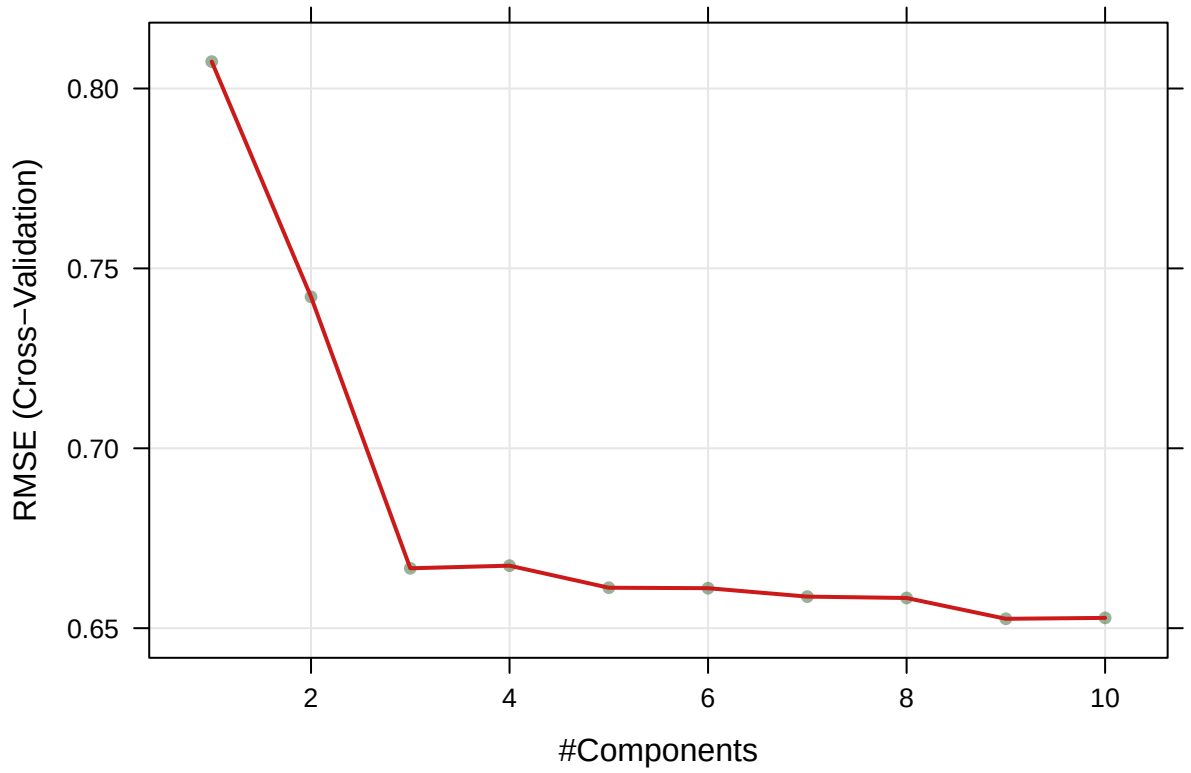
```
pcr_fit$bestTune
```

```
##   ncomp
## 9     9
```

The value of M selected by cross-validation is 9.

Plot

```
plot(pcr_fit)
```



Report the test error

```
pcr_predict_Y = predict.train(pcr_fit, test_X)
pcr_test_mse = mean((test_Y - pcr_predict_Y)^2)

pcr_test_mse
```

```
## [1] 0.4188731
```

Smoothing Spline Model

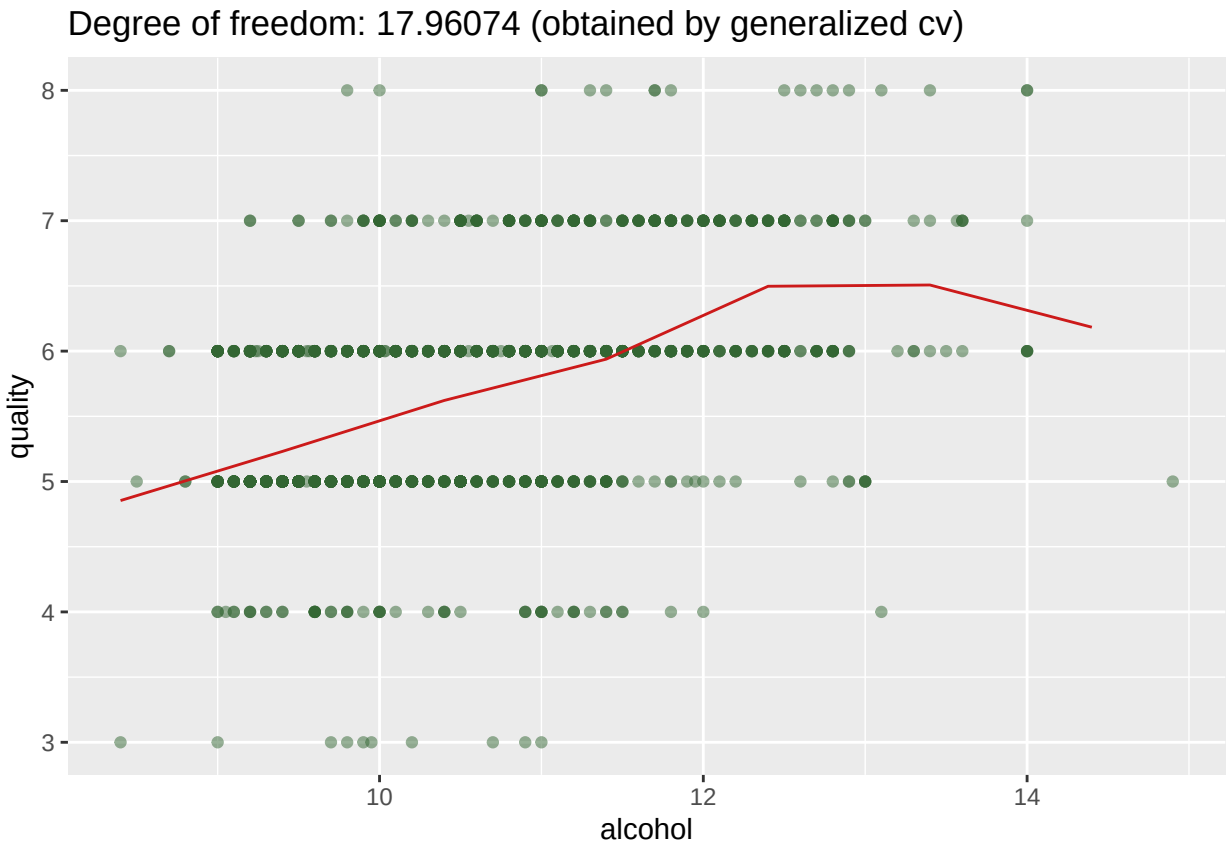
The degree of freedom obtained by generalized cv

```
fit.ss = smooth.spline(wine_df$alcohol, wine_df$quality)
fit.ss$df
```

```
## [1] 17.96074
```

Plot the resulting fit

```
alcohollims = range(wine_df$alcohol)
alcohol.grid = seq(from = alcohollims[1],to = alcohollims[2])
pred.ss = predict(fit.ss,
                  x = alcohol.grid)
pred.ss.df = data.frame(pred = pred.ss$y,
                        alcohol = alcohol.grid)
p_0 = ggplot(data = wine_df, aes(x = alcohol, y = quality)) +
  geom_point(color = rgb(.2, .4, .2, .5))
p_ss = p_0 +
  geom_line(aes(x = alcohol, y = pred), data = pred.ss.df,
          color = rgb(.8, .1, .1, 1)) +
  labs(title = "Degree of freedom: 17.96074 (obtained by generalized cv)")
p_ss
```



Generalized Additive Model

Fit GAM model

```
wine_df1 = wine_df %>%
  rename(fixed_acidity = `fixed acidity`,
         volatile_acidity = `volatile acidity`,
         citric_acid = `citric acid`,
         residual_sugar =`residual sugar`,
         free_sulfur_dioxide = `free sulfur dioxide`,
         total_sulfur_dioxide =`total sulfur dioxide`)

full1_X = model.matrix(quality ~ .,wine_df1)[,-1]
full1_Y = wine_df1$quality

gam_fit = train(full1_X, full1_Y,
                method = "gam",
                tuneGrid = data.frame(method = "GCV.Cp",
                                      select = c(TRUE,FALSE)),
                trControl = train_control)
```

Summary

```
gam_fit$bestTune
```

```
##   select method
## 2   TRUE GCV.Cp
```

```
gam_fit$finalModel
```

```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## .outcome ~ s(free_sulfur_dioxide) + s(alcohol) + s(citric_acid) +
##     s(pH) + s(residual_sugar) + s(fixed_acidity) + s(sulphates) +
##     s(volatile_acidity) + s(total_sulfur_dioxide) + s(chlorides) +
##     s(density)
##
## Estimated degrees of freedom:
## 2.935 7.168 4.027 0.783 4.598 1.850 4.223
## 6.929 6.872 7.485 7.333  total = 55.2
##
## GCV score: 0.394785
```

```
summary(gam_fit)
```

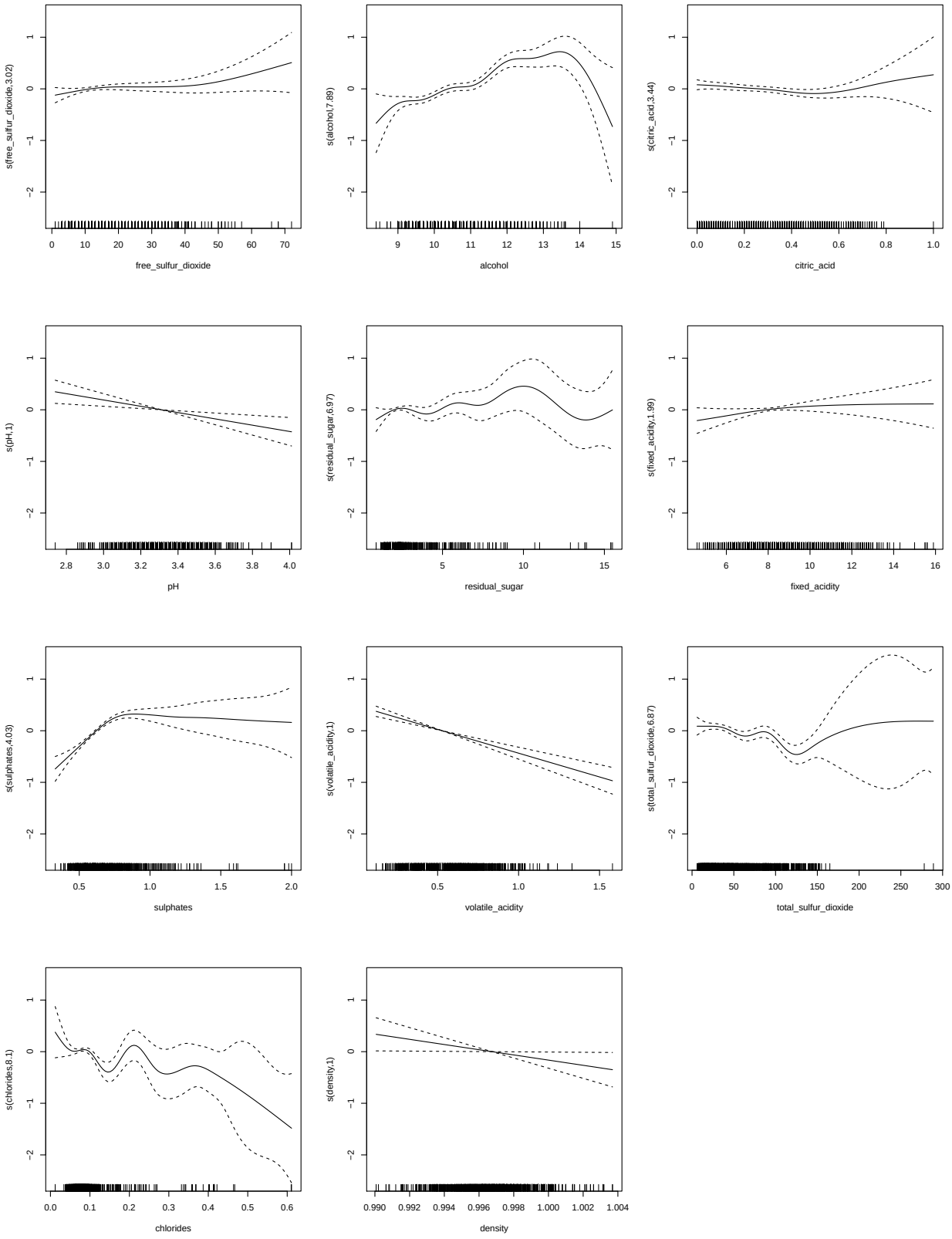
```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## .outcome ~ s(free_sulfur_dioxide) + s(alcohol) + s(citric_acid) +
##     s(pH) + s(residual_sugar) + s(fixed_acidity) + s(sulphates) +
##     s(volatile_acidity) + s(total_sulfur_dioxide) + s(chlorides) +
##     s(density)
##
## Parametric coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  5.63602    0.01544     365   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Approximate significance of smooth terms:
##                            edf Ref.df      F  p-value
## s(free_sulfur_dioxide)  2.9348      9  0.573 0.124101
## s(alcohol)              7.1676      9  9.953  < 2e-16 ***
## s(citric_acid)          4.0274      9  0.791 0.100577
## s(pH)                   0.7828      9  0.968 0.000317 ***
## s(residual_sugar)       4.5980      9  0.867 0.107016
## s(fixed_acidity)        1.8498      9  0.728 0.009892 **
```

```
## s(sulphates)            4.2230      9 15.909  < 2e-16 ***
## s(volatile_acidity)     6.9289      9  7.711 2.38e-13 ***
## s(total_sulfur_dioxide) 6.8725      9  3.719 5.91e-06 ***
## s(chlorides)            7.4846      9  2.745 0.000576 ***
## s(density)              7.3334      9  1.687 0.023025 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.416   Deviance explained = 43.5%
## GCV = 0.39479  Scale est. = 0.38116   n = 1599
```

Plot

```
gam = gam(quality ~ s(free_sulfur_dioxide) + s(alcohol) + s(citric_acid) +
    s(pH) + s(residual_sugar) + s(fixed_acidity) + s(sulphates) +
    s(volatile_acidity) + s(total_sulfur_dioxide) + s(chlorides) +
    s(density), data = wine_df1)

par(mfrow = c(4,3))
plot(gam)
```


s(free_sulfur_dioxide,3.02)
free_sulfur_dioxide
s(alcohol,7.89)
alcohol
s(citric_acid,3.44)
citric_acid
s(pH,1)
pH
s(residual_sugar,6.97)
residual_sugar
s(fixed_acidity,1.99)
fixed_acidity
s(sulphates,4.03)
sulphates
s(volatile_acidity,1)
volatile_acidity
s(total_sulfur_dioxide,6.87)
total_sulfur_dioxide
s(chlorides,8.1)
chlorides
s(density,1)
density

Multivariate Adaptive Regression Splines Model

Fit MARS model

```
mars_grid = expand.grid(degree = 1:2,
                        nprune = 2:10)

mars_fit = train(train_X, train_Y,
                 method = "earth",
                 tuneGrid = mars_grid,
                 trControl = train_control)
```

Summary

```
mars_fit$bestTune
```

```
##    nprune degree
## 12      4      2
```

```
coef(mars_fit$finalModel)
```

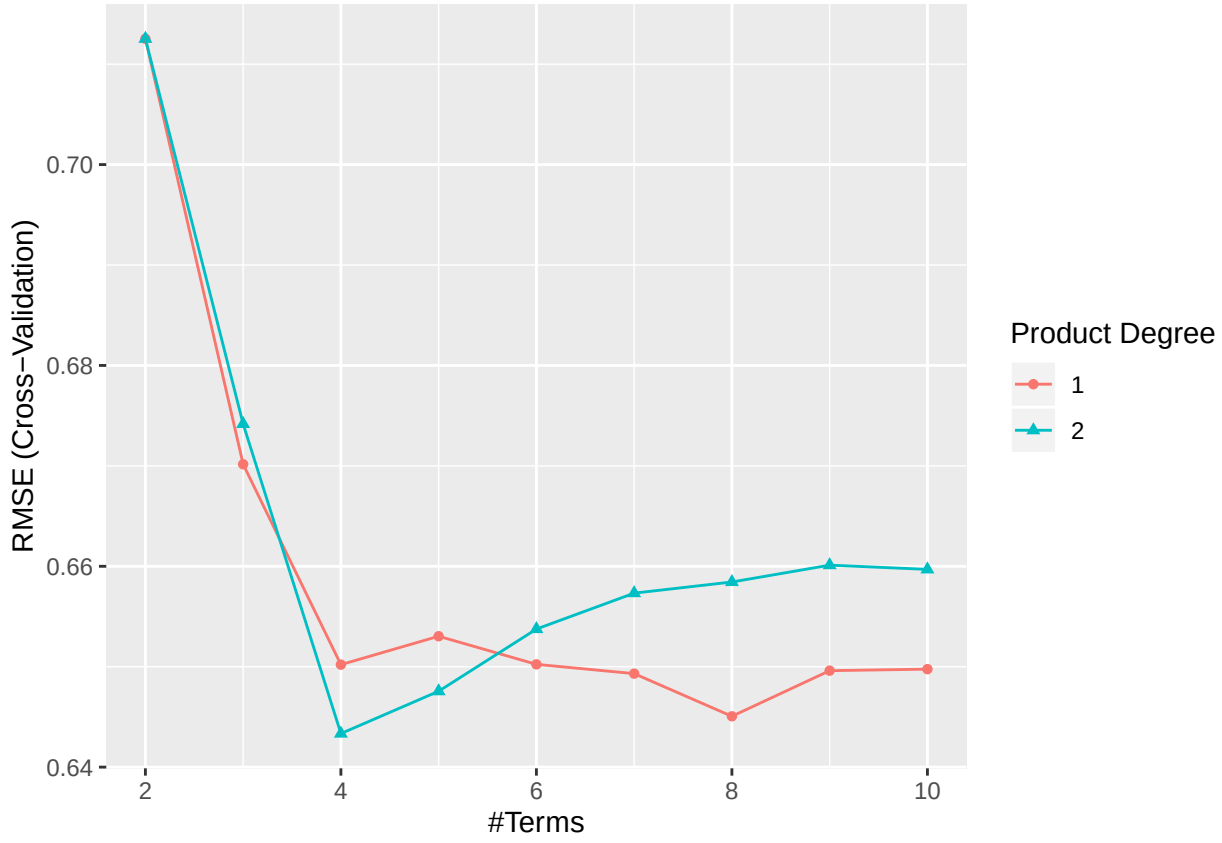
```
##                                           (Intercept)
##                                            6.00559962
##                                       h(12.1-alcohol)
##                                           -0.34227883
## h(0.84-volatile acidity) * h(126-total sulfur dioxide)
##                                            0.01489138
##         h(65-total sulfur dioxide) * h(0.76-sulphates)
##                                           -0.04808887
```

```
summary(mars_fit)
```

```
## Call: earth(x=matrix[1200,11], y=c(5,5,5,6,5,5,7...), keepxy=TRUE,
##             degree=2, nprune=4)
##
##                                                      coefficients
## (Intercept)                                             6.0055996
## h(12.1-alcohol)                                        -0.3422788
## h(0.84-volatile acidity) * h(126-total sulfur dioxide)  0.0148914
## h(65-total sulfur dioxide) * h(0.76-sulphates)         -0.0480889
##
## Selected 4 of 23 terms, and 4 of 11 predictors
## Termination condition: Reached nk 23
## Importance: alcohol, sulphates, `volatileacidity`, ...
## Number of terms at each degree of interaction: 1 1 2
## GCV 0.4161648    RSS 492.3481    GRSq 0.3728199    RSq 0.3806417
```

Plot

```
ggplot(mars_fit)
```



Compare different models

```
resamp = resamples(list(lm = lm_fit,
                        ridge = ridge_fit,
                        lasso = lasso_fit,
                        pcr = pcr_fit,
                        gam = gam_fit,
                        mars = mars_fit))

summary(resamp)
```

```
##
## Call:
## summary.resamples(object = resamp)
##
## Models: lm, ridge, lasso, pcr, gam, mars
## Number of resamples: 10
##
## MAE
##            Min.    1st Qu.     Median       Mean    3rd Qu.       Max. NA's
```

```
## lm    0.4342319 0.4691431 0.5042714 0.5017788 0.5330365 0.5665433    0
## ridge 0.4534667 0.4832119 0.4903573 0.5029094 0.5155260 0.5952779    0
## lasso 0.4591527 0.4707148 0.4900415 0.5033725 0.5284439 0.5858150    0
## pcr   0.4364074 0.4775725 0.4986497 0.5018887 0.5150067 0.5757639    0
## gam   0.4580594 0.4837320 0.4944497 0.5005825 0.5148585 0.5578730    0
## mars  0.4401873 0.4776442 0.4987160 0.5004253 0.5267184 0.5586196    0
##
## RMSE
##           Min.   1st Qu.    Median      Mean   3rd Qu.      Max. NA's
## lm    0.5779289 0.6250236 0.6626994 0.6532942 0.6847714 0.7083816    0
## ridge 0.5906911 0.6309376 0.6499327 0.6531035 0.6717569 0.7400069    0
## lasso 0.5790587 0.6133455 0.6333915 0.6515125 0.6842411 0.7574095    0
## pcr   0.5848335 0.6080756 0.6518623 0.6526109 0.6975966 0.7223157    0
## gam   0.6019513 0.6246506 0.6403150 0.6432048 0.6616430 0.7017351    0
## mars  0.5698264 0.6199849 0.6338825 0.6433405 0.6791219 0.7237716    0
##
## Rsquared
##           Min.   1st Qu.    Median      Mean   3rd Qu.      Max. NA's
## lm    0.2542892 0.3192557 0.3552967 0.3589953 0.3952502 0.4436765    0
## ridge 0.2604142 0.3098512 0.3667993 0.3595150 0.4166652 0.4284589    0
## lasso 0.2889841 0.3386261 0.3652842 0.3632421 0.3891152 0.4203412    0
## pcr   0.2202585 0.3613208 0.3802730 0.3632000 0.3925286 0.4118652    0
## gam   0.3182767 0.3427707 0.3611970 0.3670815 0.3891866 0.4361561    0
## mars  0.3041553 0.3266000 0.3694167 0.3771093 0.4234499 0.4952056    0
```

```
bwplot(resamp, metric = "RMSE")
```