

case_study_report

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Introduction

Background Information

Turbulence is highly versatile motion that is often times difficult to predict and understanding fluid motion and its effect on natural problems poses a great challenge. Interpreting turbulence data is an incredibly important task in the engineering from understanding the cosmos to the cosmic cycle.

Parametric modeling is effective when we want to compactly represent features as model parameters. Unlike certain “black box” machine learning techniques, it offers a higher level of interpretability, which is especially useful for a practical setting. Rather than simply outputting a classification result, a parametric model allows us to investigate in more detail which aspects of turbulence differ between high and low particle cluster volumes.

In our project, we use linear and (...) and apply it to interpret the difference in model parameters in order to achieve the the following objectives:

1. Build a model that predict its particle cluster volume distribution in terms of the moments.
2. Investigate and interpret how model parameters affects the probability distribution for particle cluster volumes

Data

The data set procured for this case study consists of information about cluster volumes. In total, it contains 89 observations with 7 variables. Details of each variable is specified in Table 1.1. The original response variable, a probability distribution for particle cluster volumes, is difficult to interpret, and therefore is summarized into its first 4 raw moments.

Table 1: Table 1.1 Description Table of Data set variables

Metric		Value	Description
St		$0 < St < 3$	Particle property: effect on inertia (e.g. size, density)
Re		90, 224, 398	Reynolds Number: turbulent flow property
Fr		Infinity, 0, 3	Particle propety: gravitational acceleration
R moment 1	Continuous response variable		First raw moment of probability distribution
R moment 2	Continuous response variable		Second raw moment of volume probability distribution
R moment 3	Continuous response variable		Third raw moment of volume probability distribution
R moment 4	Continuous response variable		Fourth raw moment of volume probability distribution

Performing some exploratory data analysis, we can observe from Figure 1 that St , with the exception of the 0 values, follow a linear relationship with the first moment, while for Re , there is high variability for the first moment when $Re = 90$, and low variability otherwise. There is high variability across all Fr values with respect to the first moment. Some of these insights influenced our decisions for modelling approaches which will be further discussed in the Methods section.

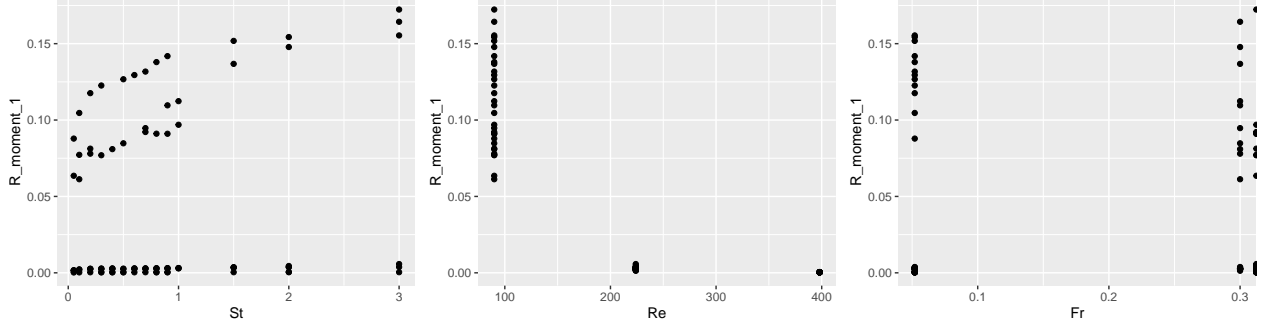


Figure 1: Exploratory data analysis plots on predictors vs first moment

Finally, since Fr contains values of infinity, we decided to inverse-logit the variable, thus creating a new variable called $Fr.logit$. We use this new variable in our models so as to decrease the originally broad range of Fr and improve our predictions.

Methodology

For the approach to modeling the first moment, we first conducted a simple linear regression with a logit transformation on Fr (this was used to address the Fr points labeled ‘Inf’) while keeping Re and St the same. However this model had a low R-squared value with a pattern found in the residuals. The next approach was conducted with the addition of interaction terms, and the results were similar: low R-squared value and pattern in the residuals.

Referring back to the exploratory data analysis, we saw that the $Fr.logit$ and Re behaved more like categorical variables with only 3 unique data points for each. Therefore, for the next approach, we made Fr and Re as factors and created a model with both the simple linear regression and the addition of interaction terms. The factored model with interaction terms resulted in the best R-squared value (.982), a low RMSE (.0087), and a more reasonably random residuals plot. The improved summary, error, and model statistics while maintaining the interpretability of the model makes this factored linear regression with interaction terms model especially appealing.

To see if we can find a better model, we also conducted a Ridge Regression and Generalized Additive Model, but these resulted in very high MSE for higher moments.

For our chosen linear regression model, we can write this in statistical notation below:

$$Moment_x = \beta_0 + \beta_1 * St + \sum_{i=2}^4 \beta_i * Re_i + \sum_{j=5}^7 \beta_j * Fr.logit_j + \sum_{k=8}^{10} \beta_k * (\text{all two-way interactions between } St, Re \text{ and } Fr.logit)$$

For $1 \leq x \leq 4$,

Considering the nature of our response variables, since each moment is derived from the same probability distribution, we decided to perform log transformations for the higher-order moments ($Moment_2$, $Moment_3$

and $Moment_4$). Furthermore, our design decision to include interaction effects stem from the exploratory data plot showing certain correlations between the predictor variables, so as to allow our model to be more interpretable to the collinearity between pair of predictors. It is important to note that the baseline level for the now categorical variable `Fr.logit` is 0.51, whereas the baseline level for the categorical variable `Re` is 90 in all of our models.

Results

For the model implemented with the log of the second moment as the response variable, we see that all predictor variables and the interaction effects between `Fr` and `Re` to be significant (p-values <0.05). A high adjusted R-squared value of 0.889 shows that the model explains a large amount of variability in its predictions considering multiple predictors and their collinearity. There Residual Mean-squared Error is 1.237, which is low, meaning that the model is fit well. Holding all else constant, a unit increase in `St` results in a $e^{(0.8586)}$ increase of the second moment. When `Fr` is 0.574 and 1, there is a $e^{(-6.678)}$ and $e^{(-6.737)}$ change of the second moment respectively. Similar when `Re` is 224 and 398, there is a $e^{(-7.43451)}$ and $e^{(-10.7873)}$ change of the second moment respectively. Additionally, when `Fr` is 0.574 and `Re` is 224 and 398, there is a $e^{(4.477)}$ change in the second moment. When `Fr` is 1, and `Re` is 224 and 398, there an additional $e^{(4.694)}$ and $e^{(6.883)}$ change in the second moment.

```
set.seed(1)

data_ctrl <- trainControl(method = "cv", number = 5)
model_caret3 <- train(log(R_moment_3) ~ St + Fr.logit + Re + St*Fr.logit + St*Re + Fr.logit*Re, data=tr,
                      trControl = data_ctrl,                # folds
                      method = "lm",                        # specifying regression model
                      na.action = na.pass)

model_caret3
summary(model_caret3$finalModel)
```

For the third moment, we can see that 4 of the interaction terms, the different combinations of `St:Fr.logit` and `St:Re`, are no longer significant compared to their baseline levels, although their main effects are still significant at an alpha level of 0.05. Holding all else constant,

```
set.seed(1)

data_ctrl <- trainControl(method = "cv", number = 5)
model_caret4 <- train(log(R_moment_4) ~ St + Fr.logit + Re + St*Fr.logit + St*Re + Fr.logit*Re, data=tr,
                      trControl = data_ctrl,                # folds
                      method = "lm",                        # specifying regression model
                      na.action = na.pass)

summary(model_caret4)
```

For the fourth moment, we can similarly see that the interaction terms including `St` are no longer significant, while their main effects are still significant. The Residual standard error is 2.693 which is higher than other models, but is expected since moment 4 is a higher-order derivation of the probability distribution compared to moments 1,2 and 3. However, a high adjusted R-squared value of 0.8784 tells us that the model explains much of the variability in the predictive capabilities of the model, but is significant lower than the other models with lower-order moments. Holding all else constant, a unit increase in `St` causes a $e^{(1.7147)}$ increase in the 4th moment. When `Fr`= 0.5744 and 1, there is an $e^{(0.3206)}$ and $e^{(0.0065)}$ increase in the 4th moment respectively. When `Re` = 224 and 398, there is an $e^{(0.1384)}$ and $e^{(-1.3817)}$ increase in the 4th moment respectively. Additionally, when `Fr`=0.5744, and `Re` = 224, there is an additional $e^{(12.435)}$ increase in the 4th moment. When `Fr` = , and `Re` = 224 and 398, there is an additional $e^{(12.719)}$ and $e^{(19.134)}$

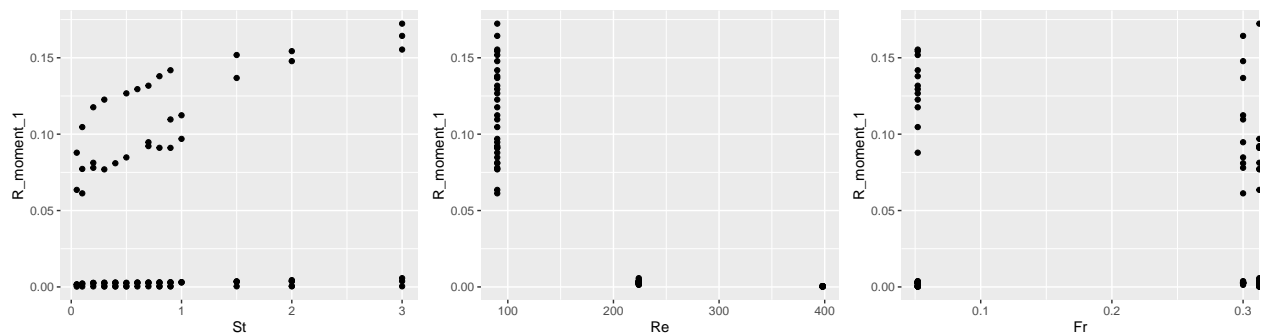
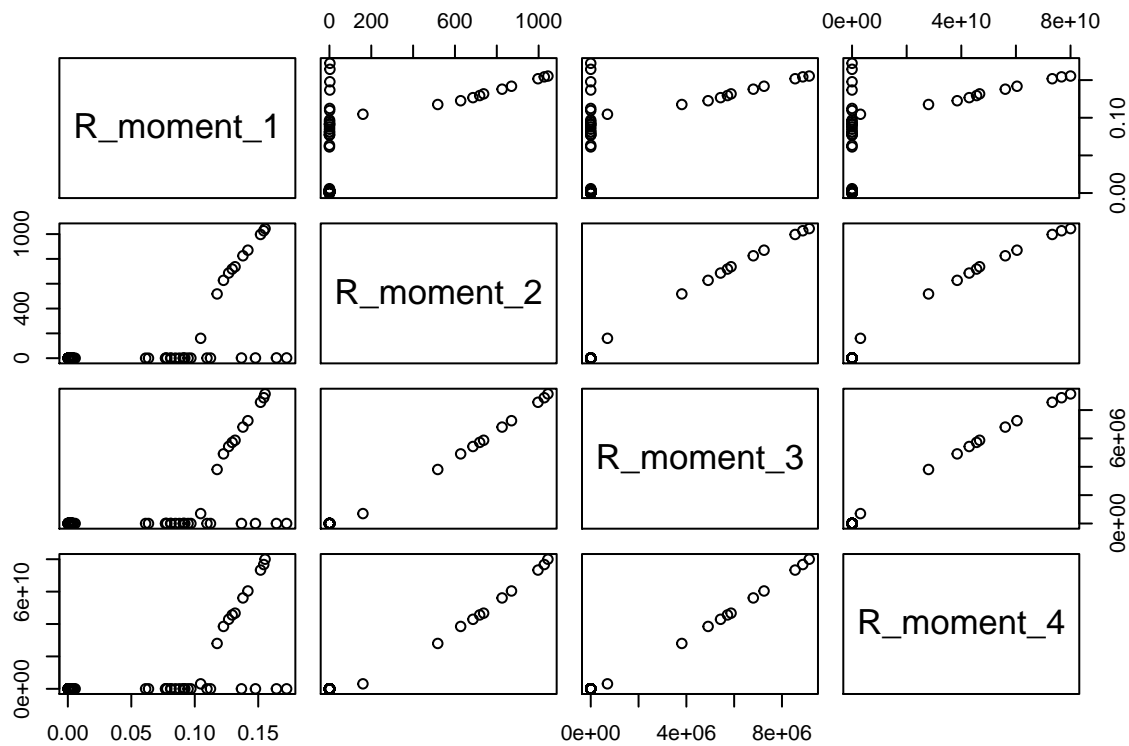
increase in the 4th moment respectively.

Conclusion

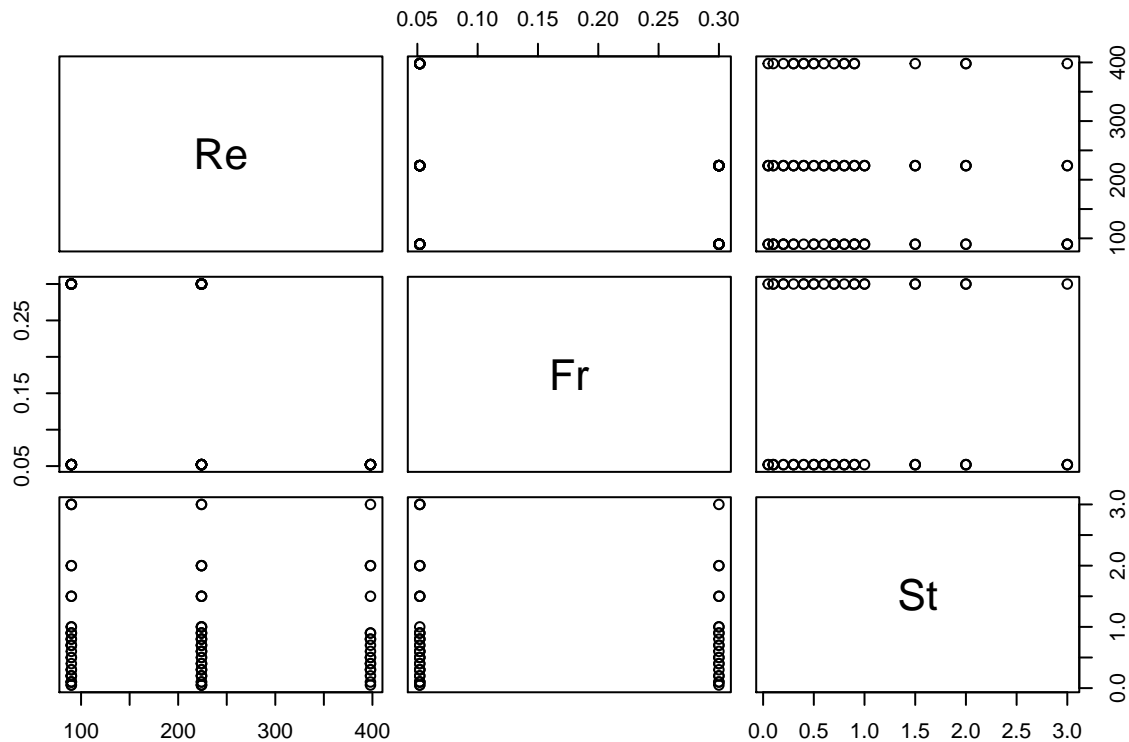
Appendix

EDA

```
#pairs plot to show correlation between response variables  
train_response <- data.frame(train[,c("R_moment_1", "R_moment_2", "R_moment_3", "R_moment_4")])  
pairs(train_response)
```



```
#correlation between predictor variables (in case we need to include interaction effects)  
train_predictors <- data.frame(train[,c("Re", "Fr", "St")])  
pairs(train_predictors)
```



Modeling

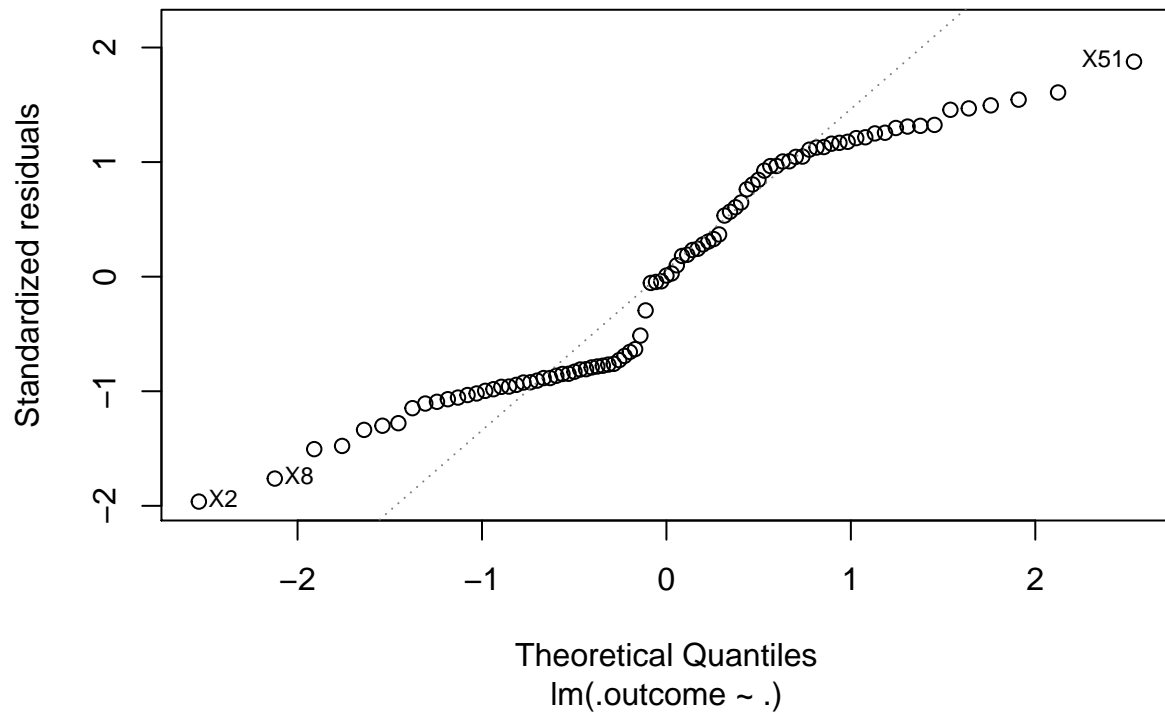
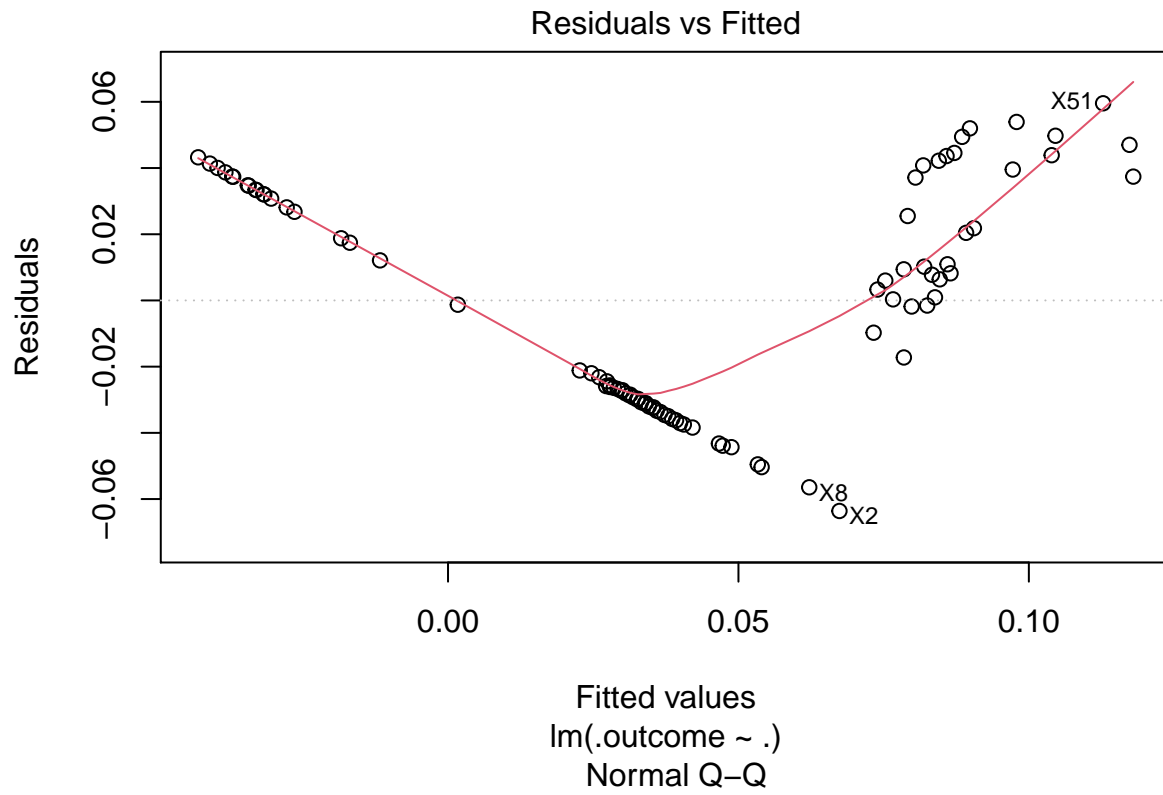
```
data_ctrl <- trainControl(method = "cv", number = 5)
model_caret <- train(R_moment_1 ~ St + Fr.logit + Re, data=train,
                     trControl = data_ctrl,                # folds
                     method = "lm",                       # specifying regression model
                     na.action = na.pass)
```

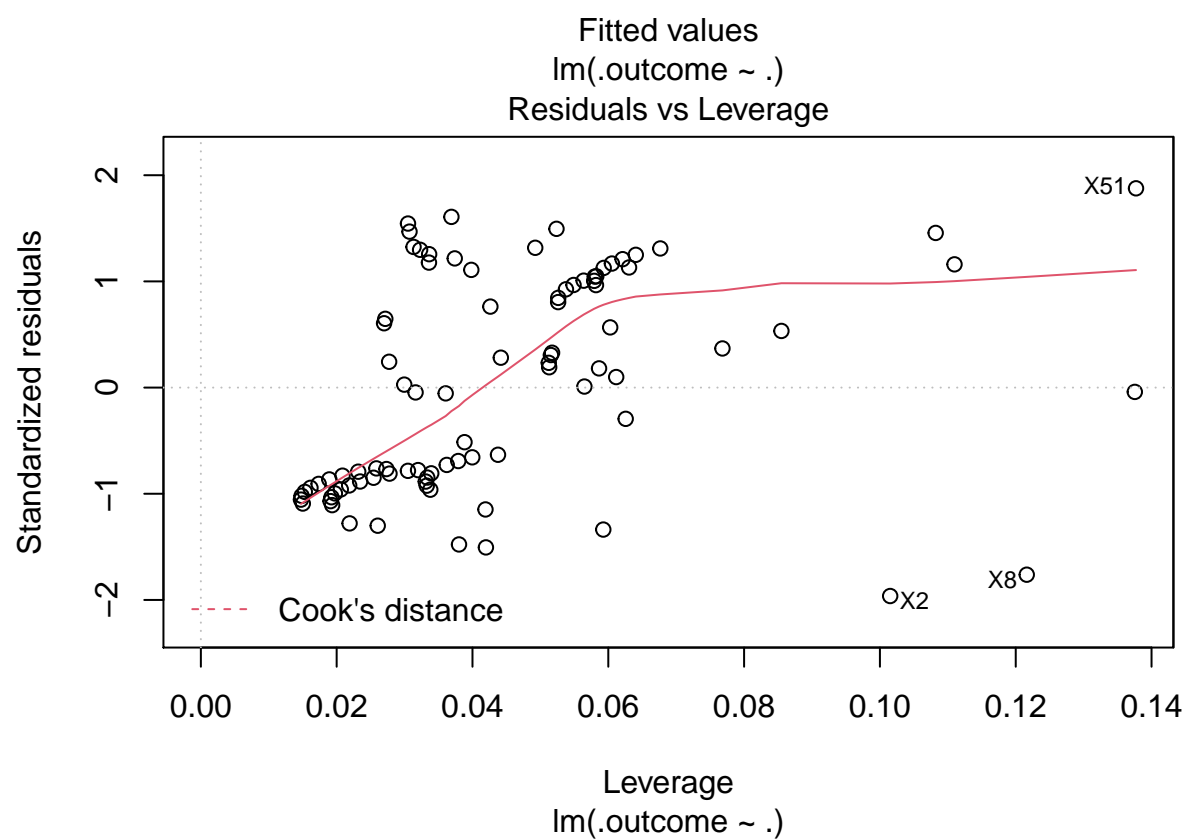
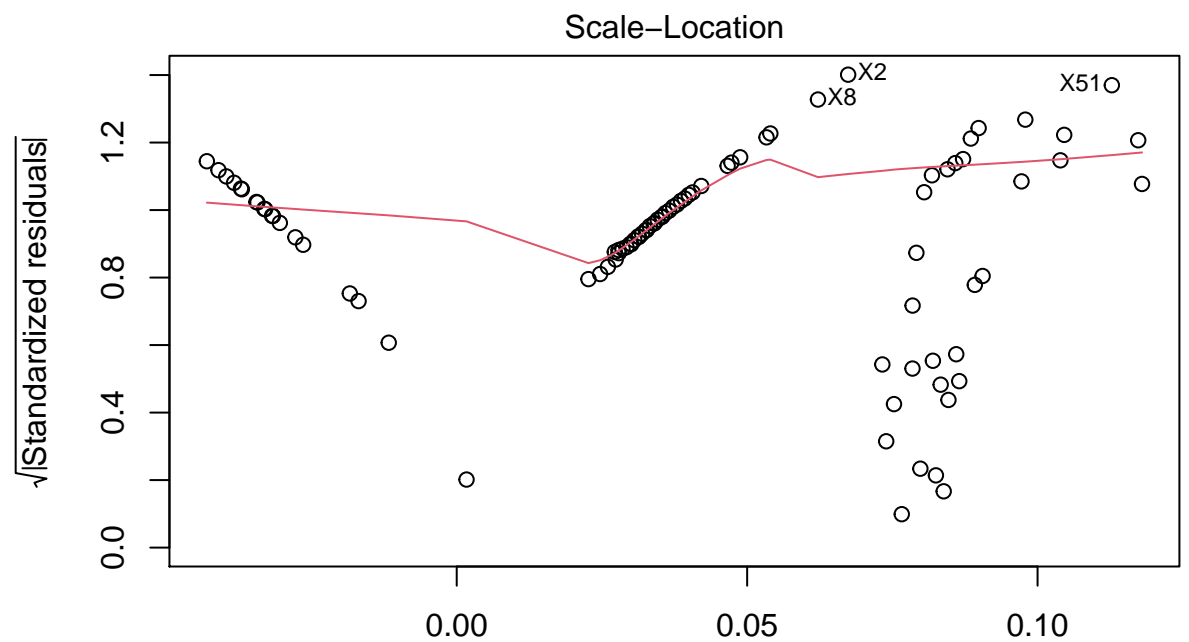
model_caret

Simple linear modeling

```
## Linear Regression
##
## 89 samples
## 3 predictor
##
## No pre-processing
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 72, 70, 71, 72, 71
## Resampling results:
##
##   RMSE          Rsquared    MAE
## 0.03386142 0.6321532 0.03063486
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

plot(model_caret\$finalModel)





```
x <- model.matrix(R_moment_1~St + Fr.logit + Re,data=train)[,-1]

set.seed(17)
train.samp <- sample(1:nrow(train), 4 * nrow(train)/5)
```

```
test <- (-train.samp)
y.test <- train$R_moment_1[test]

preds <- predict(lm_m1_int, newdata = as.data.frame(train[test,]))
mean((preds - y.test)^2)
```

Interaction effects

```
## [1] 0.0009855535

data_ctrl <- trainControl(method = "cv", number = 5)
model_caret <- train(R_moment_1 ~ St + Fr.logit + Re + St*Fr.logit + St*Re + Fr.logit*Re, data=train,
                     trControl = data_ctrl,                      # folds
                     method = "lm",                             # specifying regression model
                     na.action = na.pass)

summary(model_caret)

##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.064305 -0.028656  0.006188  0.026969  0.056868
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   1.346e-01  2.947e-02   4.568 1.72e-05 ***
## St             4.392e-02  1.656e-02   2.653  0.00958 **
## Fr.logit      -6.140e-02  3.881e-02  -1.582  0.11750
## Re            -4.801e-04  1.115e-04  -4.305 4.60e-05 ***
## `St:Fr.logit` -1.434e-02  1.997e-02  -0.718  0.47469
## `St:Re`       -1.008e-04  3.913e-05  -2.577  0.01177 *
## `Fr.logit:Re`  2.660e-04  1.351e-04   1.968  0.05242 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0323 on 82 degrees of freedom
## Multiple R-squared:  0.6883, Adjusted R-squared:  0.6655
## F-statistic: 30.18 on 6 and 82 DF,  p-value: < 2.2e-16
```

```
#linear regression with factored Re and Fr.logit
train1 <- train
train1$Re <- as.factor(train$Re)
train1$Fr.logit <- as.factor(train$Fr.logit)
lm1_m1 <- lm(R_moment_1 ~ St + Fr.logit + Re, data=train1)
lm2_m1 <- lm(R_moment_2 ~ St + Fr.logit + Re, data=train1)
lm3_m1 <- lm(R_moment_3 ~ St + Fr.logit + Re, data=train1)
lm4_m1 <- lm(R_moment_4 ~ St + Fr.logit + Re, data=train1)

set.seed(17)
train.samp <- sample(1:nrow(train), 4 * nrow(train)/5)
```



```
test <- (-train.samp)
y.test <- train$R_moment_1[test]

preds <- predict(lm1_m1, newdata = as.data.frame(train1[test,]))
mean((preds - y.test)^2)
```

Predictors as factors

```
## [1] 0.0001623039

lm1_m1_int <- lm(R_moment_1 ~ St + Fr.logit + Re + St*Fr.logit + St*Re + Fr.logit*Re, data=train1)
lm2_m1_int <- lm(R_moment_2 ~ St + Fr.logit + Re + St*Fr.logit + St*Re + Fr.logit*Re, data=train1)
lm3_m1_int <- lm(R_moment_3 ~ St + Fr.logit + Re + St*Fr.logit + St*Re + Fr.logit*Re, data=train1)
lm4_m1_int <- lm(R_moment_4 ~ St + Fr.logit + Re + St*Fr.logit + St*Re + Fr.logit*Re, data=train1)

set.seed(1)
data_ctrl <- trainControl(method = "cv", number = 5)
model_caret <- train(R_moment_1 ~ St + Fr.logit + Re + St*Fr.logit + St*Re + Fr.logit*Re, data=train1,
                     trControl = data_ctrl,                      # folds
                     method = "lm",                             # specifying regression model
                     na.action = na.pass)

## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

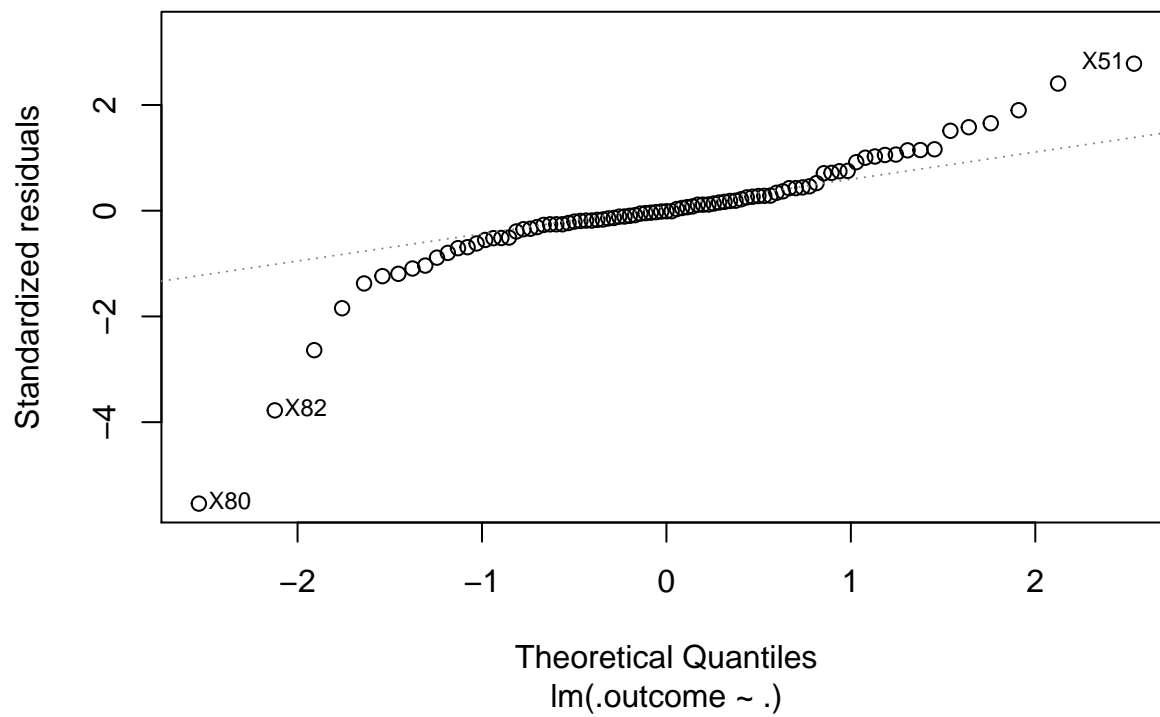
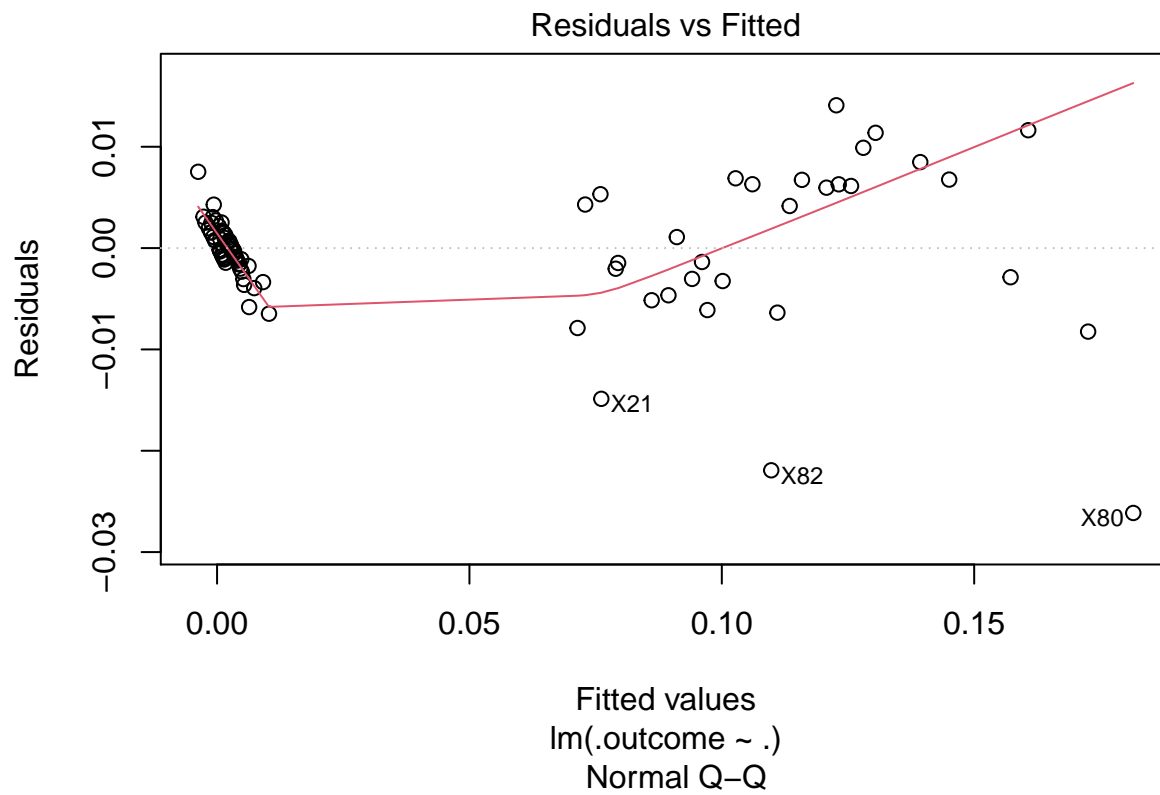
## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

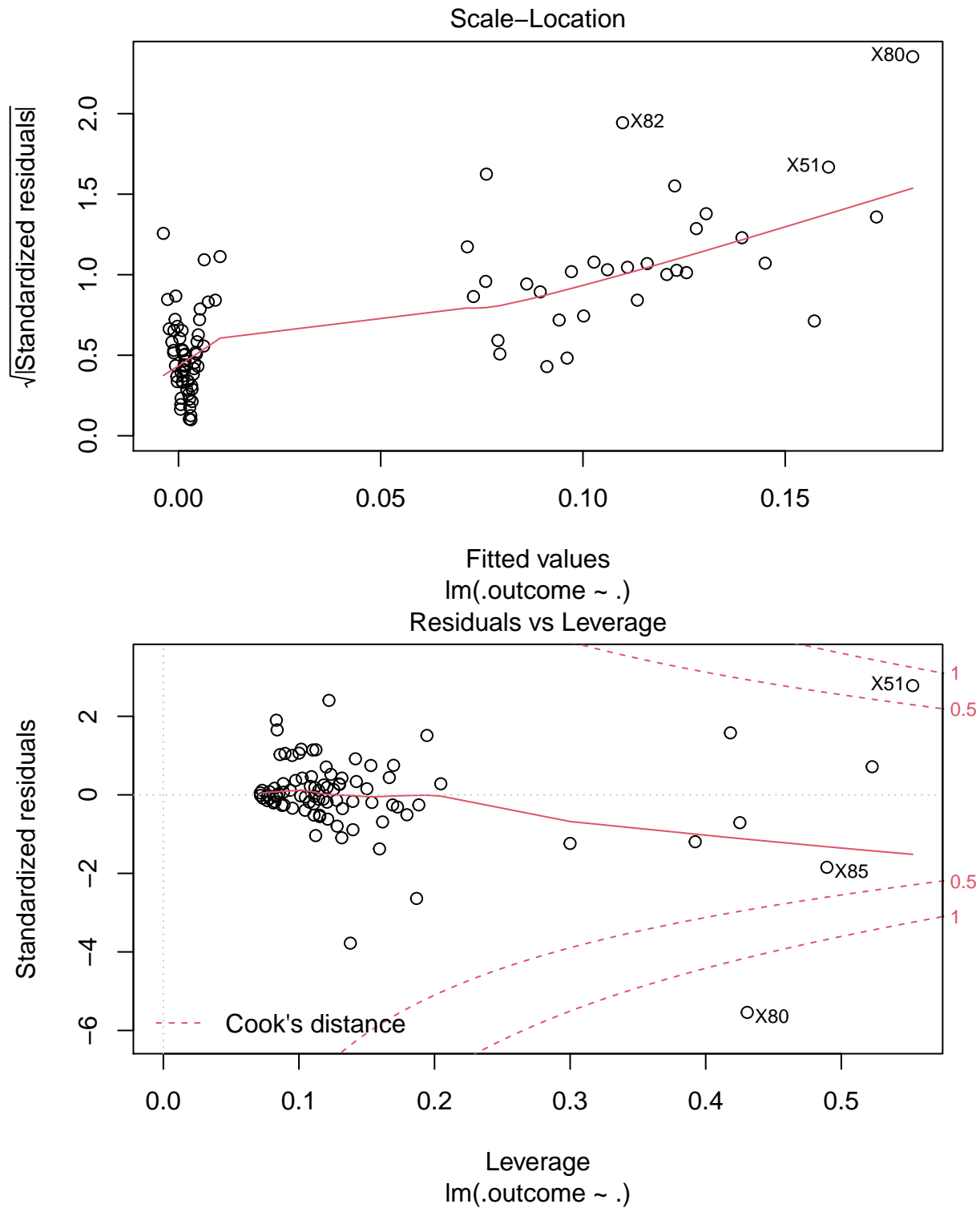
## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

model_caret

## Linear Regression
##
## 89 samples
## 3 predictor
##
## No pre-processing
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 71, 72, 71, 70, 72
## Resampling results:
##
##      RMSE          Rsquared    MAE
## 0.008673306 0.9820262 0.004945823
##
## Tuning parameter 'intercept' was held constant at a value of TRUE

plot(model_caret$finalModel)
```





```
summary(model_caret$finalModel)
```

```
##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
```

```
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.0261390 -0.0016048 -0.0000646  0.0024878  0.0140925
##
## Coefficients: (1 not defined because of singularities)
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    0.108581   0.002378  45.662 < 2e-16 ***
## St             0.024313   0.001744  13.939 < 2e-16 ***
## Fr.logit0.574442516811659 -0.035778   0.003540 -10.105 1.05e-15 ***
## Fr.logit1      -0.038679   0.003219 -12.015 < 2e-16 ***
## Re224          -0.103060   0.002987 -34.498 < 2e-16 ***
## Re398          -0.106710   0.003603 -29.616 < 2e-16 ***
## `St:Fr.logit0.574442516811659` 0.008944   0.002380   3.759 0.000333 ***
## `St:Fr.logit1`    0.005956   0.001995   2.985 0.003812 **
## `St:Re224`       -0.027400   0.001938 -14.136 < 2e-16 ***
## `St:Re398`       -0.025834   0.002506 -10.309 4.34e-16 ***
## `Fr.logit0.574442516811659:Re224` 0.028831   0.003657   7.884 1.84e-11 ***
## `Fr.logit1:Re224` 0.033657   0.003705   9.084 9.21e-14 ***
## `Fr.logit0.574442516811659:Re398` NA         NA         NA         NA
## `Fr.logit1:Re398` 0.034294   0.004051   8.465 1.41e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.006253 on 76 degrees of freedom
## Multiple R-squared:  0.9892, Adjusted R-squared:  0.9875
## F-statistic: 578.6 on 12 and 76 DF, p-value: < 2.2e-16

model_caret_2 <- train(log(R_moment_2) ~ St + Fr.logit + Re + St*Fr.logit + St*Re + Fr.logit*Re, data=t,
                      trControl = data_ctrl,                # folds
                      method = "lm",                        # specifying regression model
                      na.action = na.pass)

## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

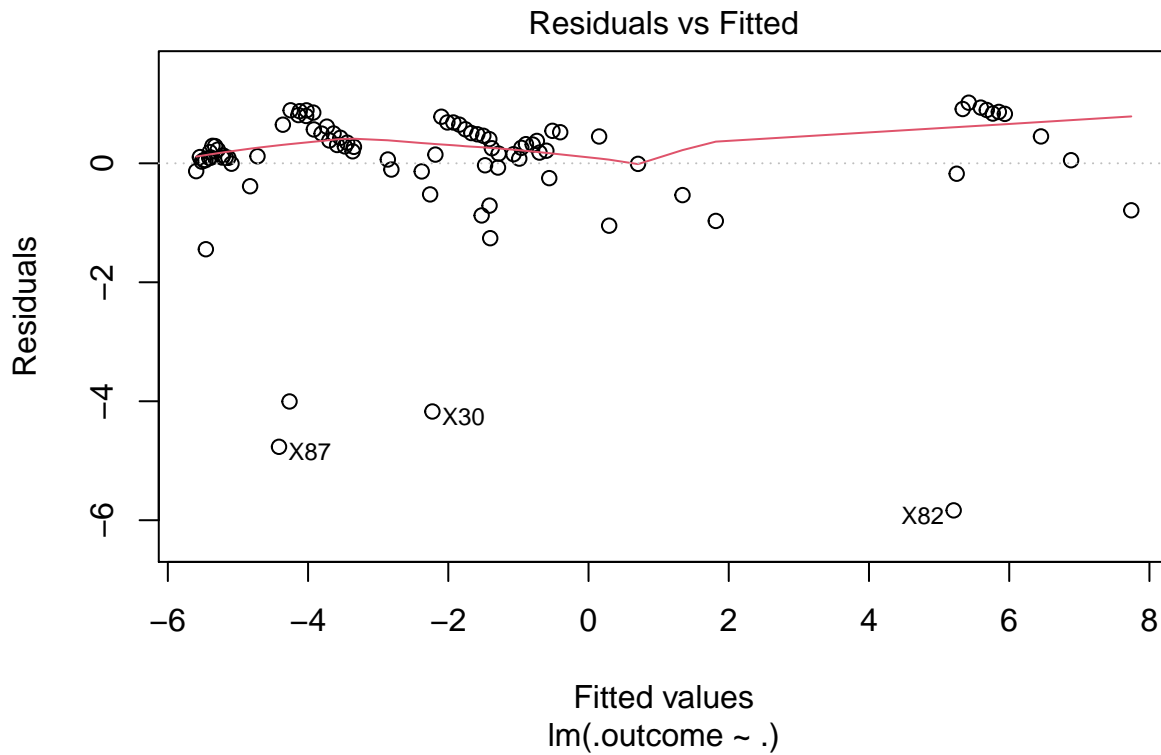
## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

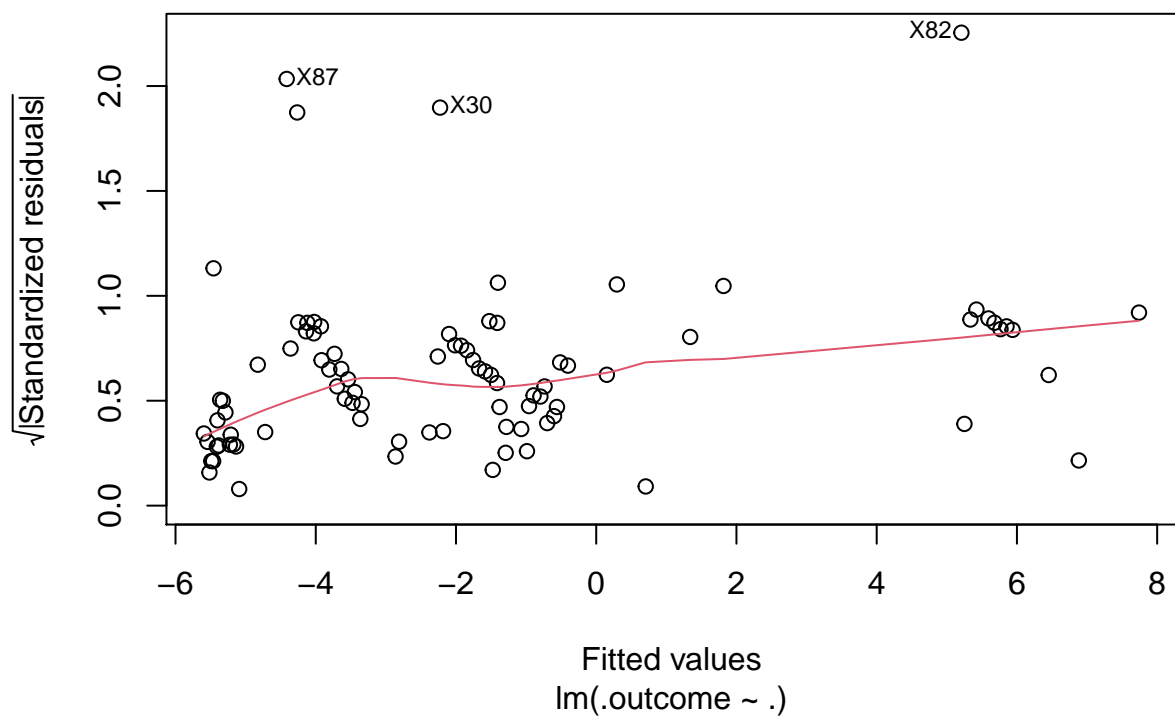
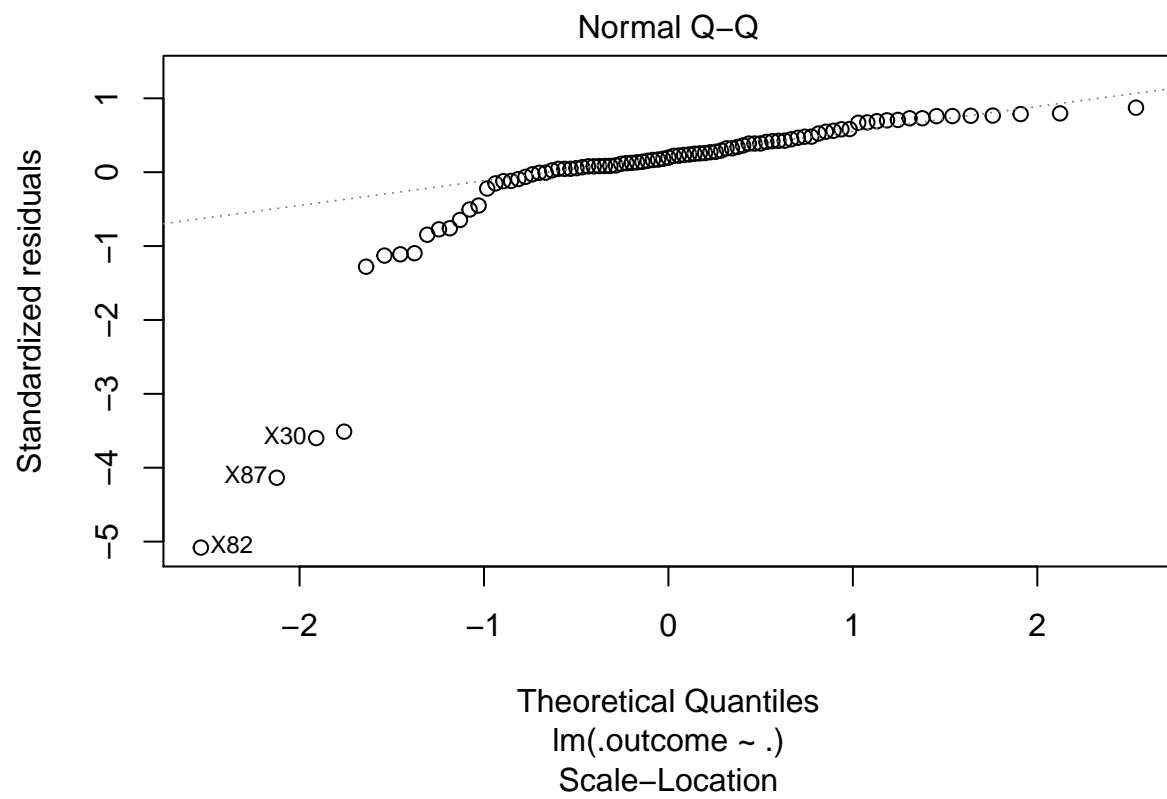
## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

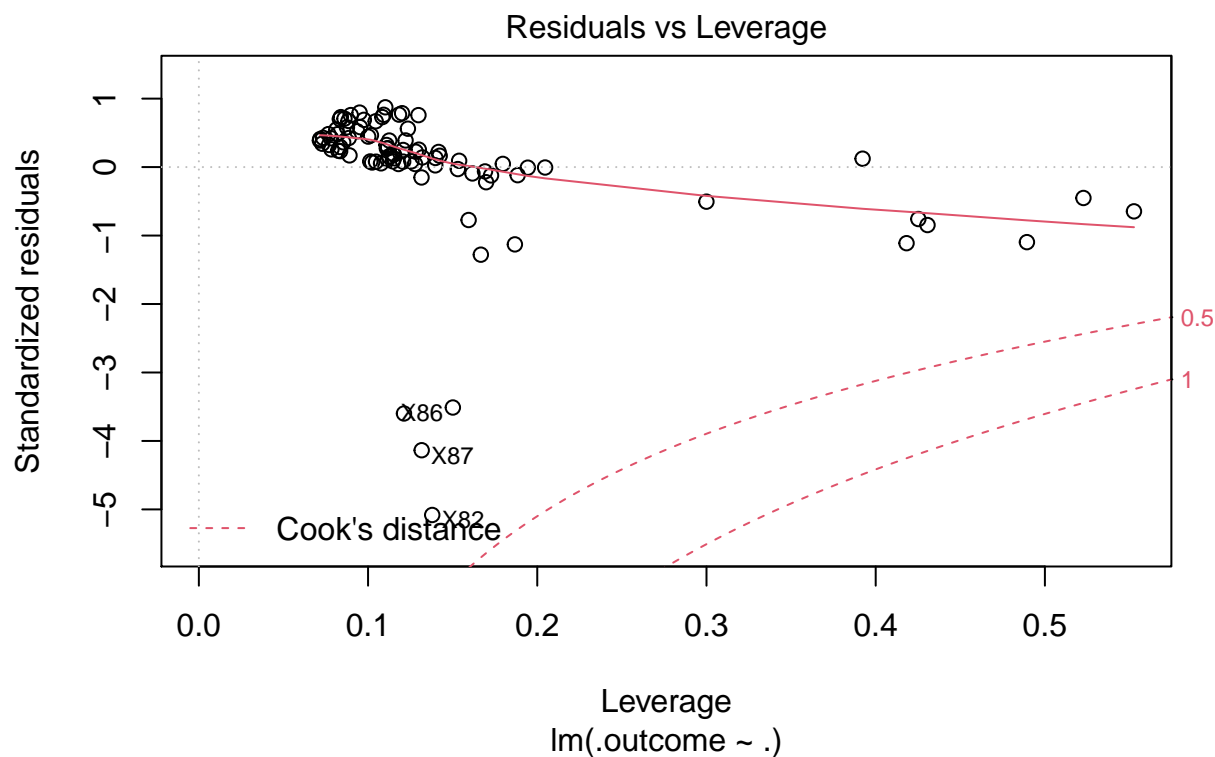
model_caret_2

## Linear Regression
##
## 89 samples
## 3 predictor
##
## No pre-processing
```

```
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 69, 72, 72, 71, 72
## Resampling results:
##
##   RMSE      Rsquared   MAE
##  1.236948  0.8834658  0.7745262
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
plot(model_caret_2$finalModel)
```







```
summary(model_caret_2$finalModel)
```

```
##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -5.8344 -0.0069  0.2296  0.5224  1.0188
##
## Coefficients: (1 not defined because of singularities)
##
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    5.164989   0.470307  10.982 < 2e-16 ***
## St              0.858695   0.344985   2.489  0.015 *
## Fr.logit0.574442516811659 -6.678147   0.700244  -9.537 1.26e-14 ***
## Fr.logit1      -6.737794   0.636727 -10.582 < 2e-16 ***
## Re224          -7.434512   0.590851 -12.583 < 2e-16 ***
## Re398         -10.787379   0.712633 -15.137 < 2e-16 ***
## `St:Fr.logit0.574442516811659`  0.250783   0.470653   0.533  0.596
## `St:Fr.logit1`    0.112392   0.394615   0.285  0.777
## `St:Re224`       -0.004091   0.383357  -0.011  0.992
## `St:Re398`       -0.593466   0.495640  -1.197  0.235
## `Fr.logit0.574442516811659:Re224`  4.477795   0.723295   6.191 2.81e-08 ***
## `Fr.logit1:Re224`  4.694433   0.732788   6.406 1.13e-08 ***
## `Fr.logit0.574442516811659:Re398`    NA         NA         NA      NA
## `Fr.logit1:Re398`  6.883436   0.801251   8.591 8.12e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.237 on 76 degrees of freedom
```

```
## Multiple R-squared:  0.9041, Adjusted R-squared:  0.889
## F-statistic: 59.73 on 12 and 76 DF,  p-value: < 2.2e-16
```

The model's coefficients are all negative except the St and Fr.logit:Re coefficients, which align with our prior beliefs. A larger particle size could increase the probability distribution for particle cluster volumes. Further, the coefficients of significance are St, Re and their interaction.

The R-squared value of 0.6883 shows the factors in the model successfully explain the most of the variance.

```
x <- model.matrix(R_moment_1~St + Fr.logit + Re,data=train)[-1]
y <- train$R_moment_1

set.seed(17)
train.samp <- sample(1:nrow(x), nrow(x)/2)
test.samp <- (-train.samp)
y.test <- y[test.samp]

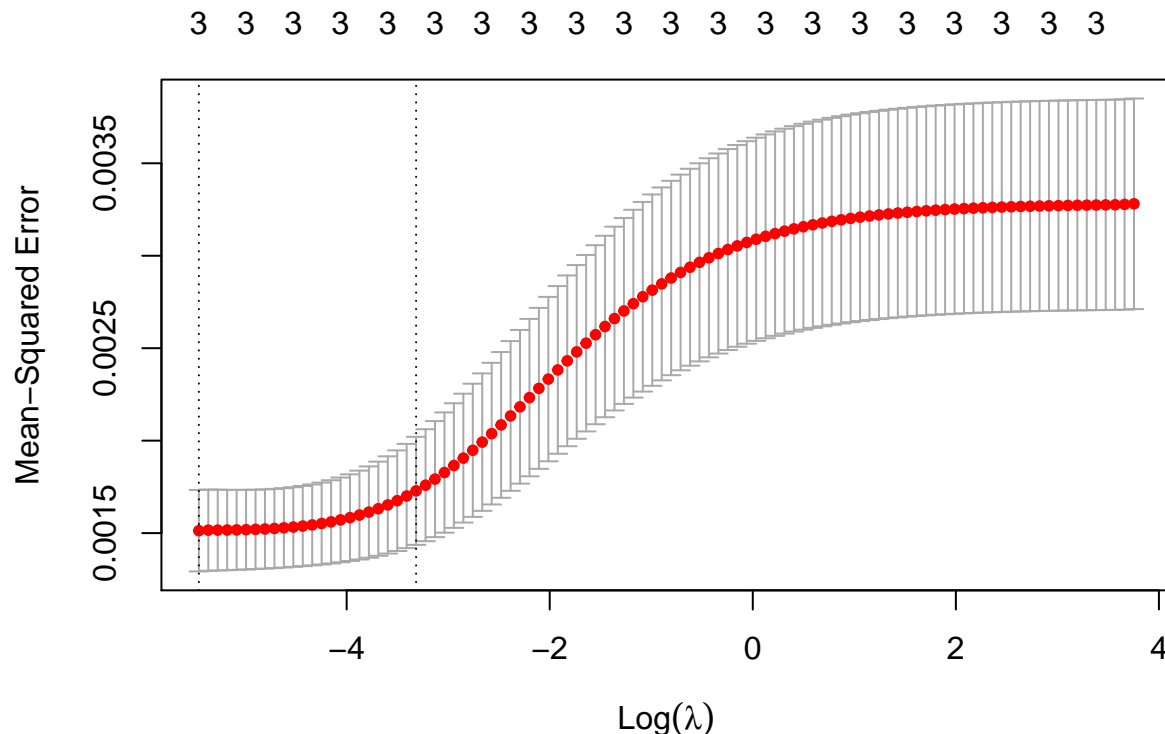
grid <- 10^seq(10, -2, length = 100) # grid of values for lambda param

ridge.mod <- glmnet(x[train.samp,], y[train.samp], alpha = 0, lambda = grid, thresh = 1e-12)
ridge.pred <- predict(ridge.mod, s=0, x = x[train.samp,], y = y[train.samp],
                      newx = x[test.samp,], exact = T)
mean((ridge.pred - y.test)^2) ## calculate MSE
```

Ridge Regression

```
## [1] 0.001078549
```

```
set.seed(1)
cv.out <- cv.glmnet(x[train.samp,], y[train.samp], alpha = 0)
plot(cv.out)
```




```
bestlam <- cv.out$lambda.min
bestlam
```

```
## [1] 0.004272015
```

```
ridge.pred <- predict(ridge.mod, s = bestlam, newx = x[test.samp,])
mean((ridge.pred - y.test)^2)
```

```
## [1] 0.001091239
```

MSE stays basically the same

```
x2 <- model.matrix(R_moment_2 ~ St + Fr.logit + Re + poly(St,2) + poly(Fr.logit,2) + poly(Re,2) + St:Re,
y2 <- train$R_moment_2
```

```
set.seed(17)
```

```
train2 <- sample(1:nrow(x2), 4 * nrow(x2)/5)
```

```
test2 <- (-train2)
```

```
y.test2 <- y2[test2]
```

```
grid <- 10^seq(10, -2, length = 100) # grid of values for lambda param
```

```
ridge.mod2 <- glmnet(x2[train2,], y2[train2], alpha = 0, lambda = grid, thresh = 1e-12)
```

```
ridge.pred2 <- predict(ridge.mod2, s=0, x = x2[train2,], y = y2[train2],
newx = x2[test2,], exact = T)
```

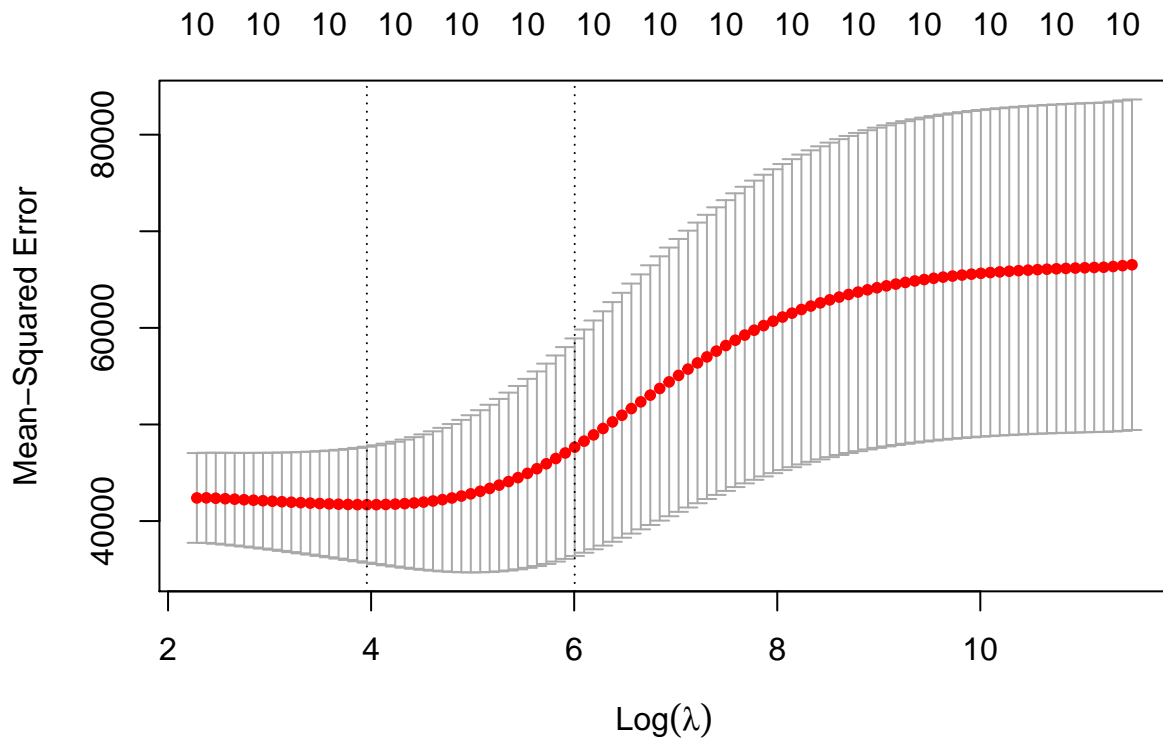
```
mean((ridge.pred2 - y.test2)^2) ## calculate MSE
```

```
## [1] 43396.09
```

```
set.seed(1)
```

```
cv.out2 <- cv.glmnet(x2[train2,], y2[train2], alpha = 0)
```

```
plot(cv.out2)
```



```

bestlam2 <- cv.out2$lambda.min
bestlam2

## [1] 52.36596

ridge.pred2 <- predict(ridge.mod2, s = bestlam2, newx = x2[test2,])
mean((ridge.pred2 - y.test2)^2)

## [1] 46196.89

x3 <- model.matrix(R_moment_3~St + Fr.logit + Re,data=train)[,-1]
y3 <- train$R_moment_3

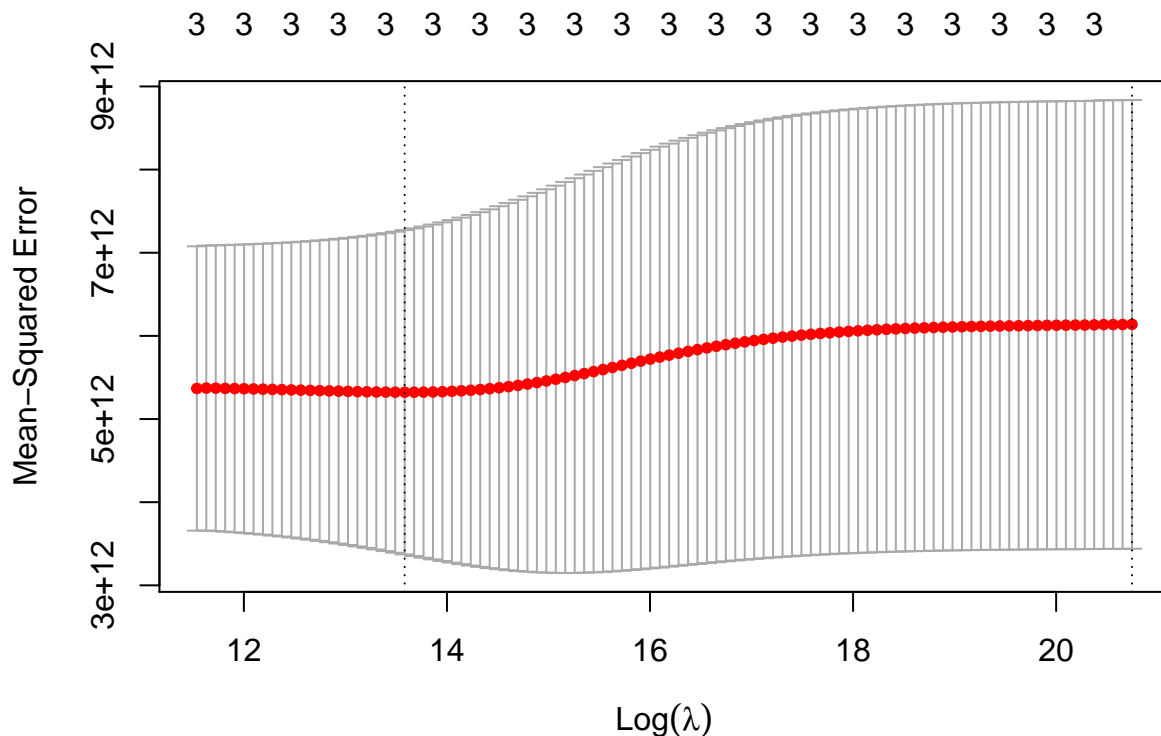
set.seed(17)
train3 <- sample(1:nrow(x3), nrow(x3)/2)
test3 <- (-train3)
y.test3 <- y3[test3]

ridge.mod3 <- glmnet(x3[train3,], y3[train3], alpha = 0, lambda = grid, thresh = 1e-12)
ridge.pred3 <- predict(ridge.mod3, s = 0, newx = x3[test3,])
mean((ridge.pred3 - y.test3)^2) ## calculate MSE

## [1] 3.166732e+12

set.seed(1)
cv.out3 <- cv.glmnet(x3[train3,], y3[train3], alpha = 0)
plot(cv.out3)

```



```

bestlam3 <- cv.out3$lambda.min
bestlam3

## [1] 792973.2

```

```

ridge.pred3 <- predict(ridge.mod3, s = bestlam3, newx = x3[test3,])
mean((ridge.pred3 - y.test3)^2)

## [1] 3.007604e+12

x4 <- model.matrix(R_moment_4~as.factor(St) + as.factor(Fr.logit) + as.factor(Re),data=train)[,-1]
y4 <- train$R_moment_4

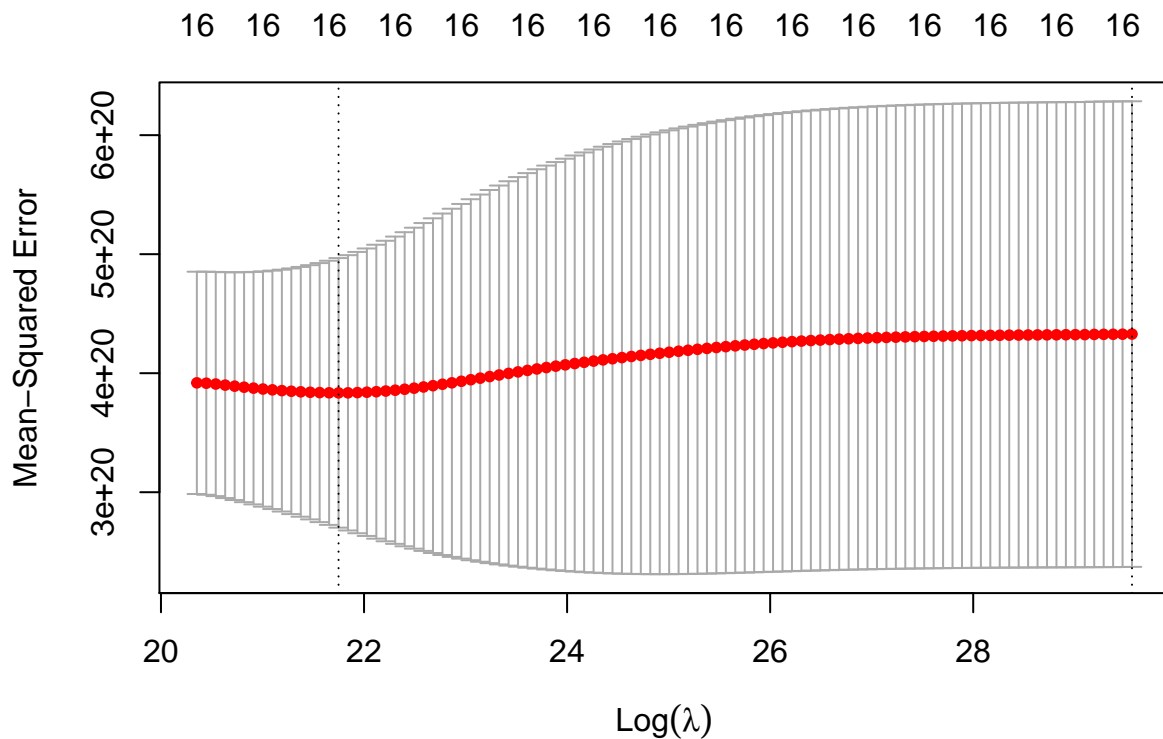
set.seed(17)
train4 <- sample(1:nrow(x4), nrow(x4)/2)
test4 <- (-train4)
y.test4 <- y[test4]

ridge.mod4 <- glmnet(x4[train4,], y4[train4], alpha = 0, lambda = grid, thresh = 1e-12)
ridge.pred4 <- predict(ridge.mod4, s = 0, newx = x4[test4,])
mean((ridge.pred4 - y.test4)^2) ## calculate MSE

## [1] 3.509278e+20

set.seed(1)
cv.out4 <- cv.glmnet(x4[train4,], y4[train4], alpha = 0)
plot(cv.out4)

```



```

bestlam4 <- cv.out4$lambda.min
bestlam4

## [1] 2789083228

ridge.pred4 <- predict(ridge.mod4, s = bestlam4, newx = x4[test4,])
mean((ridge.pred4 - y.test4)^2)

## [1] 2.039584e+20

```

improvement? still large

```
x <- model.matrix(R_moment_1~St + Fr.logit + Re,data=train)[,-1]

set.seed(17)
train.samp <- sample(1:nrow(train), 4 * nrow(train)/5)
test <- (-train.samp)
y.test <- train$R_moment_1[test]

gam1 <- lm(R_moment_1 ~ ns(St, 1) + ns(Re, 1) + ns(Fr.logit, 1), data = train, subset = train.samp)
preds <- predict(gam1, newdata = as.data.frame(x[test,]))
mean((preds - y.test)^2)
```

GAMS

```
## [1] 0.001226049
```

```
x <- model.matrix(R_moment_2 ~ St + Fr.logit + Re,data=train)[,-1]

set.seed(17)
train.samp <- sample(1:nrow(train), 4 * nrow(train)/5)
test <- (-train.samp)
y.test <- train$R_moment_2[test]

gam2 <- lm(R_moment_2 ~ ns(St, 2) + ns(Re, 2) + ns(Fr.logit, 2), data = train, subset = train.samp)
preds <- predict(gam2, newdata = as.data.frame(x[test,]))
mean((preds - y.test)^2)
```

```
## [1] 48573.71
```

```
set.seed(17)
train.samp <- sample(1:nrow(train), 4 * nrow(train)/5)
test <- (-train.samp)
y.test <- train$R_moment_4[test]

gam4 <- lm(R_moment_4 ~ ns(St, 2) + ns(Re, 2) + ns(Fr.logit, 2), data = train, subset = train.samp)
preds <- predict(gam4, newdata = as.data.frame(train[test,]))
mean((preds - y.test)^2)
```

Fourth moment

```
## [1] 2.819773e+20
```

```
lm4_m1_int <- lm(R_moment_4 ~ St + Fr.logit + Re + St*Fr.logit + St*Re + Fr.logit*Re, data=train1)
```

```
set.seed(1)
```

```
data_ctrl <- trainControl(method = "cv", number = 5)
model_caret <- train(log(R_moment_3) ~ St + Fr.logit + Re + St*Fr.logit + St*Re + Fr.logit*Re, data=train,
                     trControl = data_ctrl,                # folds
                     method = "lm",                        # specifying regression model
                     na.action = na.pass)
```

```
## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
```

```

## may be misleading

## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

## Warning in predict.lm(modelFit, newdata): prediction from a rank-deficient fit
## may be misleading

model_caret

## Linear Regression
##
## 89 samples
## 3 predictor
##
## No pre-processing
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 71, 72, 71, 70, 72
## Resampling results:
##
##   RMSE      Rsquared   MAE
##  2.133444  0.8595854  1.201479
##
## Tuning parameter 'intercept' was held constant at a value of TRUE

# plot(model_caret$finalModel)
# summary(model_caret$finalModel)

```