Cryoocyte Test Project

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Import Libraries

```
library(ggplot2)   # data visualization
library(tidyverse) # a set of module for data manipulation
library(leaps)
library(gridExtra)
```

Import Data

```
my_data = read_csv('data/train.csv')
my_test_data = read_csv('data/test.csv')
```

Linear Model selection

The data is being randomly split into training and testing sets in the 70/30 ratio. The forward selection method is implemented to determine the best final model. In the intial round of machine learning analysis, the full (with all 100 variables included) linear model has an R2 score up to **0.999**. In this section, I aim to find a simpler liner model which has an R2 score larger than **0.995** but use less features.

Forward selection

```
n = 20 # 20x cross valiation: train/test = 70/30

#-------first run-------
index = sample(1:nrow(my_data), size = round(0.7*nrow(my_data)))
train = my_data[index, ]
test = my_data[-index, ]
regfit.fwd = regsubsets(y~., data = train, nvmax = 1000, method = "forward")
regfit.fwd.summary = summary(regfit.fwd)

# save train and test errors
best_num_of_variables = head(which(regfit.fwd.summary$adjr2 > 0.995), 1)
best_variables = paste0(names(coef(regfit.fwd, best_num_of_variables))[-1], collapse=',')
best_models = data.frame(best_num_of_variables, best_variables, stringsAsFactors = FALSE)
selected_columns = c(names(coef(regfit.fwd, best_num_of_variables)[-1]), 'y')
lm.fit = lm(y~., data = train[selected_columns])
train_pred = predict(lm.fit, newdata = train[selected_columns])
test_pred = predict(lm.fit, newdata = test[selected_columns])
train_error = (train$y - train_pred)^2
test_error = (test$y - test_pred)^2
errors_df = data.frame(run_01=c(train_error, test_error))
```

```r
# save performance metrics
RSS_df = data.frame(run_01 = regfit.fwd.summary$rss)
RSq_df = data.frame(run_01 = regfit.fwd.summary$adjr2)
Cp_df = data.frame(run_01 = regfit.fwd.summary$cp)
BIC_df = data.frame(run_01 = regfit.fwd.summary$bic)

#-------second to n runs------
for (i in 2:n) {
  index = sample(1:nrow(my_data), size = round(0.7*nrow(my_data)))
  train = my_data[index, ]
  test = my_data[-index, ]
  regfit.fwd = regsubsets(y~., data = train, nvmax = 1000, method = "forward")
  regfit.fwd.summary = summary(regfit.fwd)
  if (i < 10) {
    col_name = paste0('run_0', i)
  } else {
    col_name = paste0('run_', i)
  }

  # save train and test errors
  best_num_of_variables = head(which(regfit.fwd.summary$adjr2 > 0.995), 1)
  best_variables = paste0(names(coef(regfit.fwd, best_num_of_variables))[-1], collapse=',')
  best_models[i, ] = c(best_num_of_variables, best_variables)
  selected_columns = c(names(coef(regfit.fwd, best_num_of_variables)[-1]), 'y')
  lm.fit = lm(y~., data = train[selected_columns])
  train_pred = predict(lm.fit, newdata = train[selected_columns])
  test_pred = predict(lm.fit, newdata = test[selected_columns])
  train_error = (train$y - train_pred)^2
  test_error = (test$y - test_pred)^2
  errors_df[col_name] = data.frame(run_1=c(train_error, test_error))

  # save performance metrics
  RSS_df[col_name] = regfit.fwd.summary$rss
  RSq_df[col_name] = regfit.fwd.summary$adjr2
  Cp_df[col_name] = regfit.fwd.summary$cp
  BIC_df[col_name] = regfit.fwd.summary$bic
}
```

Determine which variables should be kept in the final linear model

After randomly spliting the data and implementing the forward selection 20 times, we can determine what's the best number of variables to keep and which variables they are if we want to have an R2 score up to 0.995.

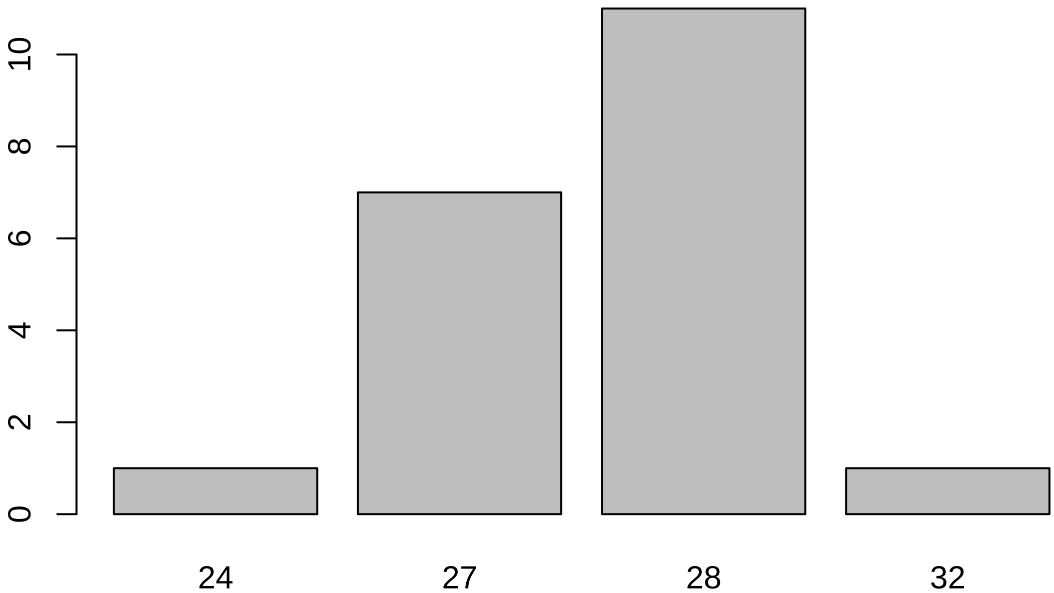
The best of number of features to keep

```r
# frequency of best number of variables
table(best_models$best_num_of_variables)
```

```
##
## 24 27 28 32
```

```
## 1  7 11  1
```

```r
barplot(table(best_models$best_num_of_variables))
```



The most important features

```r
# most important variables
highest_best_num = as.integer(names(which.max(table(best_models$best_num_of_variables))))
most_important_features = sort(table(strsplit(paste0(best_models$best_variables, collapse=','), ',')[[1
     decreasing = TRUE)[1:highest_best_num]
most_important_features
```

```
##
##  x1 x15 x19  x2 x25 x29 x31 x42  x5 x59 x62 x72 x74 x76 x84 x87 x98 x99
##  20  20  20  20  20  20  20  20  20  20  20  20  20  20  20  20  20  20
##  x7 x53 x55 x69 x28  x3 x14 x78 x79 x80
##  17  16  14  14  13  13  12  12  11  11
```

The relationship between the number of variables and the metrics of model performance

```r
# RSS
gather_RSS_df = gather(RSS_df)
gather_RSS_df['x'] = rep(1:nrow(RSS_df), n)
p1 = ggplot(data = gather_RSS_df, aes(x=x, y=value, color=key)) +
  geom_line() +
  geom_vline(xintercept = highest_best_num) +
  xlab("Number of Variables") +
  ylab("RSS") +
  theme(legend.position="none")
```

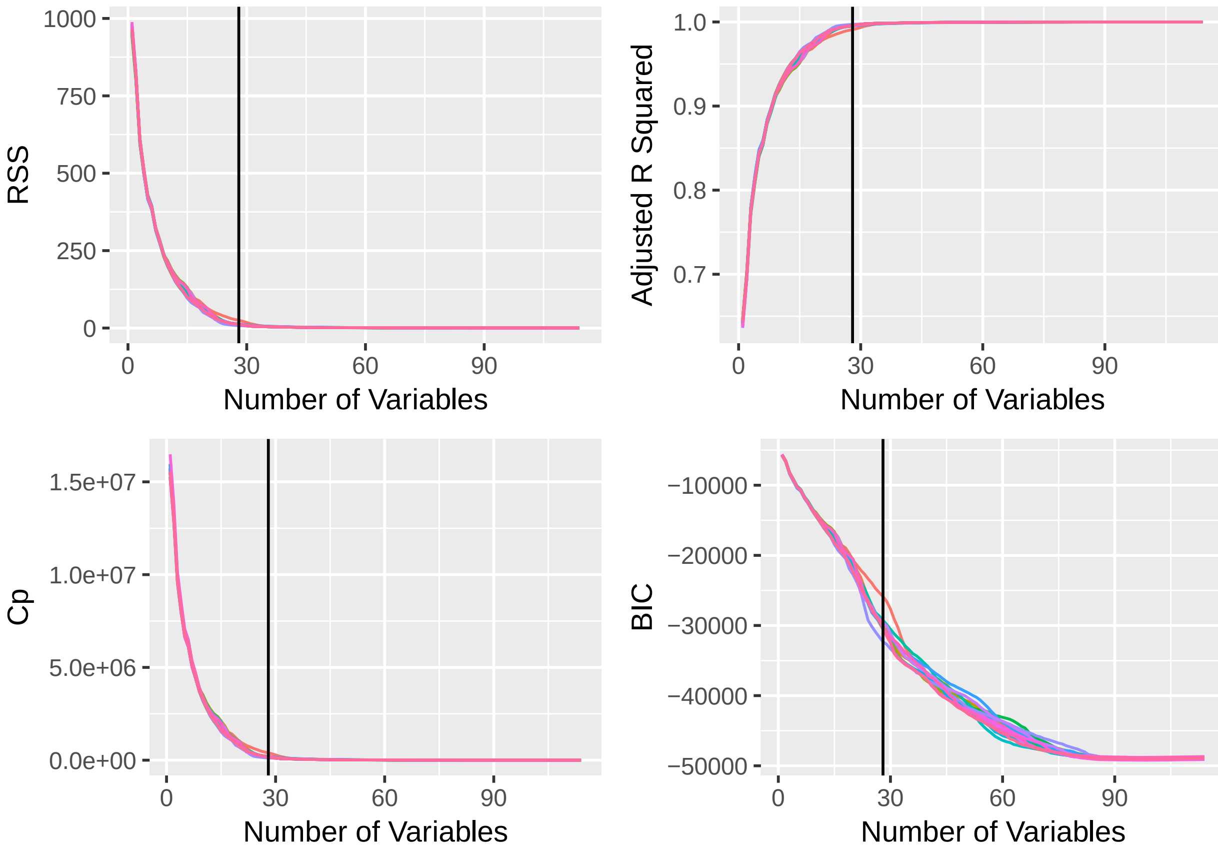
```r
# RSq
gather_RSq_df = gather(RSq_df)
gather_RSq_df['x'] = rep(1:nrow(RSq_df), n)
p2 = ggplot(data = gather_RSq_df, aes(x=x, y=value, color=key)) +
  geom_line() +
  geom_vline(xintercept = highest_best_num) +
  xlab("Number of Variables") +
  ylab("Adjusted R Squared") +
  theme(legend.position="none")

# grid.arrange(p1, p2, ncol=2)

# Cp
gather_Cp_df = gather(Cp_df)
gather_Cp_df['x'] = rep(1:nrow(Cp_df), n)
p3 = ggplot(data = gather_Cp_df, aes(x=x, y=value, color=key)) +
  geom_line() +
  geom_vline(xintercept = highest_best_num) +
  xlab("Number of Variables") +
  ylab("Cp") +
  theme(legend.position="none")

# BIC
gather_BIC_df = gather(BIC_df)
gather_BIC_df['x'] = rep(1:nrow(BIC_df), n)
p4 = ggplot(data = gather_BIC_df, aes(x=x, y=value, color=key)) +
  geom_line() +
  geom_vline(xintercept = highest_best_num) +
  xlab("Number of Variables") +
  ylab("BIC") +
  theme(legend.position="none")

grid.arrange(p1, p2, p3, p4, nrow=2, ncol=2)
```

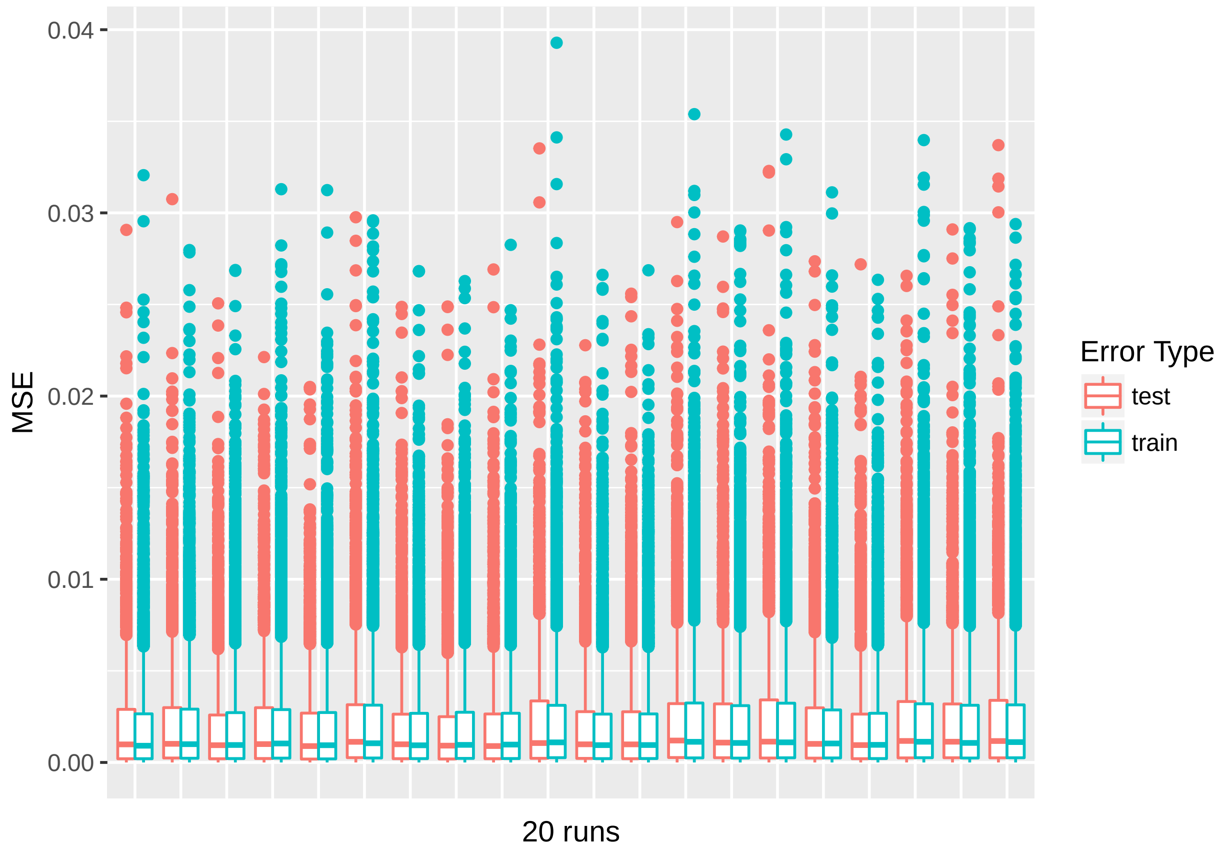


Training vs. Test errors

The plot below shows that the training and test errors are very low and pretty close to each other across all 20 runs, which means that model fits both the training and test data sets well.

```r
# Erros DataFrame
errors_df$error_type = c(rep('train', nrow(train)), rep('test', nrow(test)))
gather_errors_df = gather(errors_df, key = "key", value = "value",
                          setdiff(names(errors_df), 'error_type'))

ggplot(data = gather_errors_df, aes(x = key, y = value, color=error_type)) +
  geom_boxplot() +
  xlab(paste0(n, ' runs')) +
  ylab('MSE') +
  scale_color_discrete(name = "Error Type") +
  theme(axis.text.x=element_blank(),
        axis.ticks.x=element_blank())
```



Final Linear Model

```
final_lm = lm(y~., my_data[c(names(most_important_features), 'y')])
# remove non significant terms
update_final_lm = update(final_lm, . ~ . -1)
final_lm_summary = summary(update_final_lm)
final_lm_summary
```

```
##
## Call:
## lm(formula = y ~ x1 + x15 + x19 + x2 + x25 + x29 + x31 + x42 +
##     x5 + x59 + x62 + x72 + x74 + x76 + x84 + x87 + x98 + x99 +
##     x7 + x53 + x55 + x69 + x28 + x3 + x14 + x78 + x79 + x80 -
##     1, data = my_data[c(names(most_important_features), "y")])
##
## Residuals:
##       Min        1Q    Median        3Q       Max
## -0.163727 -0.030440 -0.000535  0.031158  0.153906
##
## Coefficients:
##     Estimate Std. Error t value Pr(>|t|)
## x1   60.4968     0.4121  146.78   <2e-16 ***
## x15  15.9961     0.4926   32.47   <2e-16 ***
## x19 108.4670     0.6177  175.60   <2e-16 ***
## x2   93.0995     0.5141  181.08   <2e-16 ***
```

```
## x25  49.2793     0.5781   85.25   <2e-16 ***
## x29 122.7685     0.7440  165.00   <2e-16 ***
## x31  68.2603     0.6282  108.66   <2e-16 ***
## x42  95.4224     0.6816  139.99   <2e-16 ***
## x5   91.1176     0.6440  141.50   <2e-16 ***
## x59  68.9285     0.5926  116.32   <2e-16 ***
## x62  11.9256     0.5778   20.64   <2e-16 ***
## x72  84.4303     0.6670  126.59   <2e-16 ***
## x74  77.5597     0.5447  142.39   <2e-16 ***
## x76  39.7352     0.8160   48.69   <2e-16 ***
## x84  69.4174     0.6315  109.93   <2e-16 ***
## x87  45.4966     0.6790   67.00   <2e-16 ***
## x98  94.4588     0.9910   95.31   <2e-16 ***
## x99  50.1494     0.7275   68.94   <2e-16 ***
## x7   22.0609     0.5439   40.56   <2e-16 ***
## x53  18.7576     0.4198   44.68   <2e-16 ***
## x55 -27.7065     0.6633  -41.77   <2e-16 ***
## x69 -31.9632     0.4915  -65.03   <2e-16 ***
## x28  76.8208     0.6607  116.27   <2e-16 ***
## x3   25.7173     0.6238   41.23   <2e-16 ***
## x14  28.8451     0.5550   51.98   <2e-16 ***
## x78  27.0942     0.6231   43.48   <2e-16 ***
## x79  45.1815     0.7092   63.71   <2e-16 ***
## x80  21.9096     0.5603   39.10   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.04514 on 7949 degrees of freedom
##   (23 observations deleted due to missingness)
## Multiple R-squared:  0.9958, Adjusted R-squared:  0.9958
## F-statistic: 6.802e+04 on 28 and 7949 DF,  p-value: < 2.2e-16
```

The final linear model includes 28 features: x1, x15, x19, x2, x25, x29, x31, x42, x5, x59, x62, x72, x74, x76, x84, x87, x98, x99, x7, x53, x55, x69, x28, x3, x14, x78, x79, x80.