Introduction to Machine Learning

Lab 2

Rasmus Holm

2016-11-11

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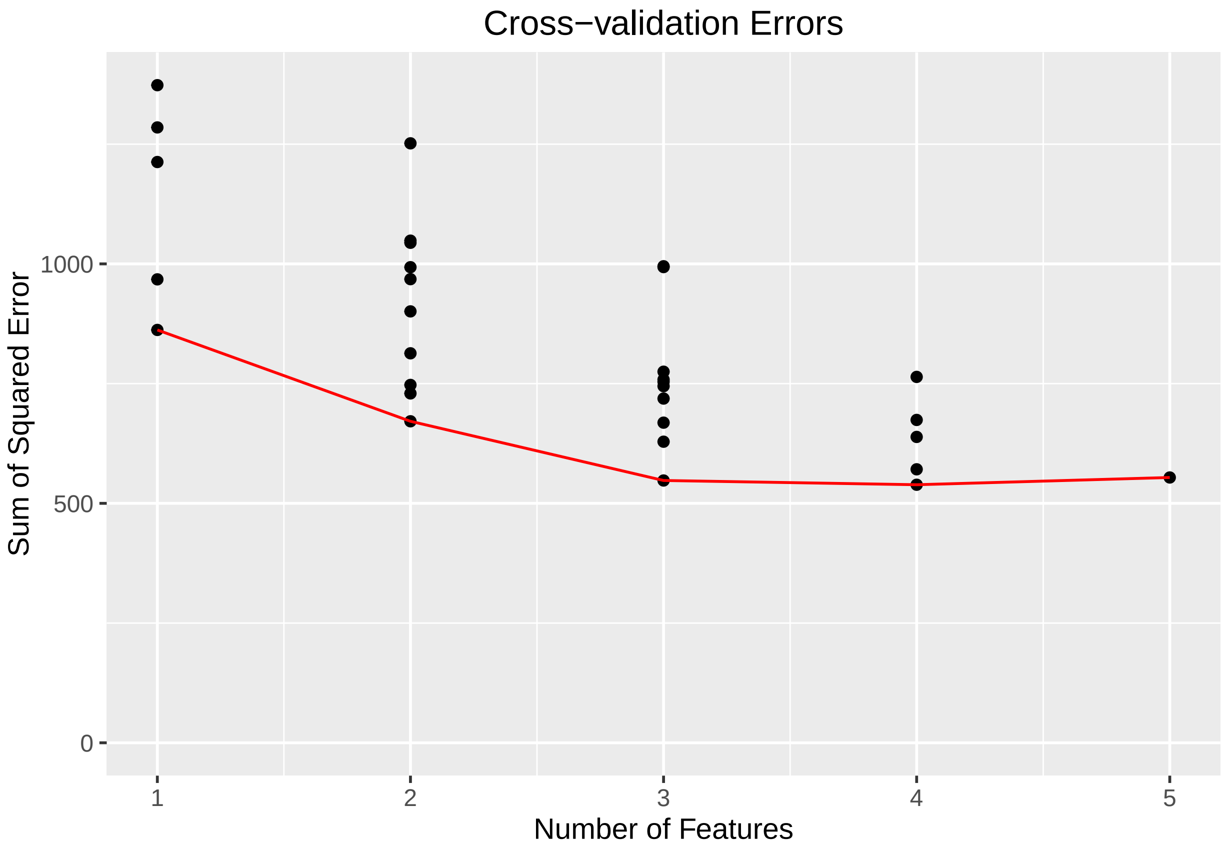
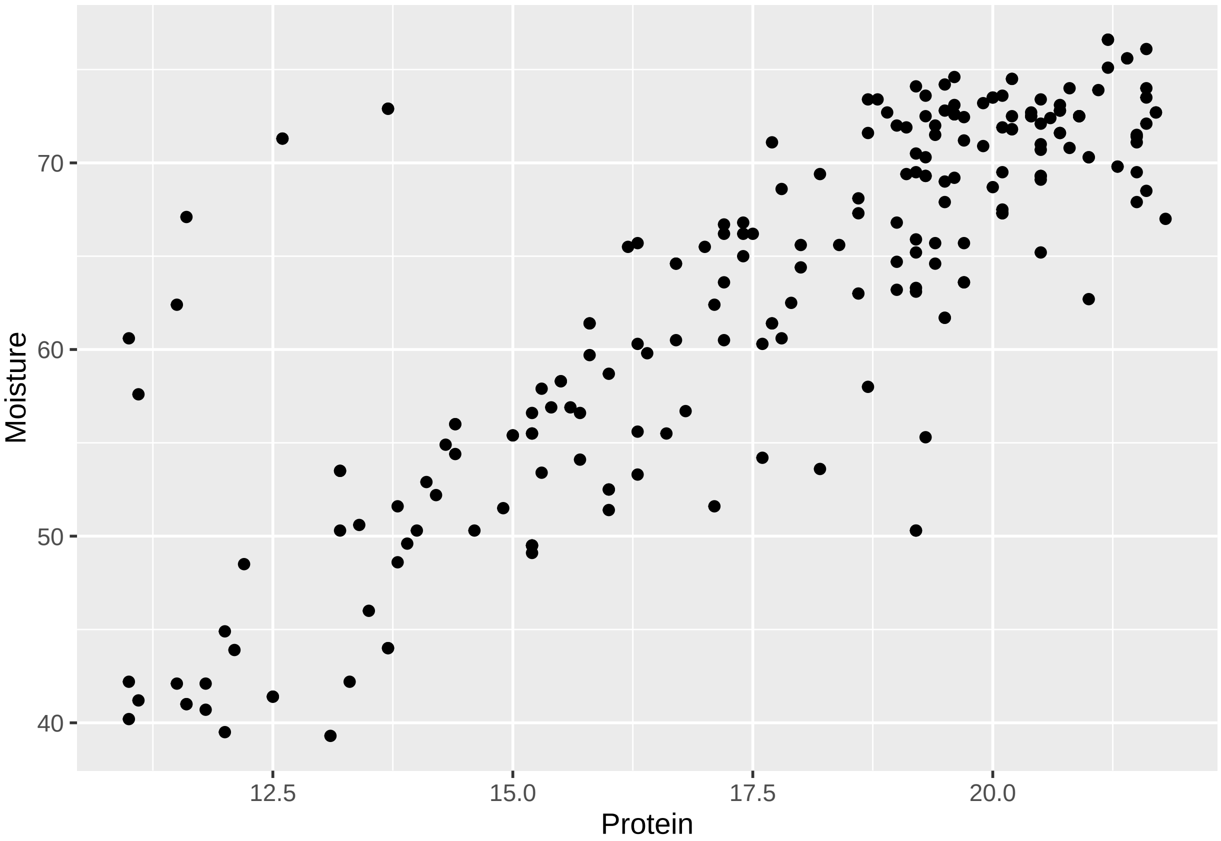


Assignment 2

1

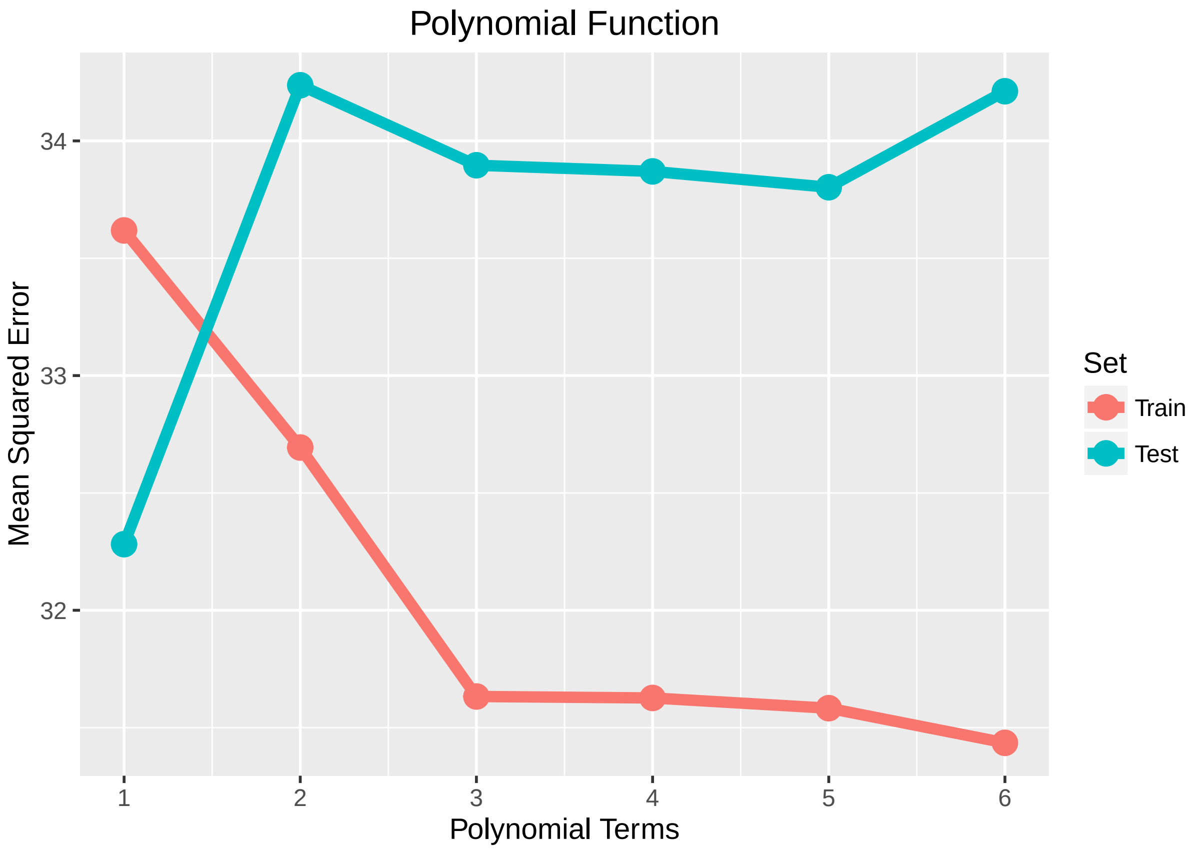


2

$$\mathrm{E}[y(x,w)] = \sum_{i=0}^{p} w_i \phi_i(x) + \epsilon_i$$

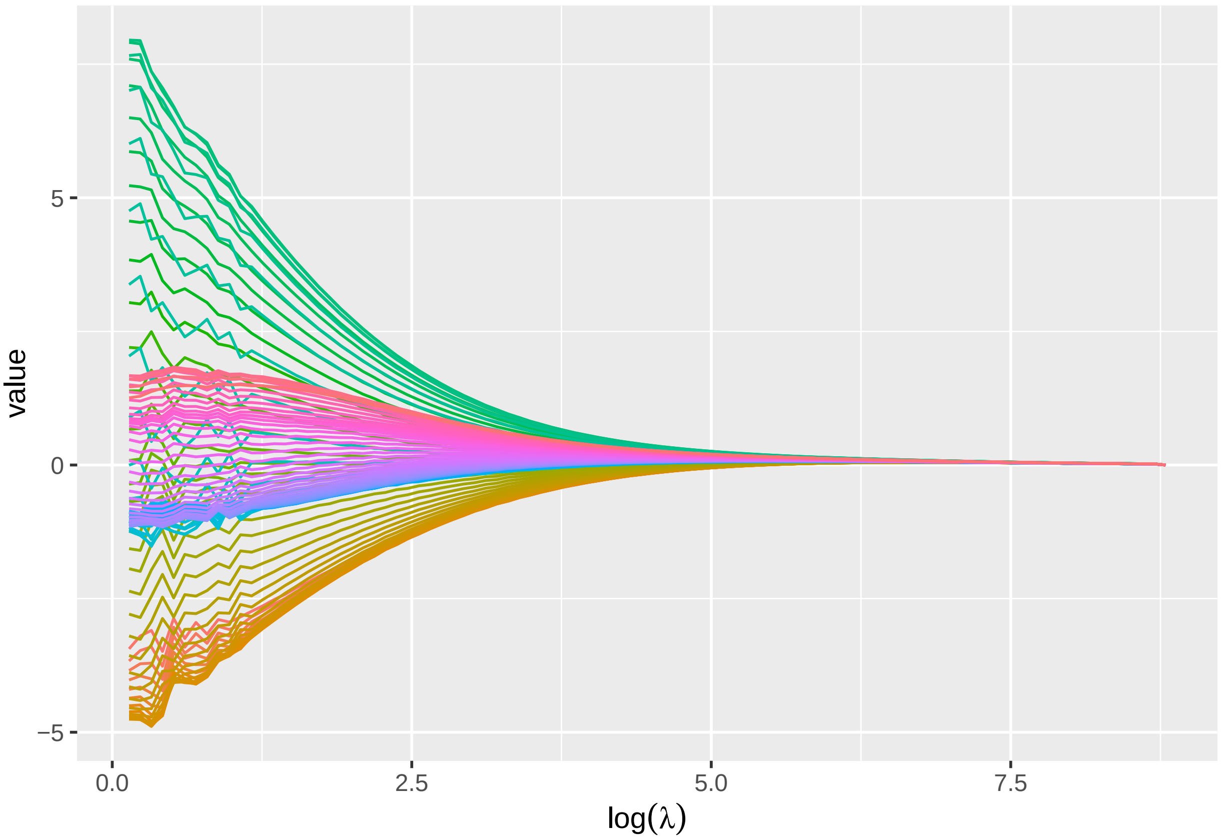
where $\phi_i(x) = x^i$. SEE Pattern Recognition 3.1.1

3

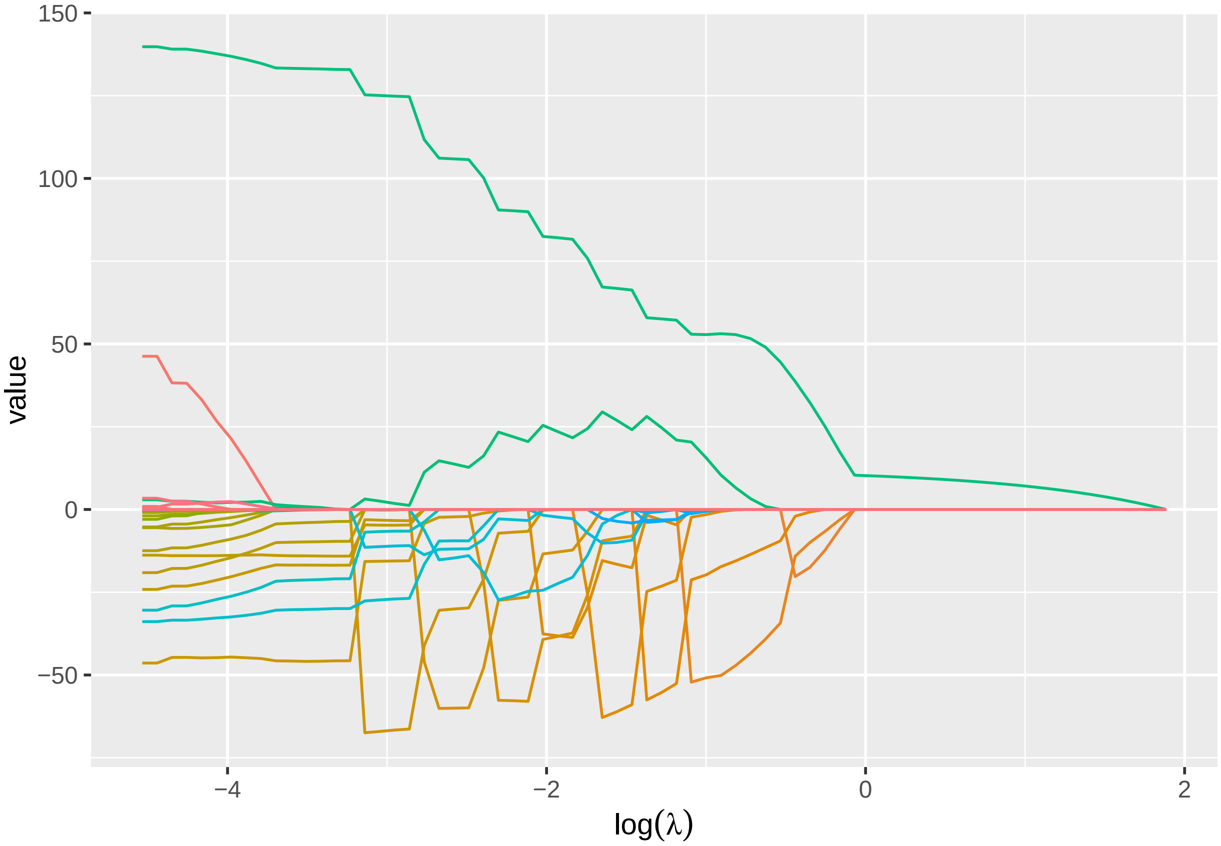

Polynomial Function
Mean Squared Error
34
33
32
1
2
3
4
5
6
Polynomial Terms
Set
Train
Test

4

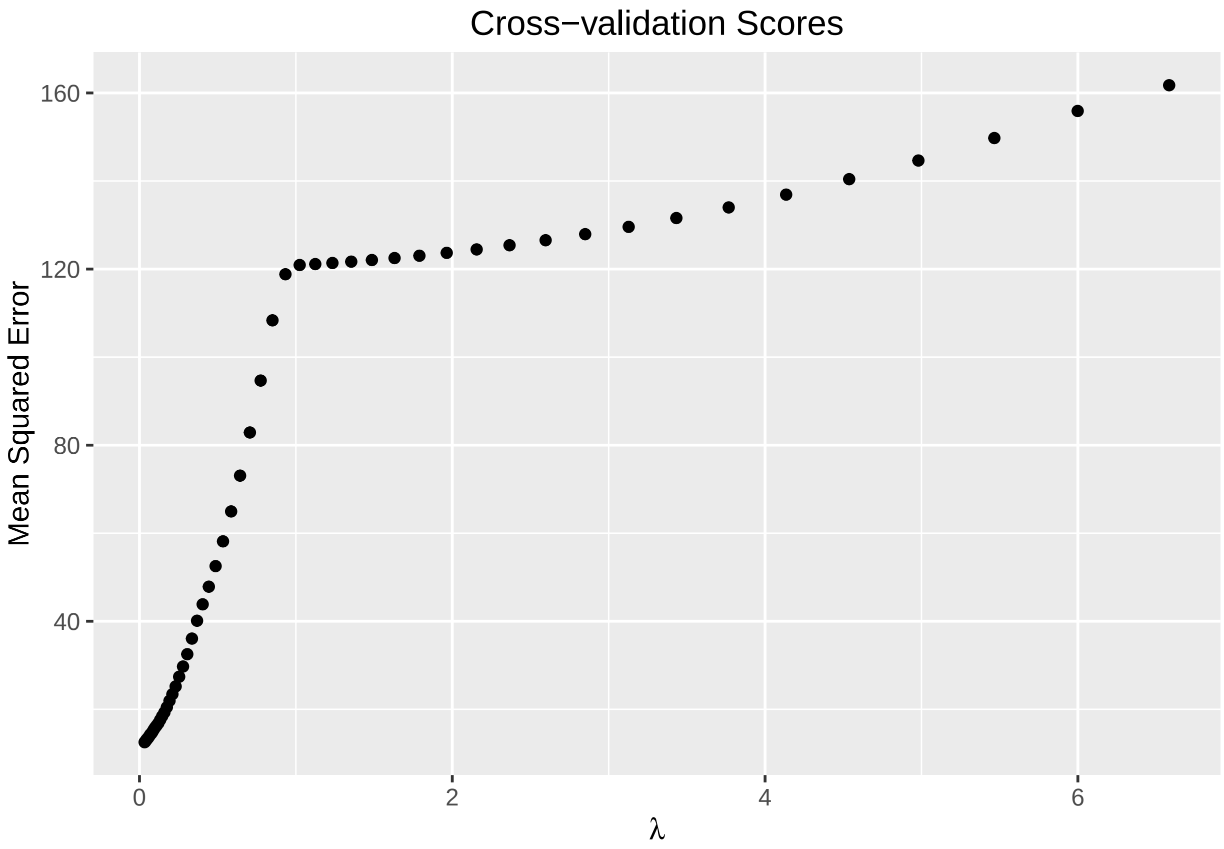
5



6



7


Cross−validation Scores
Mean Squared Error
160
120
80
40
0
2
4
6
λ

8

Appendix

Code for Assignment 1

```
library(ggplot2)

best_subset_selection <- function(X, y, folds) {
    n <- nrow(X)
    p <- ncol(X)

    stopifnot(folds <= n)

    sampled_idx <- sample(1:n, n)
    sets <- cross_validation_sets(n, folds)

    X <- X[sampled_idx,]
    y <- y[sampled_idx]

    best_features <- list()
    cv_scores <- rep(list(c()), p)

    for (j in 1:p) {
        feature_combinations <- combinations(p, j)
        errors <- c()
        for (feature_idx in 1:nrow(feature_combinations)) {
            features <- feature_combinations[feature_idx, ] == 1
            current_errors <- c()
            for (i in 1:folds) {
                test_validation_idx <- sets[i, 1]:sets[i, 2]
                test_idx <- test_validation_idx
                training_idx <- (1:n)[-test_validation_idx]

                lmfit <- linear_regression(as.matrix(X[training_idx, features]),
                                           y[training_idx],
                                           as.matrix(X[test_idx, features]),
                                           y[test_idx])
                current_errors <- c(current_errors, lmfit$SSE)
            }
            errors <- c(errors, mean(current_errors))
            cv_scores[[j]] <- c(cv_scores[[j]], mean(current_errors))
        }
        best_features[[j]] <- list(features=feature_combinations[which.min(errors),],
                                   SSE=min(errors))
    }

    list(bf=best_features, cvs=cv_scores)
}

cross_validation_sets <- function(n, folds) {
    set_size <- as.integer(n / folds)
    remaining <- n - folds * set_size

    idx <- matrix(0, nrow=folds, ncol=2)
    idx[1, 1] <- 1
    idx[1, 2] <- set_size

    for (i in 2:folds) {
        idx[i, 1] <- idx[i - 1, 2] + 1
        idx[i, 2] <- idx[i, 1] + (set_size - 1)

        if (remaining > 0) {
            idx[i, 2] <- idx[i, 2] + 1
            remaining <- remaining - 1
        }
    }

    idx
}

linear_regression <- function(X_train, y_train, X_test, y_test) {
    X_train <- cbind(rep(1, nrow(X_train)), X_train)
    X_test <- cbind(rep(1, nrow(X_test)), X_test)

    coefficients <- solve(t(X_train) %*% X_train) %*% t(X_train) %*% y_train
    coefficients <- as.vector(coefficients)
    fitted_values <- X_test %*% coefficients
    SSE <- sum((y_test - fitted_values)^2)
    list(coefficients=coefficients, fitted_values=fitted_values, SSE=SSE)
}

combinations <- function(n, m) {
    t(apply(combn(1:n, m=m), 2, function(x) replace(rep(0, n), x, 1)))
}

data <- swiss
x <- data[, -1]
y <- data[, 1]
folds <- 5
set.seed(12345)
result <- best_subset_selection(x, y, folds)
best_features <- result$bf
cv_scores <- result$cvs

best_setting <- best_features[[which.min(sapply(best_features, function(x) x$SSE))]]

lmfit <- linear_regression(as.matrix(x[, best_setting$features == 1]), y,
                           as.matrix(x[, best_setting$features == 1]), y)
## lmfit$coefficients
## colnames(x)[best_setting$features == 1]
coordinates <- lapply(1:length(cv_scores), function(feature_count) {
    cbind(x=feature_count, y=cv_scores[[feature_count]])
})
plot_data <- as.data.frame(do.call(rbind, coordinates))

best_coordinates <- lapply(1:length(cv_scores), function(feature_count) {
    cbind(x=feature_count, y=min(cv_scores[[feature_count]]))
})
plot_line <- as.data.frame(do.call(rbind, best_coordinates))

ggplot(plot_data) +
    ggtitle("Cross-validation Errors") +
    xlab("Number of Features") +
    ylab("Sum of Squared Error") +
    geom_point(aes(x=x, y=y)) +
    geom_line(data=plot_line, aes(x=x, y=y), color="red") +
    theme(plot.title = element_text(hjust=0.5)) +
    scale_y_continuous(limits=c(0, max(plot_data$y)))
```

Code for Assignment 2

```
library(MASS)
library(glmnet)
library(readxl)
library(ggplot2)
library(Matrix)
library(reshape2)

data <- read_excel("../data/tecator.xlsx")
ggplot(data) +
    geom_point(aes(x=Protein, y=Moisture))
set.seed(12345)
n <- nrow(data)
training_idx <- sample(1:n, size=floor(n * 0.5))

train <- data[training_idx,]
test <- data[-training_idx,]

power <- 6

train_mse <- rep(0, power)
test_mse <- rep(0, power)

for (i in 1:power) {
    model <- lm(Moisture ~ poly(Protein, i), data=train)

    train_mse[i] <- mean((train$Moisture - predict(model, train))^2)
    test_mse[i] <- mean((test$Moisture - predict(model, test))^2)
}

plot_data <- data.frame(x=1:power, Train=train_mse, Test=test_mse)
plot_data <- melt(plot_data, id="x", variable.name="Set")

ggplot(plot_data) +
    geom_line(aes(x=x, y=value, color=Set), lwd=2) +
    geom_point(aes(x=x, y=value, color=Set), size=4) +
    ggtitle("Polynomial Function") +
    xlab("Polynomial Terms") + ylab("Mean Squared Error") +
    scale_x_continuous(breaks=1:power)
```

```r
linear_model <- lm(Fat ~ . - Protein - Moisture - Sample, data=data)
aic <- stepAIC(linear_model, direction="both", trace=FALSE)
feature_selection_count <- length(aic$coefficients) - 1
response <- as.matrix(data[, setdiff(names(data), c("Sample", "Protein", "Moisture", "Fat"))])
target <- data[, "Fat"]

## Ridge Regression
ridge_model <- glmnet(x=response, y=target, alpha=0, nlambda=100)
coefficients <- coef(ridge_model)
coefficients <- as.matrix(coefficients[-1,])
colnames(coefficients) <- ridge_model$lambda

plot_data <- melt(coefficients, id=rownames, varnames=c("feature", "lambda"))

ggplot(plot_data, aes(x=log(lambda), y=value, colour=feature)) +
    geom_line(show.legend=FALSE) +
    xlab(expression(log(lambda)))
## Lasso Regression
lasso_model <- glmnet(x=response, y=target, alpha=1, nlambda=100)
coefficients <- coef(lasso_model)
colnames(coefficients) <- lasso_model$lambda
coefficients <- as.matrix(coefficients[-1,])

plot_data <- melt(coefficients, id=rownames, varnames=c("feature", "lambda"))

ggplot(plot_data, aes(x=log(lambda), y=value, colour=feature)) +
    geom_line(show.legend=FALSE) +
    xlab(expression(log(lambda)))
lasso_model_cv <- cv.glmnet(response, target, alpha=1, keep=TRUE)
optimal_lambda <- lasso_model_cv$lambda.min
feature_selection_count <- sum(as.matrix(coef(lasso_model_cv)) != 0) - 1

plot_data <- data.frame(x=lasso_model_cv$lambda, y=lasso_model_cv$cvm)

ggplot(plot_data, aes(x=x, y=y)) + geom_point() +
    ggtitle("Cross-validation Scores") +
    xlab(expression(lambda)) +
    ylab("Mean Squared Error")
```