

Exercises week 36

Python library import

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split

def design_poly_n(x, n):
    X = np.zeros((len(x), n))
    X[:,0] = 1
    for i in range(1, n):
        X[:,i] = (x**i).T
    return X
```

R library import

```
library(tidyverse)
library(reticulate)
```

We start by generating data using the same code as last week.

```
np.random.seed(8392)
n = 100
# Make data set.
x = np.linspace(-3, 3, n).reshape(-1, 1)
y = np.exp(-x**2) + 1.5 * np.exp(-(x-2)**2) + np.random.normal(0, 0.1, x.shape)

X = design_poly_n(x, 5)
np.random.seed(524)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2)
```

Then we scale input data by subtracting the mean of each column.

```

X_colmeans = np.mean(X_train, 0)[1:]

# without intercept
X_train_scaled = X_train[:, 1:] - X_colmeans
X_test_scaled = X_test[:, 1:] - X_colmeans
y_scaler = np.mean(y_train)
y_train_scaled = y_train - y_scaler

```

First we fit with ordinary least squares

```

Bhat = np.linalg.inv(X_train_scaled.T @ X_train_scaled) @ X_train_scaled.T @ y_train_scaled

print("Beta:", Bhat.T)

```

Beta: [[0.44343093 -0.00864978 -0.0346039 -0.00467165]]

```

ytilde_train = X_train_scaled @ Bhat + y_scaler
intercept = y_scaler - X_colmeans @ Bhat

MSE_OLS_train = sum((y_train - ytilde_train)**2) / len(y_train)
print("training data MSE:", MSE_OLS_train)

```

training data MSE: [0.03319703]

```

ytilde_test = X_test_scaled @ Bhat + y_scaler
MSE_OLS_test = sum((y_test - ytilde_test)**2) / len(y_test)
print("test data MSE:", MSE_OLS_test)

```

test data MSE: [0.03824773]

And then fit the same data with ridge regression

```

# define some functions for convenience
def get_ridge_beta(X, y, lambda):
    p = X.shape[1]
    I = np.eye(p,p)

    return np.linalg.pinv(X.T @ X + (lambda * I)) @ X.T @ y

```

```

def predict(X, Beta, scaler = 0):
    return X @ Beta + scaler

def get_intercept(X, Beta, scaler):
    return scaler - np.mean(X, 0) @ Beta

def MSE(y, ytilde):
    return sum((y - ytilde)**2) / len(y)

lambdas = 10**np.arange(-4, 1, dtype = float)
MSE_train = np.zeros(len(lambdas))
MSE_test = np.zeros(len(lambdas))

for i in range(len(lambdas)):
    ridge_beta = get_ridge_beta(X_train_scaled, y_train_scaled,
                                lambdas.item(i))

    y_ridge_train = predict(X_train_scaled, ridge_beta, y_scaler)
    y_ridge_test = predict(X_test_scaled, ridge_beta, y_scaler)

    MSE_tr = MSE(y_train, y_ridge_train)
    MSE_te = MSE(y_test, y_ridge_test)
    MSE_train[i] = MSE_tr
    MSE_test[i] = MSE_te

MSE_train

array([0.03319703, 0.03319703, 0.03319704, 0.03319765, 0.03325636])

MSE_test

array([0.03824774, 0.03824787, 0.03824919, 0.03826286, 0.03844413])

plt.plot(lambdas, MSE_train, "b-", label = "training data")
plt.plot(lambdas, MSE_test, "b-.", label = "test data")
plt.xlabel("lambda")
plt.ylabel("MSE")
plt.legend()

```

```
plt.show()
```

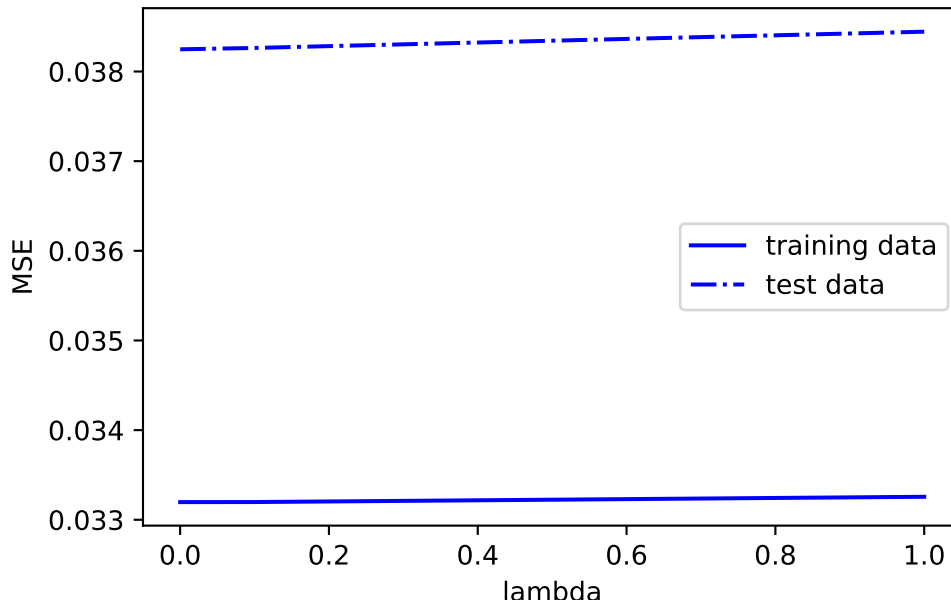


Figure 1: MSE as function of lambda for a ridge regression with predictors up to a 5th degree polynomial.

We can see that the MSE increases with increasing λ for both training and test data.

Finally, we do the same for multiple maximum polynomial degrees: 5, 10 and 15.

```
def ridge_test_lambdas(X, y, lambdas):  
  
    ## Split and scale data  
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2)  
    X_colmeans = np.mean(X_train, 0)[1:]  
  
    # without intercept  
    X_train_scaled = X_train[:, 1:] - X_colmeans  
    X_test_scaled = X_test[:, 1:] - X_colmeans  
    y_scaler = np.mean(y_train)  
    y_train_scaled = y_train - y_scaler  
  
    ## Fit models for different lambdas
```

```

MSE_train = np.zeros(len(lambdas))
MSE_test = np.zeros(len(lambdas))

for i in range(len(lambdas)):
    ridge_beta = get_ridge_beta(X_train_scaled, y_train_scaled,
                                lambdas.item(i))

    y_ridge_train = predict(X_train_scaled, ridge_beta, y_scaler)
    y_ridge_test = predict(X_test_scaled, ridge_beta, y_scaler)

    MSE_tr = MSE(y_train, y_ridge_train)
    MSE_te = MSE(y_test, y_ridge_test)
    MSE_train[i] = MSE_tr
    MSE_test[i] = MSE_te

return [MSE_train, MSE_test]

polys = [5, 10, 15]
lambdas = 10*np.arange(-4, 1, dtype = float)
MSE_train_p = np.zeros((len(lambdas), len(polys)))
MSE_test_p = np.zeros((len(lambdas), len(polys)))

for j in range(len(polys)):
    X = design_poly_n(x, polys[j])
    np.random.seed(524)
    MSE_train, MSE_test = ridge_test_lambdas(X, y, lambdas)
    MSE_train_p[:,j] = MSE_train
    MSE_test_p[:,j] = MSE_test

```

Hand over to R

```

train_data <- as.data.frame(py$MSE_train_p)
test_data <- as.data.frame(py$MSE_test_p)
names(train_data) <- names(test_data) <- paste0(py$polys)

train_data$dat <- "training"
test_data$dat <- "test"

rbind(train_data, test_data) %>%
  cbind(lmb = py$lambdas) %>%
  pivot_longer(~c(dat, lmb)) %>%

```

```

ggplot(aes(lmb, value, lty = dat)) +
  geom_line() +
  facet_wrap(~as.numeric(name), nrow = 3, scales = "free_y") +
  labs(x = expression(paste(lambda)),
       y = "MSE",
       linetype = "data") +
  theme_bw() +
  scale_x_log10()

```

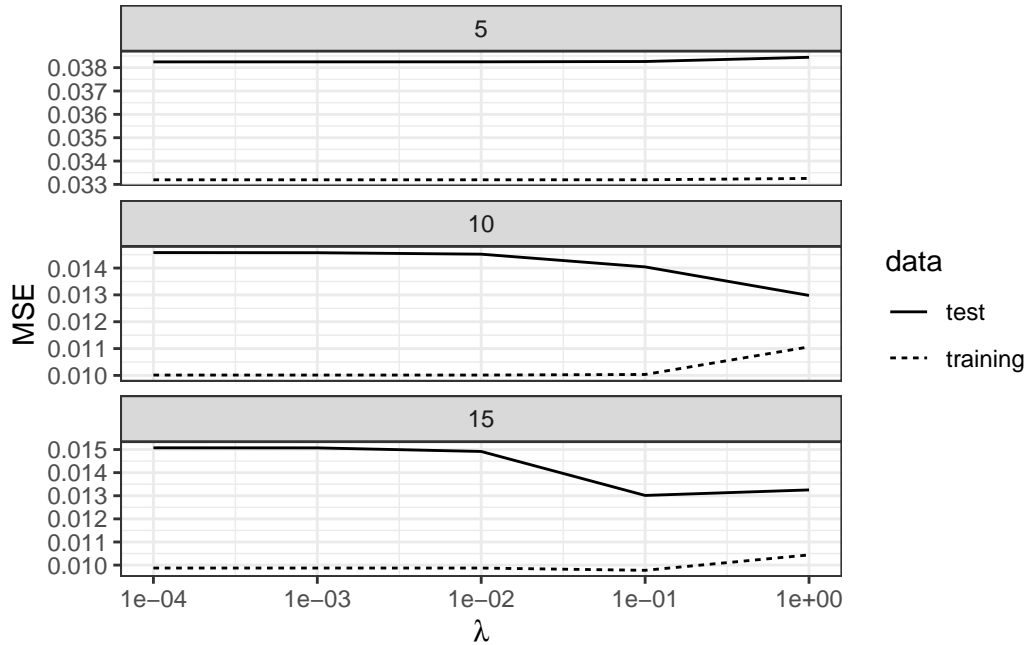


Figure 2: Mean square error for different as a function of λ for fits with predictors of polynomial degree up to 5, 10 and 15. Note individual Y-axis on each plot to emphasize patterns in the data.

In general, training data MSE increases with increasing λ . It seems that the model performs best on the test data when $\lambda \geq 0.1$ for the higher polynomial degrees, showing that the ridge regression could reduce overfitting for this data.