## PSY9511: Seminar 3

Regularization and variable selection

Esten H. Leonardsen 11.09.24



### Outline

- 1. Assignment 2
- 2. Regularization
  - · Variable selection
  - Shrinkage
- 3. Assignment 3





- 1. Download the Auto.csv dataset from the ISLP website.
- 2. Read the Auto.csv-dataset into memory.
- 3. In the horsepower-column, some values are missing. These are encoded with '?'. Remove these rows from the dataset.
- 4. Create a new column 'muscle'. This column should contain a 1 for all muscle cars (e.g. cars that have above average horsepower) and 0 for the rest.
- 5. Split the dataset into a training set and a test set, by randomly drawing 80% of the rows for the former and 20% of the rows for the latter.

http://localhost:8890/notebooks/notebooks/Assignment%202.ipynb



- 1. Fit a simple linear regression model using horsepower as the predictor and mpg as the outcome using the training data.
- 2. Create a scatter plot with horsepower on the x-axis and mpg on the y-axis using the testing data. Plot the regression line found by the model in the plot.
- 3. Use the model to generate predictions for the training set. Calculate and report the mean absolute error (MAE) of these predictions.
- 4. Use the model to generate predictions for the test set. Calculate and report the MAE of the predictions.

http://localhost:8890/notebooks/notebooks/Assignment%202.ipynb



Reflection: Is the training or testing MAE is lower? Does this match your expectation? What would be the general pattern we expect here (e.g. one is lower than the other, they are the same, etc.), and why do we expect that?



- Fit a multivariate linear regression model using horsepower, weight, displacement, and year as predictors and mpg as the outcome.
- 2. Print the intercept and coefficients of the model .
- 3. Use the model to generate predictions for the training set. Calculate and report the MAE of these predictions.
- 4. Use the model to generate predictions for the test set. Calculate and report the MAE of the predictions.

http://localhost:8890/notebooks/notebooks/Assignment%202.ipynb



Is the training MAE lower or higher than in the simple linear regression model? Does it have to be this way, or could it have been otherwise? What about the testing MAE?



- Fit a logistic regression model using weight, displacement and year as predictors and our newly created muscle-column as the outcome.
- 2. Use the model to generate predictions for the training set. Calculate and report the accuracy of these predictions.
- 3. Use the model to generate predictions for the testing set. Calculate and report the accuracy of these predictions.

http://localhost:8890/notebooks/notebooks/Assignment%202.ipynb



```
In[1]:
        import pandas as pd
        df = pd.DataFrame(...)
        train = df.sample(frac=0.8)
        test = df.drop(train.index)
```



```
In[1]:
        import pandas as pd
        df = pd.DataFrame(...)
        train = df.sample(frac=0.8)
        test = df.drop(train.index)
                                                     → MAE=3.5
```



```
In[1]:
        import pandas as pd
        df = pd.DataFrame(...)
        train = df.sample(frac=0.8)
        test = df.drop(train.index)
                                                      → MAE=9.2
```



```
In[1]:
        import pandas as pd
        import numpy as np
        np.random.seed(42)
        df = pd.DataFrame(...)
        train = df.sample(frac=0.8)
        test = df.drop(train.index)
                                                      → MAE=3.5
```



```
model <- glm(muscle ~ year + weight, data=df, family='binomial')
predict(model, df)</pre>
```



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predict(model, df)</pre>
```

```
1 2 3 4 5 6 7 8 9 10 11
1.2460 1.9245 1.0019 0.9911 1.0485 4.2506 4.1465 4.5522 2.4889 1.4578 1.6223
```



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```
1 2 3 4 5 6 7 8 9 10 11 1.2460 1.9245 1.0019 0.9911 1.0485 4.2506 4.1465 4.5522 2.4889 1.4578 1.6223
```

```
predict(model, df, type="response")
```

```
1 2 3 4 5 6 7 8 9 10 11
0.7766 0.8726 0.7314 0.7293 0.7405 0.9853 0.9844 0.9895 0.9233 0.8112 0.8352
```



```
In[1]:    model = LogisticRegression()
    model.fit(df[['year', 'weight']], df['muscle'])
    model.predict(df[['year', 'weight']])

Out[1]:    array([0, 0, 0, 0, 0, 1, 1, 1, 0, 0, 0])

In[1]:    model.predict_proba(df[['year', 'weight']])

Out[1]:    array([[0.14, 0.86], [0.08, 0.92], [0.17, 0.83], [0.18, 0.82]])
```



## Assignment 2: Eye test

```
model <- glm(muscle ~ year + weight, data=df, family='binomial')
predict(model, df)</pre>
```

```
1 2 3 4 5 6 7 8 9 10 11
1.2460 1.9245 1.0019 0.9911 1.0485 4.2506 4.1465 4.5522 2.4889 1.4578 1.6223
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## Assignment 2: Eye test

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model <- glm(muscle ~ year + weight, data=df, family='binomial')
predict(model, df)</pre>
```

```
1 2 3 4 5 6 7 8 9 10 11
1.2460 1.9245 1.0019 0.9911 1.0485 4.2506 4.1465 4.5522 2.4889 1.4578 1.6223
```

```
model <- lm(mpg ~ horsepower, df)
summary(model)</pre>
```

```
Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept) 19.59412 0.96187 20.371 < 2e-16 ***
horsepower102 0.40588 4.08087 0.099 0.920840
horsepower103 0.70588 4.08087 0.173 0.862789
horsepower105 0.90588 1.49529 0.606 0.545091
```



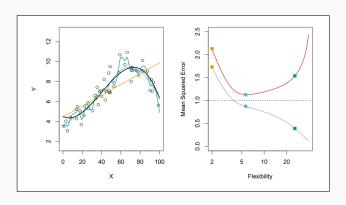
# Regularization



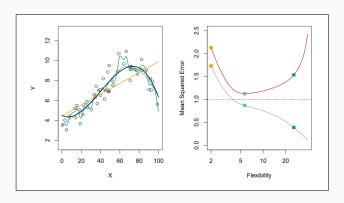
$$y \sim \beta_0 + \beta_1 * X_1 + \beta_2 * X_2$$



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$$y \sim \beta_0 + \beta_1 * X_1 + \beta_2 * X_2 + \beta_3 * X_3 + \beta_4 * X_4$$





```
In[1]: import pandas as pd

df = pd.read_csv('/Users/esten/Downloads/Auto.csv')
    train = df.iloc[:int(len(df) * 0.8)]
    validation = df.iloc[int(len(df) * 0.8):]

    print(f'Using len(train) samples for training')
    print(f'Using len(validation) samples for validation')
Out[1]: Using 317 samples for training
    Using 80 samples for validation
```



- 1. Variable selection
  - a. Best subset selection
  - b. Forward stepwise selection
  - c. Backward stepwise selection
- 2. Shrinkage
  - a. LASSO
  - b. Ridge Regression
- 3. Dimensionality reduction: Lecture 6 and self-study



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  - a. LASSO
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The number of predictors we are using in our linear model directly impacts its complexity.



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### Motivation

To reduce model complexity (and therefore risk of overfitting), avoid problems due to collinearity, and simplify subsequent interpretations we want to reduce the number of predictors.



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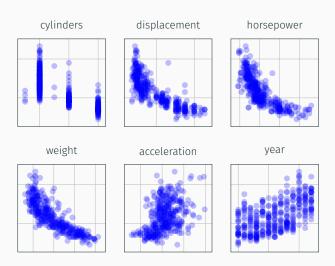
The number of predictors we are using in our linear model directly impacts its complexity.

### Motivation

To reduce model complexity (and therefore risk of overfitting), avoid problems due to collinearity, and simplify subsequent interpretations we want to reduce the number of predictors.

## Formal problem specification

We have a set of predictors  $P = \{x_0, x_1, ...\}$  and a target variable y, and we want to find the subset  $p \subseteq P$  that yields the best (linear) model for predicting y.





### Problem

We have a set of predictors  $P = \{x_0, x_1, ...\}$  and a target variable y, and we want to find the subset  $p \subseteq P$  that yields the best (linear) model for predicting y.

### Solution

Train models on all subsets *p* and select the best one.

```
In[1]:
         import numpy as np
         from itertools import chain, combinations
         from sklearn.linear model import LinearRegression
         from sklearn.metrics import mean squared error
         subsets = list(chain.from iterable(combinations(predictors. r)
                        for r in range(len(predictors)+1)))
         best = {'mse': float('inf'), 'subset': None}
         for subset in subsets:
             if len(subset) == 0:
                 continue
            model = LinearRegression()
            model.fit(train[list(subset)], train[target])
             predictions = model.predict(validation[list(subset)])
            mse = mean squared error(validation[target], predictions)
             best = best if mse > best['mse'] else {'mse': mse, 'subset': subset}
         print(f'MSE: {best["mse"]:.2f}, predictors: {best["subset"]}')
```

```
Out[1]: MSE: 29.68, predictors: ('cylinders', 'displacement', 'horsepower', 'weight', 'year')
```



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In[1]:
         import numpy as np
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             predictions = model.predict(validation[list(subset)])
            mse = mean squared error(validation[target], predictions)
             best = best if mse > best['mse'] else {'mse': mse, 'subset': subset}
         print(f'MSE: {best["mse"]:.2f}, predictors: {best["subset"]}')
```

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Out[1]: MSE: 29.68, predictors: ('cylinders', 'displacement', 'horsepower', 'weight', 'year')
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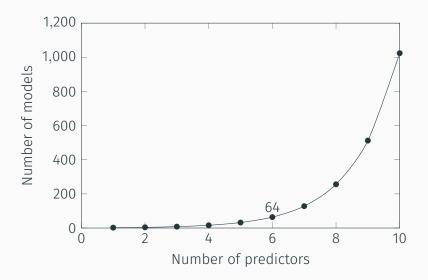
### Solution

Train models on all subsets *p* and select the best one.

- + Positives
- · Guaranteed to find the optimal solution.
- · Simple implementation
- Drawbacks
- Need to train many  $(2^{|P|})$  models.



#### Variable selection: Best subset selection





#### Problem

We have a set of predictors  $P = \{x_0, x_1, ...\}$  and a target variable y, and we want to find the subset  $p \subseteq P$  that yields the best (linear) model for predicting y.

#### Solution

Start with no predictors. Iteratively add the predictor that yields the best model until all are included.

#### Problem

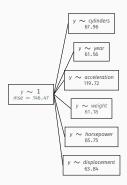
We have a set of predictors  $P = \{x_0, x_1, ...\}$  and a target variable y, and we want to find the subset  $p \subseteq P$  that yields the best (linear) model for predicting y.

#### Solution

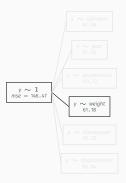
Start with no predictors. Iteratively add the predictor that yields the best model until all are included.



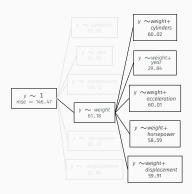




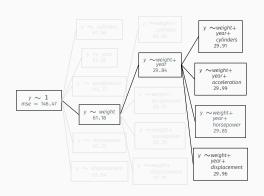




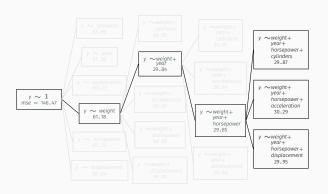




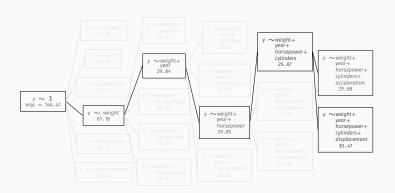




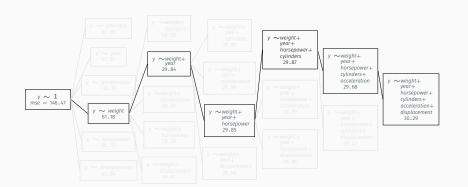




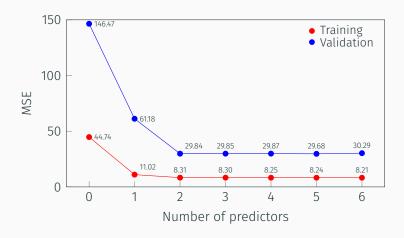














In[1]:

```
def fit and evaluate(train: pd.DataFrame, validation: pd.DataFrame,
                     predictors: List[str], target: str):
    model = LinearRegression()
    model.fit(train[predictors], train[target])
    train_predictions = model.predict(train[predictors])
    validation_predictions = model.predict(validation[predictors])
    return np.mean((train_predictions - train[target]) ** 2),
           np.mean((validation predictions - validation[target]) ** 2)
predictors = ['cylinders', 'displacement', 'horsepower', 'weight', 'acceleration', 'year']
target = 'mpg'
train['intercept'] = 1
validation['intercept'] = 1
train mse, validation mse = fit and evaluate(train, validation, predictors=['intercept'], target=target)
print(f'[]: {validation mse:.2f} ({train mse:.2f})')
chosen predictors = []
while len(chosen_predictors) < len(predictors):
    best_predictor = {'train_mse': None, 'validation_mse': float('inf'),
                       'predictor': None}
    for predictor in set(predictors) - set(chosen predictors):
        train mse, validation mse = fit and evaluate(train, validation, predictors=chosen predictors + [predictor], target=target)
        if validation mse < best predictor['validation mse']:
            best predictor = { 'train mse': train mse, 'validation mse': validation mse, 'predictor': predictor}
    chosen_predictors.append(best_predictor['predictor'])
    print(f'{chosen_predictors}: {best_predictor["validation_mse"]:.2f} ({best_predictor["train_mse"]:.2f})')
```



#### Problem

We have a set of predictors  $P = \{x_0, x_1, ...\}$  and a target variable y, and we want to find the subset  $p \subseteq P$  that yields the best (linear) model for predicting y.

#### Solution

Start with no predictors. Iteratively add the predictor that yields the best model until all are included.

- + Positives
- · Need to train fewer models.
- Drawbacks
- Not guaranteed to find the optimal solution.



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We have a set of predictors  $P = \{x_0, x_1, ...\}$  and a target variable y, and we want to find the subset  $p \subseteq P$  that yields the best (linear) model for predicting y.

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Start with all predictors. Iteratively remove the predictor that yields the best model until all you have none left.

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We have a set of predictors  $P = \{x_0, x_1, ...\}$  and a target variable y, and we want to find the subset  $p \subseteq P$  that yields the best (linear) model for predicting y.

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Start with all predictors. Iteratively remove the predictor that yields the best model until all you have none left.

- + Positives
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- Not guaranteed to find the optimal solution.



Does forward and backward stepwise selection yield the same set of predictors?



# Shrinkage



$$y \sim \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6$$



$$y \sim \beta_0 + \frac{\beta_1}{\beta_1} x_1 + \frac{\beta_2}{\beta_2} x_2 + \frac{\beta_3}{\beta_3} x_3 + \frac{\beta_4}{\beta_4} x_4 + \frac{\beta_5}{\beta_5} x_5 + \beta_6 x_6$$



$$y \sim \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_4 X_4 + \beta_5 X_5 + \beta_6 X_6$$
  
$$\beta_n \to 0$$



$$y \sim \beta_0 + \frac{\beta_1 x_1}{\beta_2 x_2} + \frac{\beta_3 x_3}{\beta_3 x_3} + \frac{\beta_4 x_4}{\beta_5 x_5} + \frac{\beta_6 x_6}{\beta_6 x_6}$$
  
 $\beta_n \to 0$ 

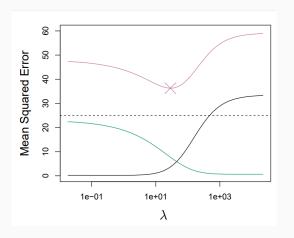
1.  $\beta_1 = 0$   $\Longrightarrow$  One less degree of freedom in our function

$$y \sim \beta_0 + \frac{\beta_1}{\beta_1} x_1 + \frac{\beta_2}{\beta_2} x_2 + \frac{\beta_3}{\beta_3} x_3 + \frac{\beta_4}{\beta_4} x_4 + \frac{\beta_5}{\beta_5} x_5 + \frac{\beta_6}{\beta_6} x_6$$
  
 $\beta_n \to 0$ 

1.  $\beta_1 = 0$   $\Longrightarrow$  One less degree of freedom in our function

mse=bias<sup>2</sup>+variance+irreducible error





mse=bias<sup>2</sup>+variance+irreducible error



$$y \sim \beta_0 + \frac{\beta_1 x_1}{\beta_2 x_2} + \frac{\beta_3 x_3}{\beta_3 x_3} + \frac{\beta_4 x_4}{\beta_5 x_5} + \frac{\beta_6 x_6}{\beta_6 x_6}$$
  
 $\beta_n \to 0$ 

- 1.  $\beta_1 = 0 \implies$  One less degree of freedom in our function
- 2. A little more bias  $\implies$  A lot less variance



$$y \sim \beta_0 + \frac{\beta_1 x_1}{\beta_2 x_2} + \frac{\beta_3 x_3}{\beta_4 x_4} + \frac{\beta_5 x_5}{\beta_6 x_6} + \frac{\beta_6 x_6}{\beta_6 x_6}$$

- 1.  $\beta_1 = 0$   $\Longrightarrow$  One less degree of freedom in our function
- 2. A little more bias  $\implies$  A lot less variance

$$y \sim \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6$$
 subject to the constraint 
$$\sum_{j=1}^p \beta_j \leq 1$$

$$y \sim \beta_0 + \frac{\beta_1 x_1}{\beta_2 x_2} + \frac{\beta_3 x_3}{\beta_4 x_4} + \frac{\beta_5 x_5}{\beta_6 x_6} + \frac{\beta_6 x_6}{\beta_6 x_6}$$

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 subject to the constraint 
$$\sum_{j=1}^p \beta_j \le 1$$

$$\beta_1 = 1, \beta_2 = 0, \beta_3 = 0, \dots$$



$$y \sim \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6$$
  
 $\beta_n \to 0$ 

- 1.  $\beta_1 = 0 \implies$  One less degree of freedom in our function
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$$y \sim \beta_0 + \frac{\beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6}{\text{subject to the constraint}}$$
$$\sum_{j=1}^p \beta_j \le 1$$



 $\beta_1 = 1, \beta_2 = 0, \beta_3 = 0, \dots$ 

$$y \sim \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6$$
  
 $\beta_n \to 0$ 

- 1.  $\beta_1 = 0$   $\Longrightarrow$  One less degree of freedom in our function
- 2. A little more bias  $\implies$  A lot less variance
- 3. Parameters depend on eachother ⇒ Fewer degrees of freedom



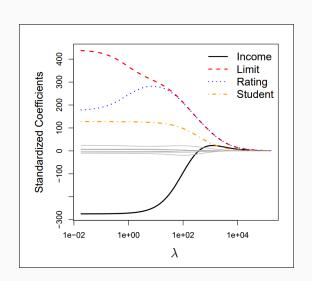
$$loss_{mse} = \sum_{i=0}^{n} \left( y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2$$



$$loss_{ridge} = \sum_{i=0}^{n} \left( y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=0}^{p} \beta_j^2$$









$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

$$\ell = \sum_{i=0}^{n} (y_i - \hat{y}_i)^2 + \lambda \sum_{j=0}^{p} \beta_j^2$$



$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

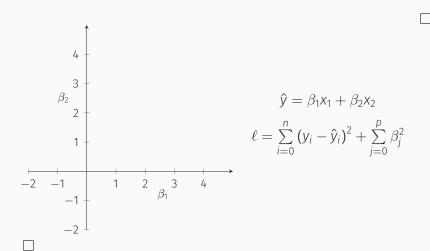
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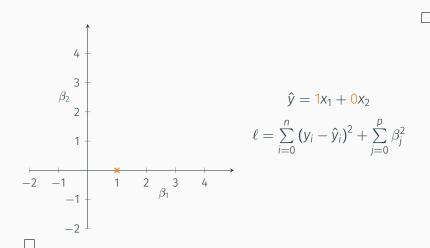
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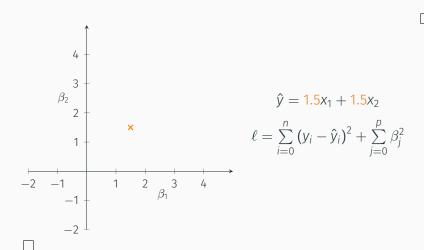










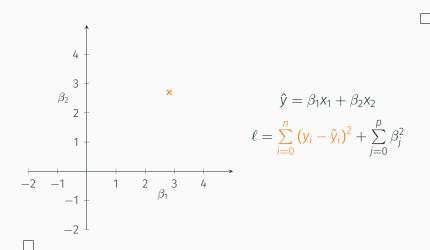




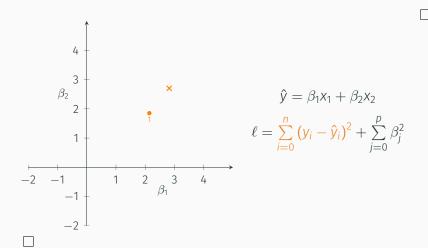
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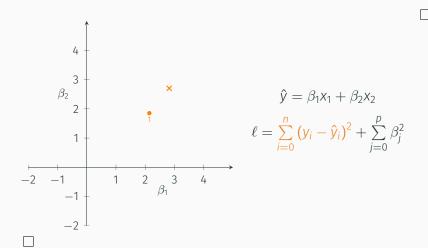




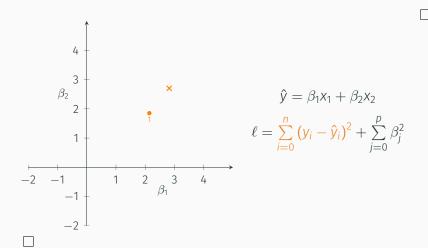




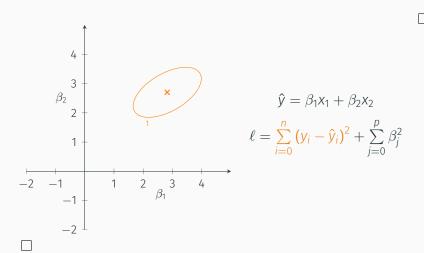




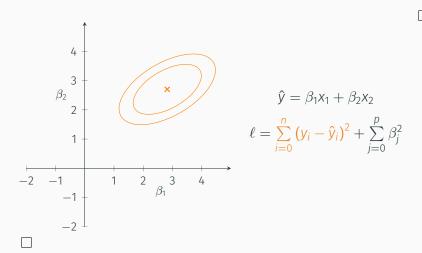




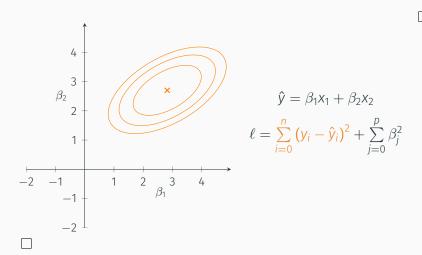




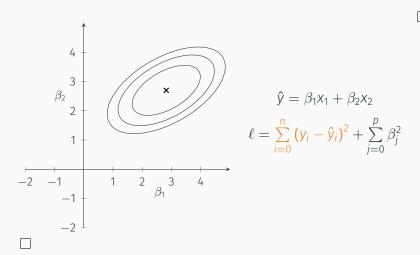




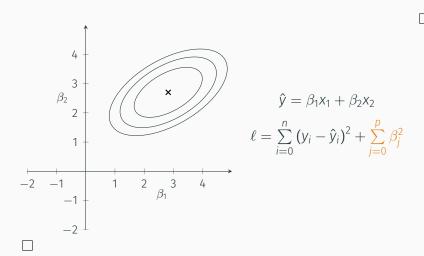




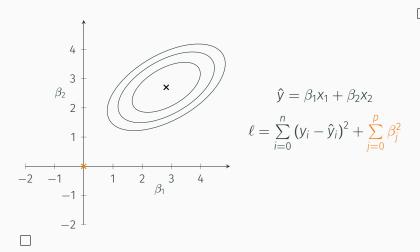




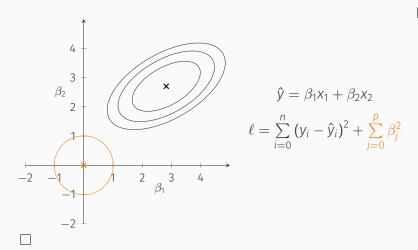




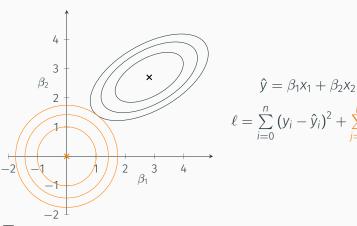


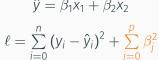


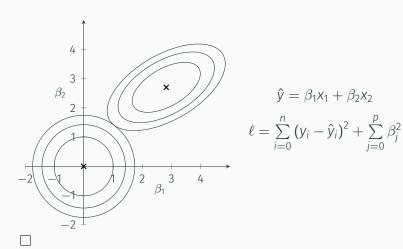




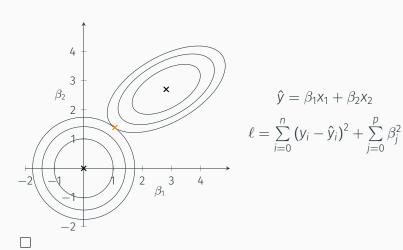












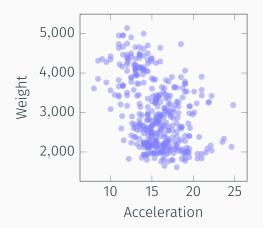


$$y \sim \beta_0 + \beta_1 x_1 + \beta_2 x_2$$
  
 $x_1 \in [0, 1], x_2 \in [0, 1000]$ 



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 $x_1 \in [0, 1], x_2 \in [0, 1000]$   
 $\downarrow \downarrow$   
 $\beta_1 \approx 1000 * \beta_2$ 







z-score standardization



#### z-score standardization

$$\mathbf{X} = \frac{\mathbf{X} - \mu_{\mathbf{X}}}{\sigma_{\mathbf{X}}}$$

#### z-score standardization

$$X = \frac{X - \mu_X}{\sigma_X}$$

```
In[1]:
          for col in predictors:
              print(f'{col}: {np.mean(df[col]):.2f} ({np.std(df[col]):.2f})')
          # z-score standardization
          for col in predictors:
              df[col] = (df[col] - np.mean(df[col])) / np.std(df[col])
          for col in predictors:
              print(f'{col} after: {np.mean(df[col]):.2f} ({np.std(df[col]):.2f})')
Out[1]:
         cylinders: 5.47 (1.70)
          displacement: 194.41 (104.51)
          horsepower: 104.47 (38.44)
          cylinders after: -0.00 (1.00)
          displacement after: -0.00 (1.00)
          horsepower after: -0.00 (1.00)
```

$$loss_{ridge} = \sum_{i=0}^{n} \left( y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=0}^{p} \beta_j^2$$

http://localhost:8888/notebooks/notebooks/Live%20coding.ipynb

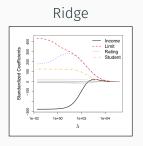


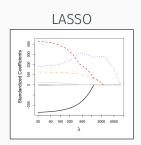
$$loss_{ridge} = \sum_{i=0}^{n} \left( y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=0}^{p} \beta_j^2$$
$$loss_{lasso} = \sum_{i=0}^{n} \left( y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=0}^{p} |\beta_j|$$

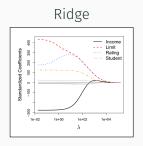


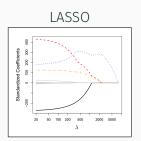
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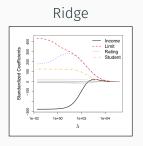


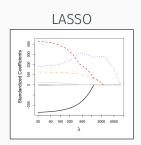


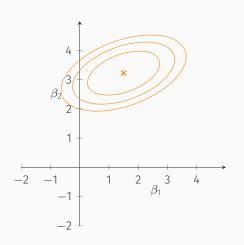




Predictor	Ridge	LASSO
Intercept	23.44	23.44
Weight	-5.59	-4.78
Year	2.75	2.00
Acceleration	0.19	0
Displacement	0.66	0

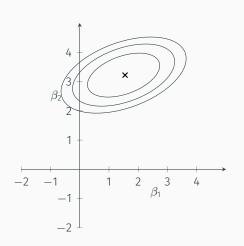






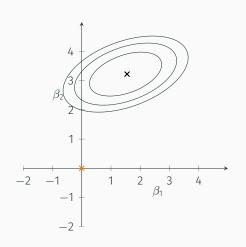
$$\hat{y} = \beta_1 x_1 + \beta_2 x_2$$

$$\ell = \sum_{i=0}^{n} (y_i - \hat{y}_i)^2 + \sum_{j=0}^{p} \beta_j^2$$



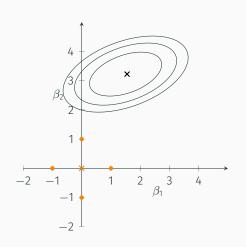
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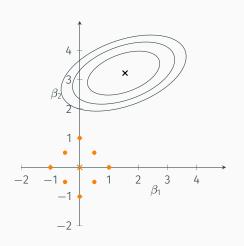
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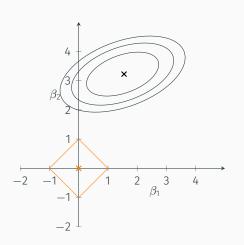
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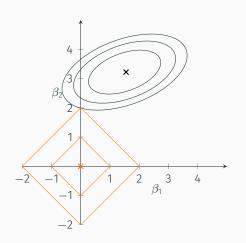
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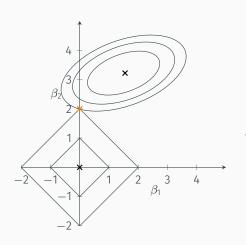
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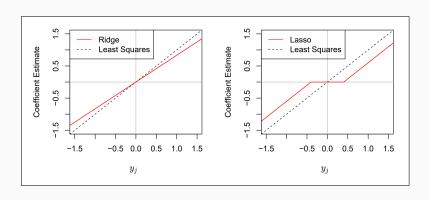
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A coefficient of 0 does not mean the predictor has no association with the outcome! Why?







## Shrinkage: Summary

$$loss_{mse} = \sum_{i=0}^{n} \left( y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2$$

Fits the **best** model to the data.

## Shrinkage: Summary

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Fits the **best** model to the data.

Fits the **best** model to the data while **shrinking** coefficients towards zero.



## Shrinkage: Summary

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Fits the **best** model to the data.

Fits the **best** model to the data while **shrinking** coefficients towards zero.

Fits the **best** model to the data while **shrinking** coefficients towards zero such that some variables are effectively **removed**.

