PSY9511: Seminar 3

Variable selection and regularization

Esten H. Leonardsen 07.09.23

1

Outline

1 Introduction

- · Python
- · Coding tips: Separation of concerns

2. Variable selection

- · Best subset selection
- · Forward stepwise selection
- · Backward stepwise selection

3. Regularization

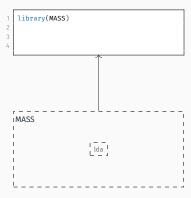
- · Ridge regression
- · Lasso
- · Elastic net

4. Dimensionality reduction

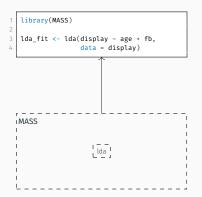
- · Principal component regression
- · Partial least squares

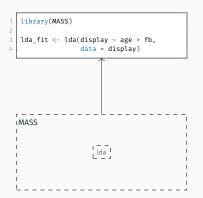
```
1 2 3 4
```

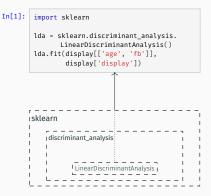
```
iMASS
```



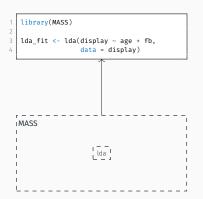
```
library(MASS)
iMASS
```

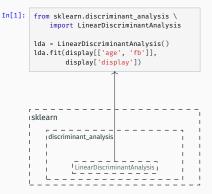






7





Python: pandas

```
path <- '/Users/esten/Downloads/Auto.csv'
df <- read.csv(path)
head(df, 10)</pre>
```

```
mpg cylinders displacement horsepower
     18
                 8
                           307.0
                                          130
                           350.0
     15
                  8
                                          165
3
     18
                  8
                           318.0
                                          150
     16
                           304.0
                                          150
                 8
5
     17
                           302.0
                                          140
                 8
     15
                           429.0
6
                 8
                                          198
     14
                  8
                           454.0
                                          220
8
     14
                  8
                           440.0
                                          215
     14
                           455.0
                                          225
9
                  8
     15
10
                 8
                           390.0
                                          190
```

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

path = '/Users/esten/Downloads/Auto.csv'
    df = pd.read_csv(path)
    df.head(10)
```

Out[1]: mpg cylinders displacement horsepower 307.0 350.0 318.0 302.0 429.0 454.0 440.0 455.0 390.0

Python: numpy

```
In[1]: import numpy as np
In[2]: np.random.seed(42)
In[3]:
        np.arange(0, 10, 1)
Out[1]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
In[4]: np.isnan([0, 1, np.nan, 3])
Out[2]: array([False, False, True, False])
In[5]: np.amin([1, 0, 3, 2])
Out[3]: 0
Out[6]: np.argmin([1, 0, 3, 2])
Out[4]: 1
In[7]: np.nanmin([1, 0, 3, np.nan])
Out[5]: 0
```

Python: statsmodels

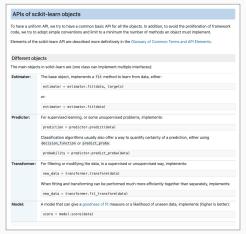
```
Coefficients:
               Estimate Std. Frror Pr(>|t|)
(Intercept) -1.454e+01 4.764e+00 0.00244 **
cvlinders
            -3.299e-01 3.321e-01 0.32122
displacement 7.678e-03 7.358e-03 0.29733
horsepower
          -3.914e-04 1.384e-02 0.97745
weight
            -6.795e-03 6.700e-04 < 2e-16 ***
acceleration 8.527e-02 1.020e-01 0.40383
             7.534e-01 5.262e-02 < 2e-16 ***
vear
Signif. codes:
              0 '***' 0.001 '**' 0.01 '*'
      0.05
```

```
Out[1]: coef std err P>|t| [0.025 0.975]

Intercept -14.5353 4.764 0.002 -23.90 -5.16
cylinders -0.3299 0.332 0.321 -0.98 0.32
displacement 0.0077 0.007 0.297 -0.00 0.02
horsepower -0.0004 0.014 0.977 -0.02 0.02
weight -0.0068 0.001 0.000 -0.00 -0.00
acceleration 0.0853 0.102 0.404 -0.11 0.28
year 0.7534 0.053 0.000 0.65 0.85
```

```
In[1]: from sklearn.linear_model import LinearRegression
        math = '/Users/esten/Downloads/Auto.csv'
        df = pd.read csv(path)
        predictors = ['cvlinders', 'displacement', 'horsepower',
                      'weight', 'acceleration', 'vear'l
        target = 'mpg'
        model = LinearRegression()
        model.fit(df[predictors], df[target])
        # Print model coefficients
        print(f'Intercept: {model.intercept }')
        print(f'Coefficients: {model.coef }')
        # Print model residuals
        predictions = model.predict(df[predictors])
        residuals = df[target] - predictions
        print(f'Residuals: {residuals.values[:5]}...')
```

```
Out[1]: Intercept: -14.53525048050604
Coefficients: [-3.29859089e-01 7.67843024e-03 -3.91355574e-04 -6.79461791e-03 8.52732469e-02 7.53367180e-01]
Residuals: [2.91708096 0.92742531 2.46368456 0.46552549 1.71359255]...
```



https://scikit-learn.org/stable/developers/develop.html

```
In[1]: from sklearn.linear_model import LinearRegression
        math = '/Users/esten/Downloads/Auto.csv'
        df = pd.read csv(path)
        predictors = ['cvlinders', 'displacement', 'horsepower',
                      'weight', 'acceleration', 'vear'l
        target = 'mpg'
        model = LinearRegression()
        model.fit(df[predictors], df[target])
        # Print model coefficients
        print(f'Intercept: {model.intercept }')
        print(f'Coefficients: {model.coef }')
        # Print model residuals
        predictions = model.predict(df[predictors])
        residuals = df[target] - predictions
        print(f'Residuals: {residuals.values[:5]}...')
```

```
Out[1]: Intercept: -14.53525048050604
Coefficients: [-3.29859089e-01 7.67843024e-03 -3.91355574e-04 -6.79461791e-03 8.52732469e-02 7.53367180e-01]
Residuals: [2.91708096 0.92742531 2.46368456 0.46552549 1.71359255]...
```

```
In[1]: from sklearn.svm import SVR
        path = '/Users/esten/Downloads/Auto.csv'
        df = pd.read csv(path)
        predictors = ['cylinders', 'displacement', 'horsepower',
                      'weight', 'acceleration', 'vear'l
        target = 'mpg'
        model = SVR(kernel='linear')
        model.fit(df[predictors], df[target])
        # Print model coefficients
        print(f'Intercept: {model.intercept }')
        print(f'Coefficients: {model.coef }')
        # Print model residuals
        predictions = model.predict(df[predictors])
        residuals = df[target] - predictions
        print(f'Residuals: {residuals.values[:5]}...')
```

Coding tips: Separation of concerns

```
In[1]: # Read and clean data
        path = '/Users/esten/Downloads/Auto.csv'
        df = pd.read csv(path)
        # Split data
        train = df.iloc[:int(len(df) * 0.8)]
        validation = df.iloc[int(len(df) * 0.8):]
        # Define input and output variables
        target = 'mpg'
        # Define necessary data structures for state
        chosen predictors = []
        mses = []
        while len(predictors) > 0:
            best_predictor = {'mse': float('inf'), 'predictor': None}
            for predictor in set(predictors) - set(chosen predictors):
               potential predictors = chosen predictors + [predictor]
               # Fit and evaluate model
               model = LinearRegression()
               model.fit(train[potential predictors], train[target])
               predictions = model.predict(validation[potential predictors])
               test_mse = np.mean((validation[target] - predictions) ** 2)
               # Compare model with previous best
               if test mse < best predictor['mse']:</pre>
                   best predictor = {'mse': test mse, 'predictor': predictor}
            # Update state
            chosen predictors.append(best predictor['predictor'])
            mses.append(best predictor['mse'])
            predictors = [p for p in predictors if p != best predictor['predictor']]
```

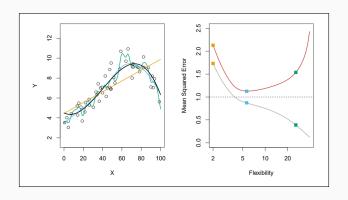
Coding tips: Separation of concerns

```
In[1]:
        # Read and clean data
        path = '/Users/esten/Downloads/Auto.csv'
        df = pd.read csv(path)
        # Split data
        train = df.iloc[:int(len(df) * 0.8)]
        validation = df.iloc[int(len(df) * 0.8):]
        # Define input and output variables
        target = 'mpg'
        # Define necessary data structures for state
        chosen predictors = []
        mses = []
        while len(predictors) > 0:
            best predictor = {'mse': float('inf'), 'predictor': None}
            for predictor in set(predictors) - set(chosen predictors):
               potential predictors = chosen predictors + [predictor]
               # Fit and evaluate model
                                                                                                             Modelling
               model = LinearRegression()
               model.fit(train[potential predictors], train[target])
               predictions = model.predict(validation[potential predictors])
               test mse = np.mean((validation[target] - predictions) ** 2)
               # Compare model with previous best
               if test mse < best predictor['mse']:</pre>
                   best predictor = {'mse': test mse, 'predictor': predictor}
            chosen predictors.append(best predictor['predictor'])
            mses.append(best predictor['mse'])
            predictors = [p for p in predictors if p != best predictor['predictor']]
```

Coding tips: Separation of concerns

```
In[1]: # Read and clean data
        path = '/Users/esten/Downloads/Auto.csv'
        df = pd.read csv(path)
        # Split data
        train = df.iloc[:int(len(df) * 0.8)]
        validation = df.iloc[int(len(df) * 0.8):]
        # Define input and output variables
        predictors = ['cylinders', 'displacement', 'horsepower',
                         'weight', 'acceleration', 'year']
        target = 'mpg'
        # Define necessary data structures for state
        chosen predictors = []
        mses = []
                                                                                                                   Modelling
        def fit and evaluate model(model: LinearRegression, train: pd.DataFrame,
                                    validation: pd.DataFrame, variables: List[str].
                                    target: str):
            """ Fit a given model on a training dataset using a given set of variables
            and return MSE from a validation dataset. ""
            model = LinearRegression()
            model.fit(train[potential predictors], train[target])
            predictions = model.predict(validation[potential predictors])
            return np.mean((validation[target] - predictions) ** 2)
        while len(predictors) > 0:
            best predictor = {'mse': float('inf'), 'predictor': None}
            for predictor in set(predictors) - set(chosen predictors):
                potential predictors = chosen predictors + [predictor]
                test mse = fit and evaluate model(LinearRegression(), train, validation,
                                                     variables=potential predictors,
                                                     target=target)
                # Compare model with previous best
                if test mse < best predictor['mse']:
                    best predictor = {'mse': test mse, 'predictor': predictor}
            # Undate state
            chosen predictors.append(best predictor['predictor'])
            mses.append(best predictor['mse'])
            predictors = [p for p in predictors if p != best predictor['predictor']]
```

Regularization: Motivation



Regularization: Out-of-sample testing

Regularization: Methods

1. Variable selection

- a. Best subset selection
- b. Forward stepwise selection
- c. Backward stepwise selection

2. Shrinkage

- a. LASSO
- b. Ridge Regression
- c. Flastic net

3. Dimensionality reduction

- a. Principal Component Regression
- b. Partial Least Squares

Variable selection: Outline

<u>Problem</u>

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.

Variable selection: Outline

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.

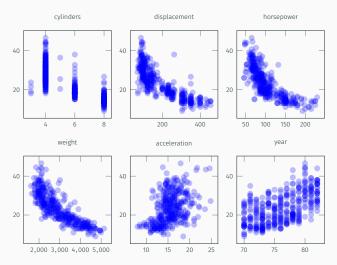
Motivation

- 1. Simplify interpretation
- 2. Reduce model complexity (overfitting)

Variable selection: Outline

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.



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.

<u>Solution</u>

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

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

```
In[1]:
       import numpy as np
       from itertools import chain, combinations
       from sklearn.linear model import LinearRegression
       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 = np.mean((predictions - validation[target]) ** 2)
            if mse < best['mse']:</pre>
                best = {'mse': mse. 'subset': subset}
       print(f'MSE: {best["mse"]:.2f}, predictors: {best["subset"]}')
Out[1]: MSE: 29.68, predictors: ('cylinders', 'displacement', 'horsepower', 'weight', 'year')
```

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.

<u>Solution</u>

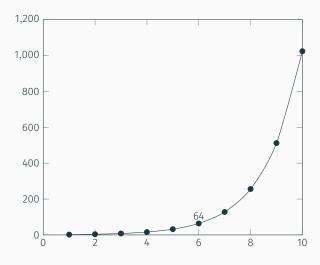
Train models on all subsets p and select the best one.

+ Positives

Guaranteed to find the optimal solution. Simple implementation

Drawbacks

Need to train many $(2^{|P|})$ models.



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.

<u>Solution</u>

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.

<u>Solution</u>

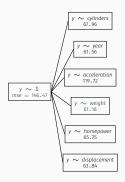
Start with no predictors. Iteratively add the predictor that yields the best model until all are included.

 $y \sim 1$ mse = 146.47

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.

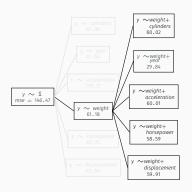
Solution



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.

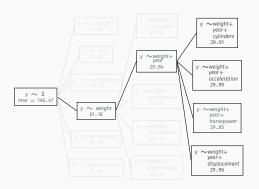
<u>Solution</u>



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.

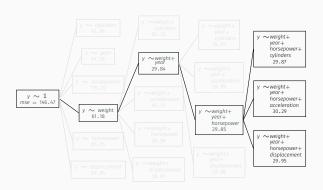
Solution



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

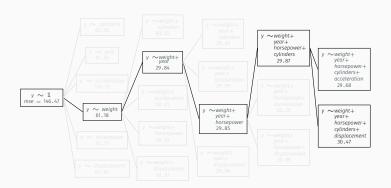


Problem

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.

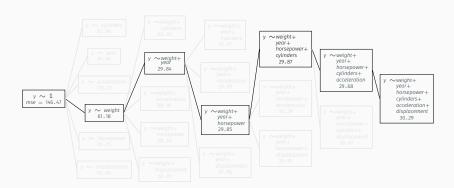


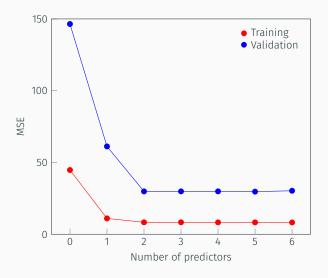
Problem

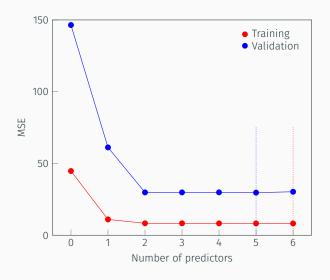
We have a set of predictors $P = \{x_0, x_1, ...\}$ and a target variable y, and we want to find the subset $p \subseteq P$ that yields the best (linear) model for predicting y.

Solution

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







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

```
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.

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

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

+ Positives

Need to train fewer models.

- Drawbacks

Not guaranteed to find the optimal solution.

Shrinkage

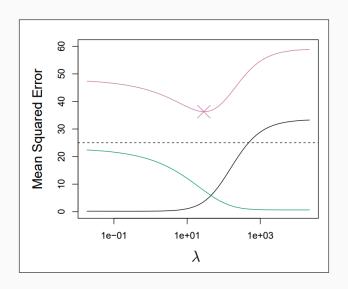
$$y \sim \beta_0 + \frac{\beta_1}{\lambda_1} x_1 + \frac{\beta_2}{\lambda_2} x_2 + \frac{\beta_3}{\lambda_3} x_3 + \frac{\beta_4}{\lambda_4} x_4 + \frac{\beta_5}{\lambda_5} x_5 + \frac{\beta_6}{\lambda_6} x_6$$

```
Out[1]: coef std err P>|t| [0.025 0.975]

Intercept -14,5353 4.764 0.002 -23.90 -5.16
cylinders -0.3299 0.332 0.321 -0.98 0.32
displacement 0.0077 0.007 0.297 -0.00 0.02
horsepower -0.0004 0.014 0.977 -0.02 0.02
weight -0.0068 0.001 0.000 -0.00 -0.00
acceleration 0.0853 0.102 0.404 -0.11 0.28
year 0.7534 0.053 0.000 0.65 0.85
```

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

 $mse = bias^2 + variance + irreducible error$



salary
$$\sim \beta_0 + \beta_1 * age$$

salary
$$\sim \beta_0 + \beta_1 * age$$

$$salary \sim 3000000 + 10000 * age$$

$$salary \sim 6000000 + 0 * age$$

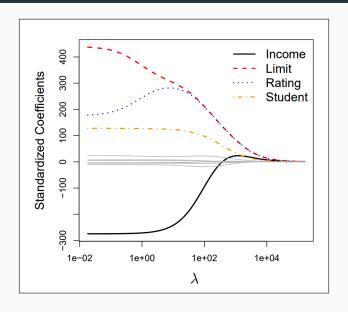
$$loss_{mse} = \sum_{i=0}^{n} \left(y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2$$

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

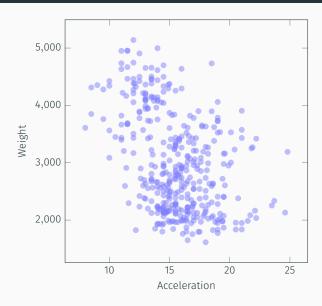
$$loss_{ridge} = \sum_{i=0}^{n} \left(y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=0}^{p} \beta_j^2$$

$$\downarrow \qquad \qquad \qquad \qquad \lambda \to \infty \Rightarrow \beta \to 0$$

Shrinkage



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



$$X = \frac{x - \mu_X}{\sigma_X^2}$$

$$X = \frac{x - \mu_X}{\sigma_X^2}$$

```
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})')
```

$$X = \frac{X - \mu_X}{\sigma_X^2}$$

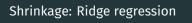
```
In[1]: for col in predictors:
    print(f'{col}: {np.mean(df[col]):.2f} ({np.std(df[col]):.2f})')

# 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)
weight: 2977.58 (848.32)
acceleration: 15.54 (2.76)
year: 75.98 (3.68)
cylinders after: -0.00 (1.00)
displacement after: -0.00 (1.00)
horsepower after: -0.00 (1.00)
weight after: -0.00 (1.00)
acceleration after: 0.00 (1.00)
year after: -0.00 (1.00)
```



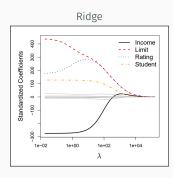
http://localhost:8888/notebooks/notebooks/Live%20coding.ipynb

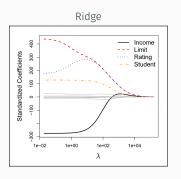
$$loss_{ridge} = \sum_{i=0}^{n} \left(y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=0}^{p} \beta_j^2$$

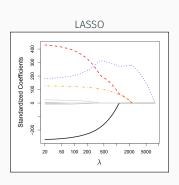
 $\label{lem:covariates} \textit{Regularization through shrinking the model covariates towards zero.}$

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

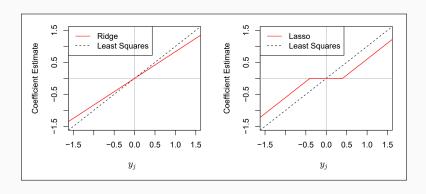
$$loss_{lasso} = \sum_{i=0}^{n} \left(y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=0}^{p} |\beta_j|$$

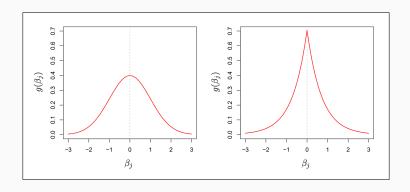






Python coefficients





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

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

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

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

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

Shrinkage: Summary

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

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

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

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**.

Dimensionality reduction: Outline

Dimensionality reduction: Principal component analysis

Dimensionality reduction: Principal component regression

Dimensionality reduction: Partial least squares