## PSY9511: Seminar 3

Variable selection and regularization

Esten H. Leonardsen 07.09.23

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## Outline

#### 1. Introduction

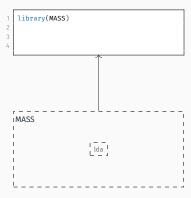
- · Python
- · Coding tips: Separation of concerns

#### 2. Regularization

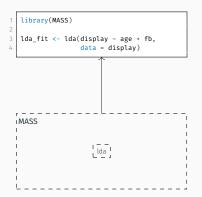
- · Variable selection
- · Shrinkage (+ live coding)
- · Dimensionality reduction

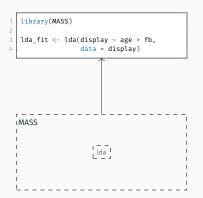
```
1 2 3 4
```

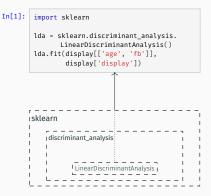
```
iMASS
```



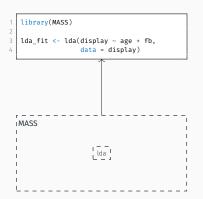
```
library(MASS)
iMASS
```

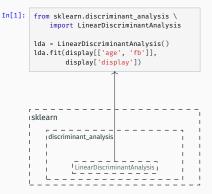






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## Python: pandas

```
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

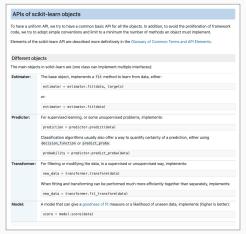
```
Coefficients:
               Estimate Std. Frror Pr(>|t|)
(Intercept) -1.454e+01 4.764e+00 0.00244 **
cvlinders
            -3.299e-01 3.321e-01 0.32122
displacement 7.678e-03 7.358e-03 0.29733
horsepower
          -3.914e-04 1.384e-02 0.97745
weight
            -6.795e-03 6.700e-04 < 2e-16 ***
acceleration 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

```
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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

```
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        path = '/Users/esten/Downloads/Auto.csv'
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               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'])
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            predictors = [p for p in predictors if p != best predictor['predictor']]
```

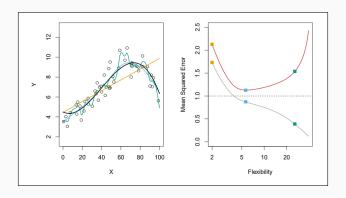
## Coding tips: Separation of concerns

```
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

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

# Regularization: Motivation



# Regularization: Out-of-sample testing

```
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
```

## Regularization: Methods

#### 1. Variable selection

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

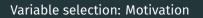
#### 2. Shrinkage

- a. LASSO
- b. Ridge Regression

#### 3. Dimensionality reduction

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

# Variable selection



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

#### 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.

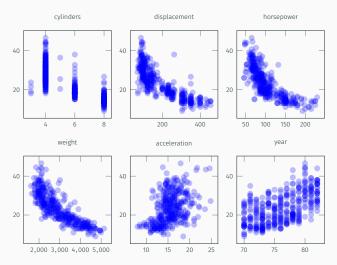
#### Motivation

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

#### 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**

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#### <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')
```

#### <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.

#### Solution

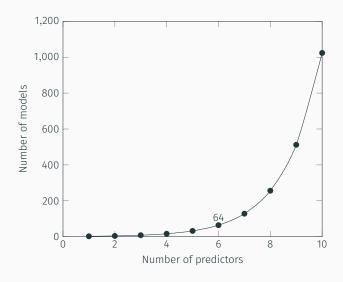
Train models on all subsets p and select the best one.

#### + Positives

Guaranteed to find the optimal solution. Simple implementation

#### - Drawbacks

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



## Variable selection: Forward stepwise 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.

## Variable selection: Forward stepwise 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.

y ∼ 1 mse = 146.47

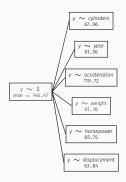
## Variable selection: Forward stepwise selection

#### **Problem**

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#### Solution

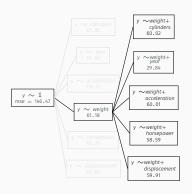
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### **Problem**

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.

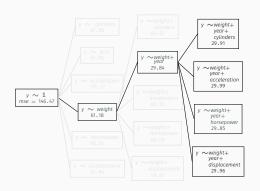
#### Solution



### **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.

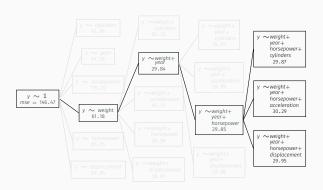
### Solution



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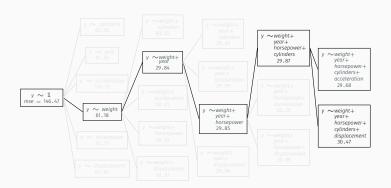
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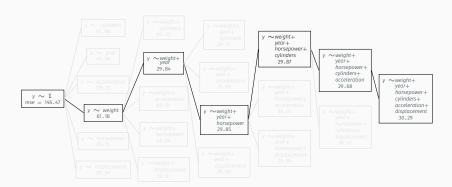
### Solution

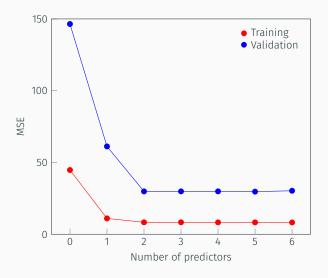


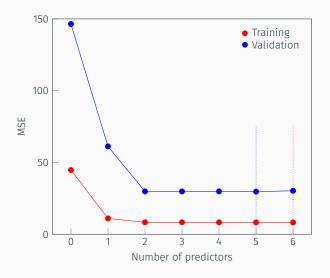
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#### Solution







#### Problem

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#### 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

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# Shrinkage

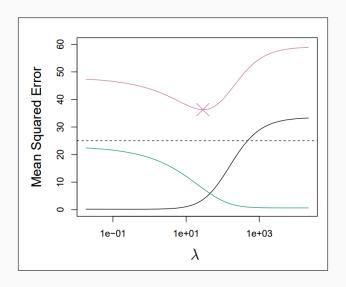
$$y \sim \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6$$

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

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

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

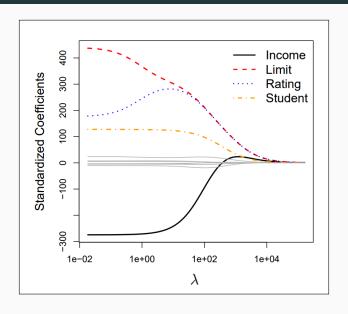
$$loss_{mse} = \sum_{i=0}^{n} \left( y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2$$

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

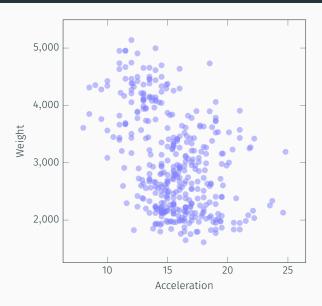
$$loss_{ridge} = \sum_{i=0}^{n} \left( y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=0}^{p} \beta_j^2$$

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

# Shrinkage



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



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

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

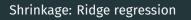
# z-score standardization
for col in predictors:
    df[col] = (df[col] - np.mean(df[col])) / np.std(df[col])

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

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

```
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)
weight after: -0.00 (1.00)
year after: -0.00 (1.00)
```



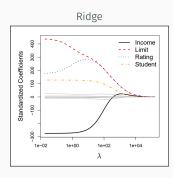
http://localhost:8888/notebooks/notebooks/Live%20coding.ipynb

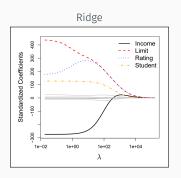
$$loss_{ridge} = \sum_{i=0}^{n} \left( y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=0}^{p} \beta_j^2$$

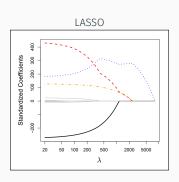
Regularization through shrinking the model covariates towards zero.

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

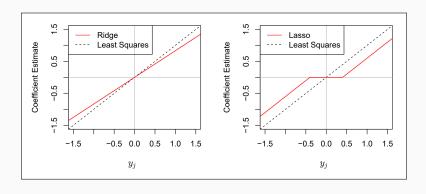
$$loss_{lasso} = \sum_{i=0}^{n} \left( y_i - \sum_{j=0}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=0}^{p} |\beta_j|$$

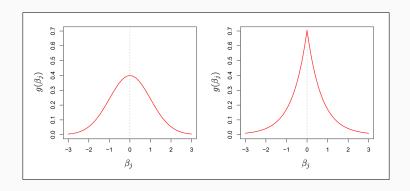






Predictor	Ridge	LASSO
Predictor	Riuge	LASSU
Intercept	23.44	23.44
Weight	-5.59	-4.78
Year	2.75	2.00
Horsepower	-0.07	-0.09
Cylinders	-0.54	0
Acceleration	0.19	0
Displacement	0.66	0





#### 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

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

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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.

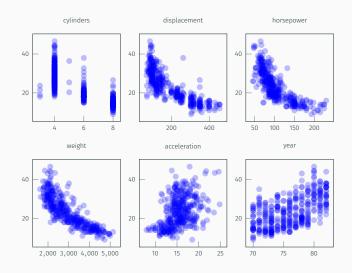
Fits the **best** model to the data while **shrinking** coefficients towards zero such that some variables are effectively **removed**.

## Dimensionality reduction

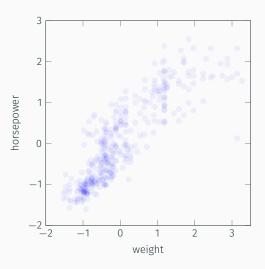
# Dimensionality reduction: Motivation

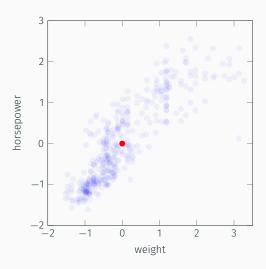
Although we have p predictors, there are actually q < p dimensions of variability in our data, and using q instead of p is going to reduce model complexity.

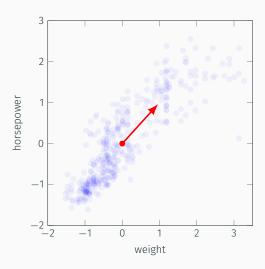
#### Dimensionality reduction: Outline

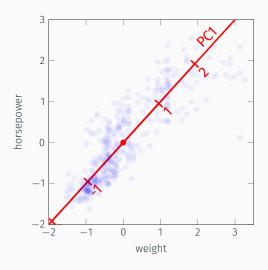


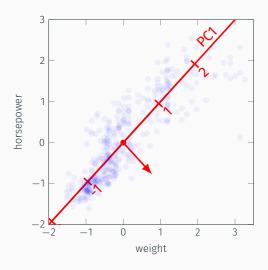
1	0.30	0.86	0.89	0.41	0.93
0.30					
0.86			0.84	0.68	0.89
0.89		0.84		0.50	0.95
0.41		0.68	0.50	1	0.54
0.93		0.89	0.95	0.54	1

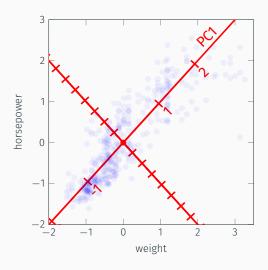


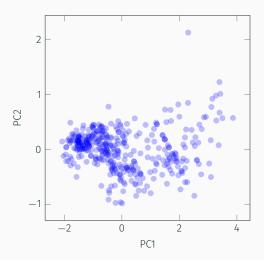












#### Dimensionality reduction: Principal component regression

mpg	horsepower	weight	PC1	PC2
18	130	3504	0.908	0.303
15	165	3693	1.709	0.517
18	150	3436	1.219	0.455
16	150	3433	1.217	0.457
17	140	3449	1.046	0.260
15	198	4341	2.856	0.583
14	220	4354	3.272	0.977

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#### Principal component regression

- 1. Fit a PCA to transform your *p* predictors into *p* principal components.
- 2. Fit a linear regression model using a subset of the principal components.

#### + Positives

- The principal components are orthogonal, so there is no issue of collinearity.
- The principal components are ordered by the amount of variance they explain, so
  we can select the early principal components to explain most of the variability in
  the predictors.

#### - Drawbacks

- · Have to select number of principal components to use.
- What if the principal components that explain the largest amount of variance as not related to the outcome?

## Dimensionality reduction: Partial least squares

Next time