PSY9511: Seminar 3

Regularization and variable selection

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11.09.24

Outline

1. Assignment 2
2. Regularization
    - Variable selection
    - Shrinkage (+ live coding 🥳)

Assignment 2

Assignment 2

Non-numeric horsepower: Expectations Interpretation of year-variable Type of prediction

Assignment 2: Data splitting

In[1]:

```
import pandas as pd


df = pd.DataFrame(...)
train = df.sample(frac=0.8)
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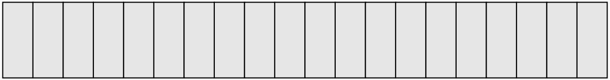

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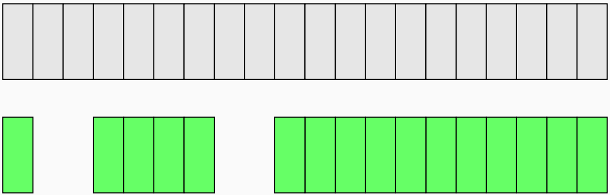

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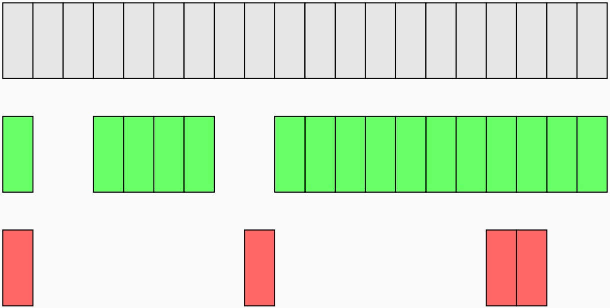
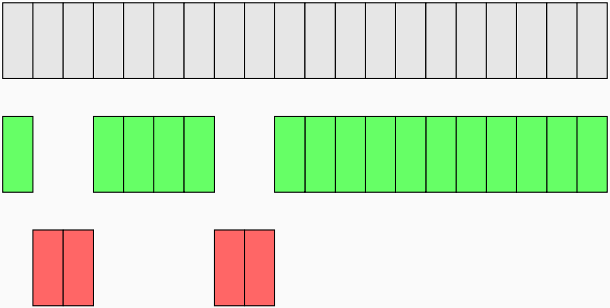


Assignment 2: Data splitting

In[1]:

```
import pandas as pd


df = pd.DataFrame(...)
train = df.sample(frac=0.8)
test = df.drop(train.index)
```



Assignment 2: Random seeds

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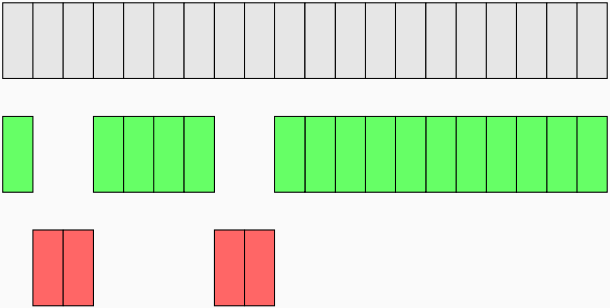

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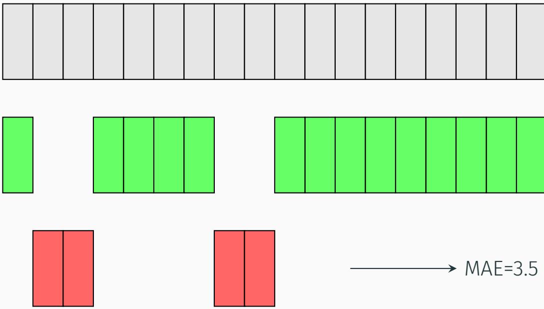

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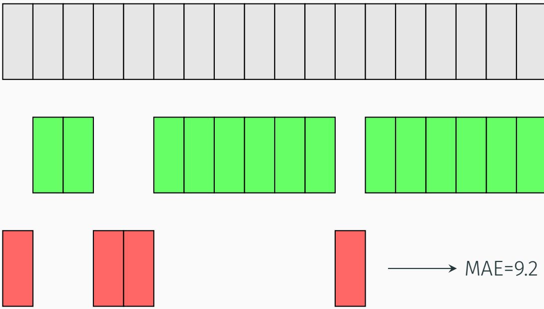
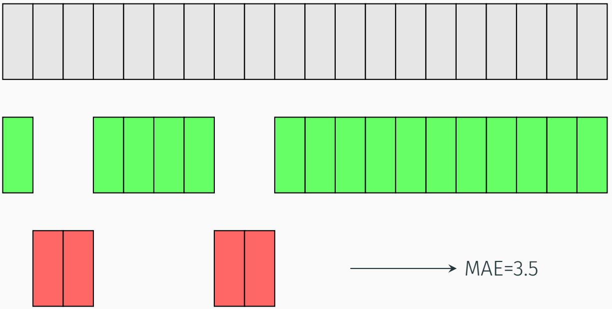


Assignment 2: Random seeds

In[1]:
```python
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)
```



Assignment 2: Log-odds vs probability vs class

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

Assignment 2: Log-odds vs probability vs class

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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
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```

```r
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 
```

Assignment 2: Log-odds vs probability vs class

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

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model <- glm(muscle ~ year + weight, data=df, family='binomial')
predict(model, df)
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```
     1      2      3      4      5      6      7      8      9     10     11
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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)
```

```
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

Regularization: Preparations

$$y \sim \beta_0 + \beta_1 * x_1 + \beta_2 * x_2$$

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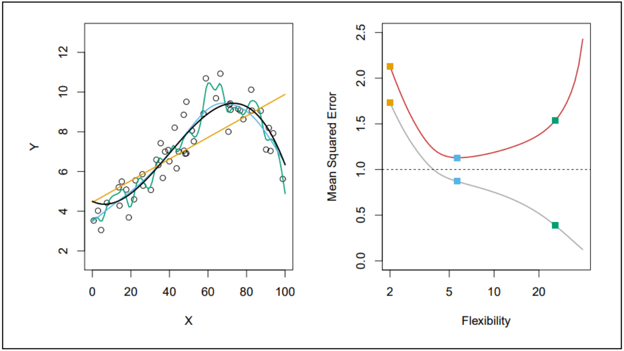
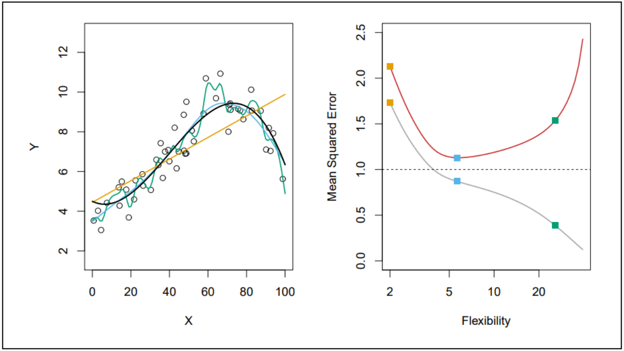


Regularization: Preparations

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



Regularization: Preparations

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

Regularization: Preparations

1. Variable selection
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Variable selection

Variable selection

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

Variable 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.

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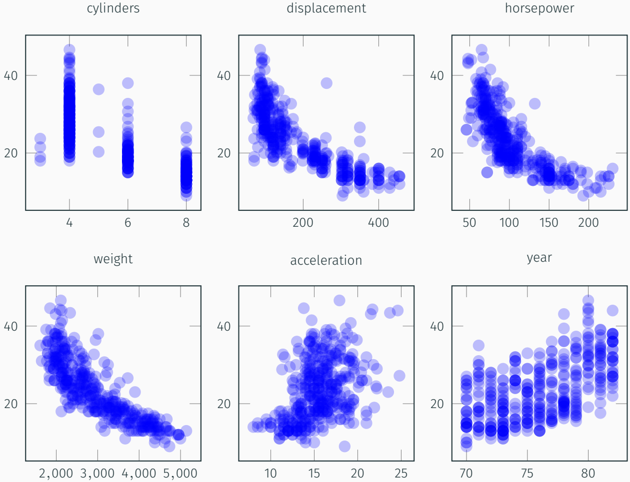
Motivation

To reduce model complexity (and therefore risk of overfitting), and to simplify subsequent interpretations.

Variable selection



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

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

Variable selection: Best subset selection

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']:
        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')
```

Variable selection: Best subset selection

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Solution

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

+ Positives

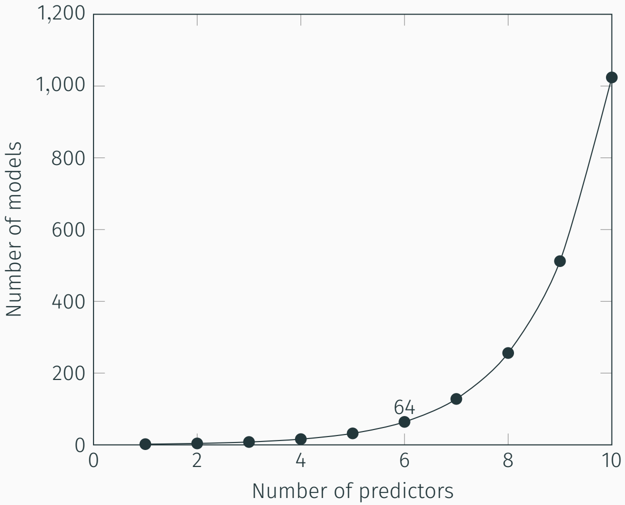
Guaranteed to find the optimal solution.

Simple implementation

- Drawbacks

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

Variable selection: Best subset selection



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.

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$$\boxed{\begin{array}{c} y \sim \mathbb{1} \\ mse = 146.47 \end{array}}$$

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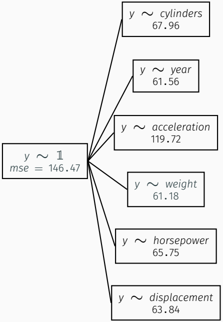

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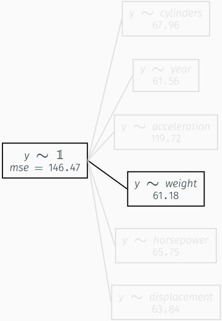

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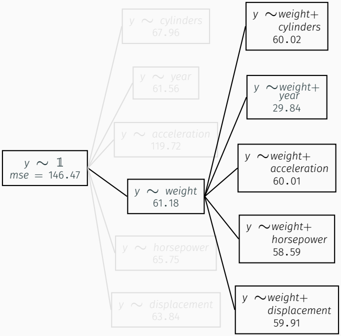

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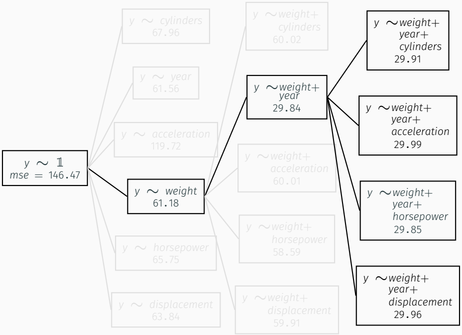

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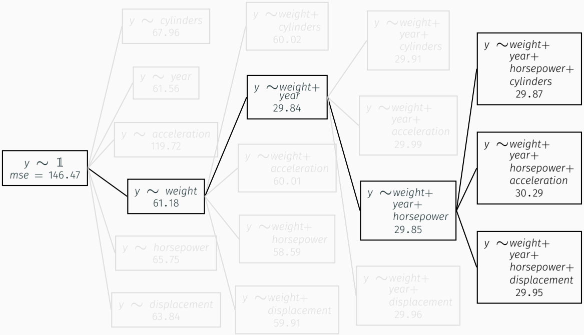

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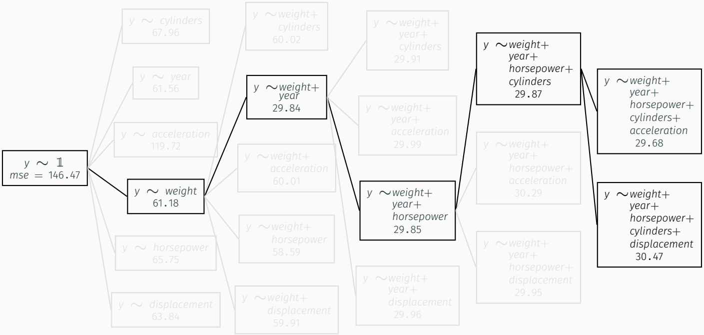

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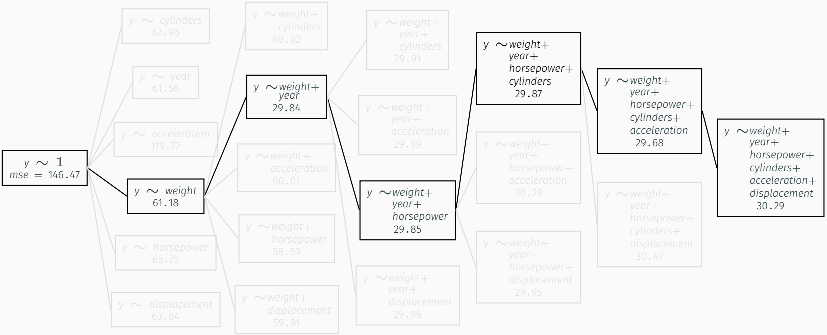

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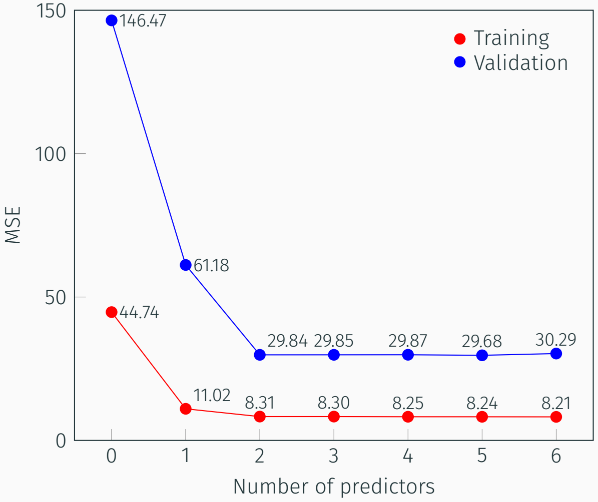

Variable selection: Forward stepwise selection

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})')
```

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.

+ Positives

Need to train fewer models.

- Drawbacks

Not guaranteed to find the optimal solution.

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

Variable selection: Backward stepwise selection

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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.

Solution

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Shrinkage

Shrinkage: Outline

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

Shrinkage: Outline

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

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$$\beta_n \rightarrow 0$$

Shrinkage: Outline

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$$\beta_n \to 0$$

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

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

Shrinkage: Outline

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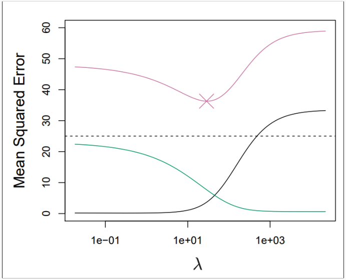

$mse = bias^2 + variance + irreducible\ error$

Shrinkage: Outline

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$$\beta_n \to 0$$

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

Shrinkage: Outline

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

Shrinkage: Outline

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

$$\beta_n \to 0$$

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

Shrinkage: Ridge regression

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

Shrinkage: Ridge regression

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

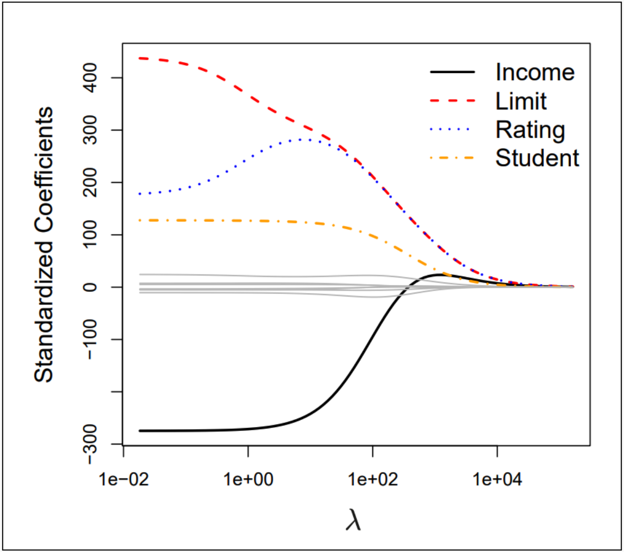
Shrinkage: Ridge regression

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

$$\Downarrow$$

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

Shrinkage: Ridge regression

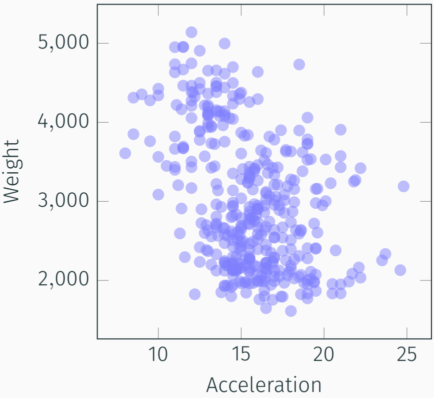


Shrinkage: Ridge regression

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

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

Shrinkage: Feature standardization



Shrinkage: Feature standardization

z-score standardization

Shrinkage: Feature standardization

z-score standardization

$$x = \frac{x - \mu_x}{\sigma_x}$$

Shrinkage: Feature standardization

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)
```

Shrinkage: Ridge regression

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

Shrinkage: Ridge regression

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Blackboard!

Shrinkage: Ridge regression

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

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

Shrinkage: Ridge regression

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

Regularization by shrinking the model covariates towards zero.

Shrinkage: LASSO

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

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

Shrinkage: LASSO

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

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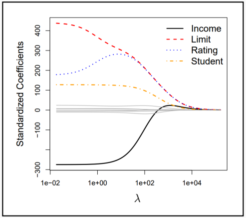
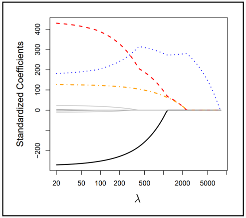
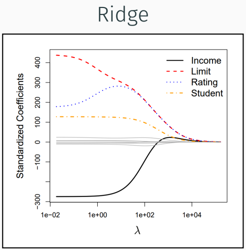
Shrinkage: LASSO

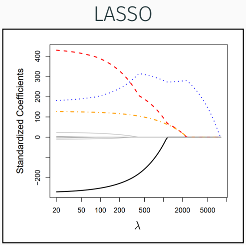
Ridge



LASSO



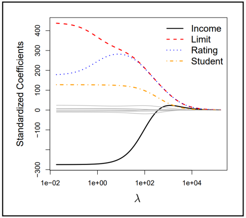




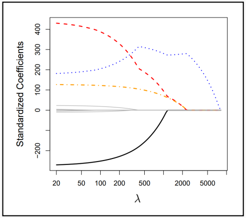
Predictor	Ridge	LASSO
Intercept	23.44	23.44
Weight	-5.59	-4.78
Year	2.75	2.00
Acceleration	0.19	0
Displacement	0.66	0

Shrinkage: LASSO

Ridge



LASSO



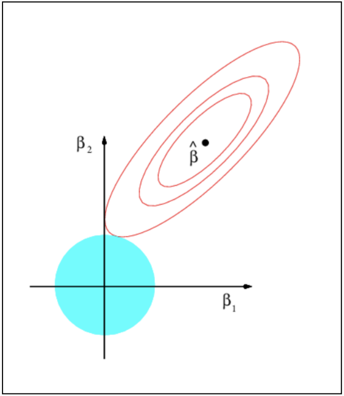
A coefficient of 0 does not mean the predictor has no association with the outcome!

Shrinkage: LASSO

Lasso

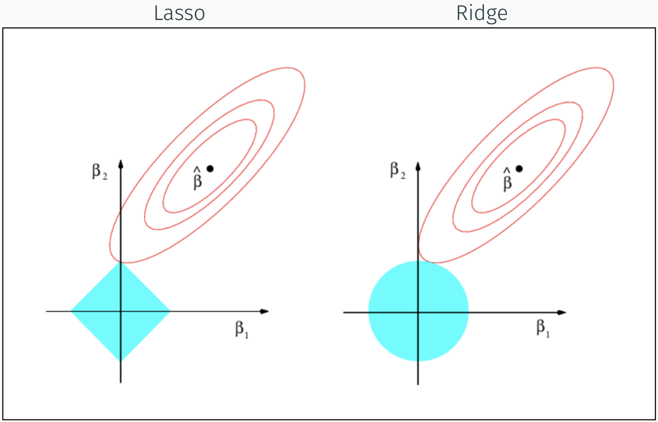
?

Ridge

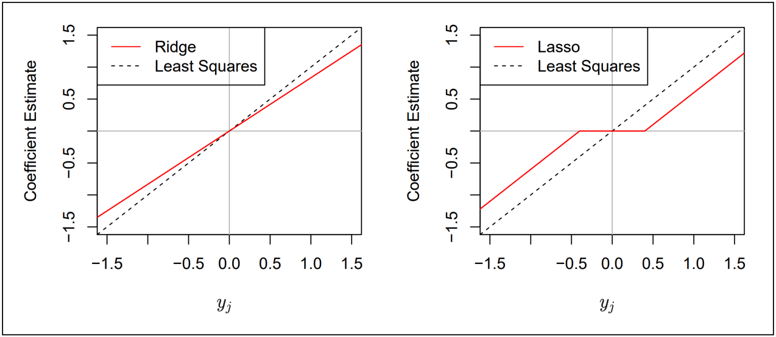


Whiteboard! 🥳

Shrinkage: LASSO



Shrinkage: LASSO



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

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

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

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

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

Shrinkage: Summary

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

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

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

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

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

Assignment 3

Assignment 3

https://uio.instructure.com/courses/53357/assignments/118667?module_item_id=962921

Coding tips: Separation of concerns

In[1]:

```python
# 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 = []

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']:
            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']]
```

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Setup

Selection

Modelling

Housekeeping

Coding tips: Separation of concerns

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predictors = ['cylinders', 'displacement', 'horsepower', 'weight', 'acceleration', 'year']
target = 'mpg'

# Define necessary data structures for state
chosen_predictors = []
mses = []

def fit_and_evaluate(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.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(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

    # Update state
    chosen_predictors.append(best_predictor['predictor'])
    mses.append(best_predictor['mse'])
    predictors = [p for p in predictors if p != best_predictor['predictor']]
```

Modelling