PSY9511: Seminar 3

Variable selection and regularization

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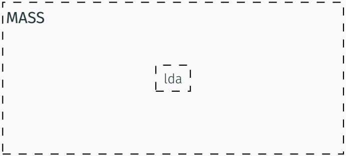
Outline

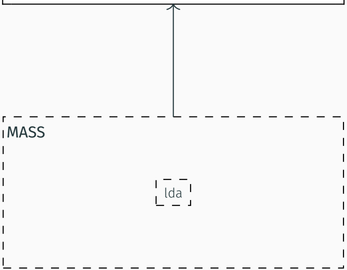
1. Introduction
    - Python
    - Coding tips: Separation of concerns
2. Regularization
    - Variable selection
    - Shrinkage (+ live coding)
    - Dimensionality reduction

Python: Imports



Python: Imports

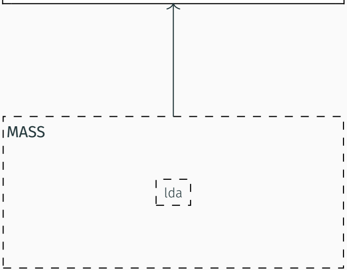
```
library(MASS)
```



Python: Imports

```r
library(MASS)

lda_fit <- lda(display ~ age + fb,
               data = display)
```



Python: Imports

```r
library(MASS)

lda_fit <- lda(display ~ age + fb,
               data = display)
```

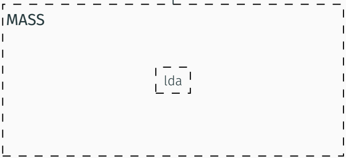
In[1]:
```python
from sklearn import *

lda = discriminant_analysis.
       LinearDiscriminantAnalysis()
lda.fit(display[['age', 'fb']],
        display['display'])
```

Python: Imports

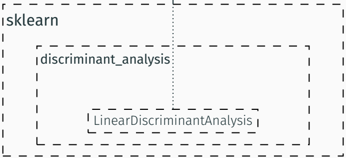
```r
library(MASS)

lda_fit <- lda(display ~ age + fb,
               data = display)
```



In[1]:
```python
import sklearn

lda = sklearn.discriminant_analysis.
       LinearDiscriminantAnalysis()
lda.fit(display[['age', 'fb']],
        display['display'])
```



```r
library(MASS)

lda_fit <- lda(display ~ age + fb,
               data = display)
```

In[1]:
```python
from sklearn.discriminant_analysis \
    import LinearDiscriminantAnalysis

lda = LinearDiscriminantAnalysis()
lda.fit(display[['age', 'fb']],
        display['display'])
```

Python: pandas

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

	mpg	cylinders	displacement	horsepower
1	18	8	307.0	130
2	15	8	350.0	165
3	18	8	318.0	150
4	16	8	304.0	150
5	17	8	302.0	140
6	15	8	429.0	198
7	14	8	454.0	220
8	14	8	440.0	215
9	14	8	455.0	225
10	15	8	390.0	190

In[1]:

```python
import pandas as pd

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

Out[1]:

	mpg	cylinders	displacement	horsepower
0	18	8	307.0	130
1	15	8	350.0	165
2	18	8	318.0	150
3	16	8	304.0	150
4	17	8	302.0	140
5	15	8	429.0	198
6	14	8	454.0	220
7	14	8	440.0	215
8	14	8	455.0	225
9	15	8	390.0	190

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

```r
path <- '/Users/esten/Downloads/Auto.csv'
data <- read.csv(path)

model <- lm(mpg ~ cylinders + displacement +
                  horsepower + weight +
                  acceleration + year,
            data=data)
summary(model)
```

In[1]:

```python
import statsmodels.formula.api as smf

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

model = smf.ols(
    formula='mpg ~ cylinders + displacement +'
            'horsepower + weight + '
            'acceleration + year',
    data=df
)
fit = model.fit()
print(fit.summary())
```

```
Coefficients:
                Estimate Std. Error Pr(>|t|)
(Intercept)  -1.454e+01  4.764e+00  0.00244 **
cylinders    -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
year          7.534e-01  5.262e-02  < 2e-16 ***
---
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
=============================================
```

Python: scikit-learn

In[1]:

```
from sklearn.linear_model import LinearRegression

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

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

model = LinearRegression()
model.fit(df[predictors], df[target])
model.summary()
```

In[1]:
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from sklearn.linear_model import LinearRegression

path = '/Users/esten/Downloads/Auto.csv'
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predictors = ['cylinders', 'displacement', 'horsepower',
              'weight', 'acceleration', 'year']
target = 'mpg'

model = LinearRegression()
model.fit(df[predictors], df[target])
model.summary()
```

Out[1]:
```
---------------------------------------------------------------------------
AttributeError                            Traceback (most recent call last)
Cell In[52], line 13
     11 model = LinearRegression()
     12 model.fit(df[predictors], df[target])
---> 13 model.summary()

AttributeError: 'LinearRegression' object has no attribute 'summary'
```

Python: scikit-learn

In[1]:

```
from sklearn.linear_model import LinearRegression

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

predictors = ['cylinders', 'displacement', 'horsepower',
              'weight', 'acceleration', 'year']
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]...
```

Python: scikit-learn

APIs of scikit-learn objects

To have a uniform API, we try to have a common basic API for all the objects. In addition, to avoid the proliferation of framework code, we try to adopt simple conventions and limit to a minimum the number of methods an object must implement.

Elements of the scikit-learn API are described more definitively in the Glossary of Common Terms and API Elements.

Different objects

The main objects in scikit-learn are (one class can implement multiple interfaces):

Estimator: The base object, implements a `fit` method to learn from data, either:

```
estimator = estimator.fit(data, targets)
```

or:

```
estimator = estimator.fit(data)
```

Predictor: For supervised learning, or some unsupervised problems, implements:

```
prediction = predictor.predict(data)
```

Classification algorithms usually also offer a way to quantify certainty of a prediction, either using `decision_function` or `predict_proba`:

```
probability = predictor.predict_proba(data)
```

Transformer: For filtering or modifying the data, in a supervised or unsupervised way, implements:

```
new_data = transformer.transform(data)
```

When fitting and transforming can be performed much more efficiently together than separately, implements:

```
new_data = transformer.fit_transform(data)
```

Model: A model that can give a goodness of fit measure or a likelihood of unseen data, implements (higher is better):

```
score = model.score(data)
```

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

Python: scikit-learn

In[1]:

```python
from sklearn.linear_model import LinearRegression

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

predictors = ['cylinders', 'displacement', 'horsepower',
              'weight', 'acceleration', 'year']
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]...
```

Python: scikit-learn

In[1]:

```python
from sklearn.svm import SVR

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

predictors = ['cylinders', 'displacement', 'horsepower',
              'weight', 'acceleration', 'year']
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]}...')
```

Out[1]:

```
Intercept: [-35.38646279]
Coefficients: [[-1.0526357   0.05910105  -0.03667206  -0.00831565   0.56218046
       0.96851648]]
Residuals: [3.0266171   0.62154228  3.10666275  1.34695011  3.07475274]...
```

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 = []

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']]
```

Coding tips: Separation of concerns

In[1]:

Setup

```
# 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 = []
```

Selection

```
while len(predictors) > 0:
    best_predictor = {'mse': float('inf'), 'predictor': None}

    for predictor in set(predictors) - set(chosen_predictors):
        potential_predictors = chosen_predictors + [predictor]
```

Modelling

```
        # 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}
```

Housekeeping

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

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 = []

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}

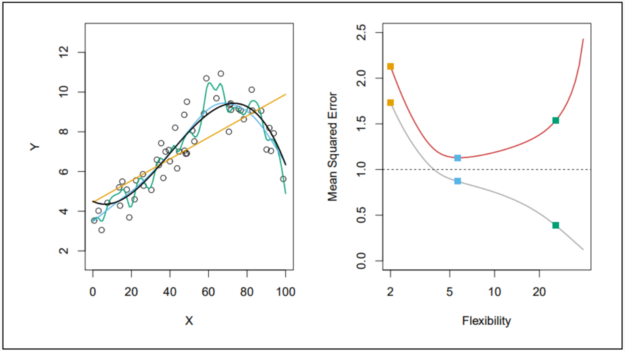
    # Update state
    chosen_predictors.append(best_predictor['predictor'])
    mses.append(best_predictor['mse'])
    predictors = [p for p in predictors if p != best_predictor['predictor']]
```

Modelling

Regularization: Motivation

$$y \sim \beta_0 + \beta_1 * x_1 + \beta_2 * x_2 + \beta_3 * x_3$$

Regularization: Motivation



Regularization: Motivation

$$y \sim \beta_0 + \beta_1 * x_1 + \beta_2 * x_2 + \beta_3 * x_3$$

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

Variable selection: Motivation

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

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.

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.

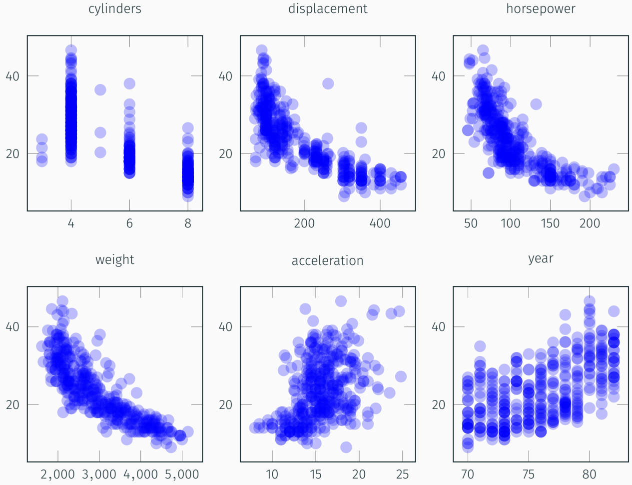
Motivation

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

Variable selection: Outline

Problem

We have a set of predictors $P = \{x_0, x_1, \ldots\}$ 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: 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

Problem

We have a set of predictors $P = \{x_0, x_1, \ldots\}$ 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']:
        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

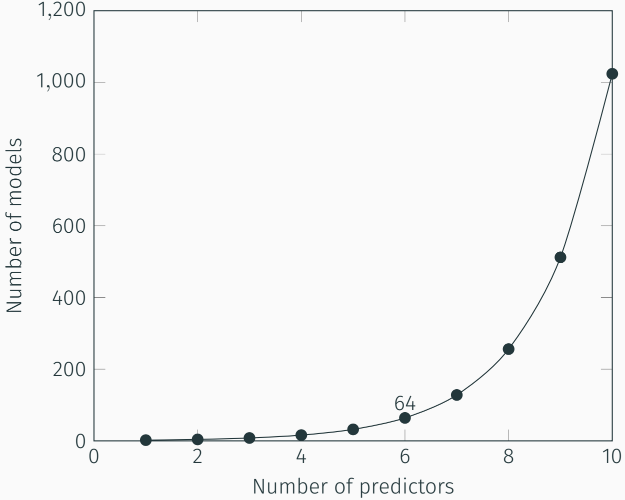
Problem
We have a set of predictors $P = \{x_0, x_1, ...\}$ and a target variable y, and we want to find the subset $p \subseteq P$ that yields the best (linear) model for predicting y.

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

+ 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.

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.

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

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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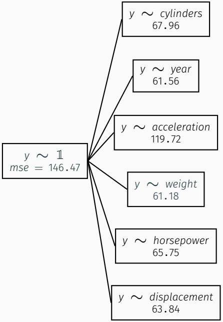

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We have a set of predictors $P = \{x_0, x_1, ...\}$ and a target variable y, and we want to find the subset $p \subseteq P$ that yields the best (linear) model for predicting y.

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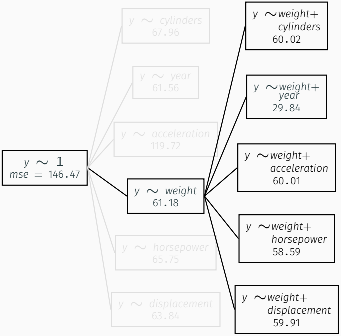

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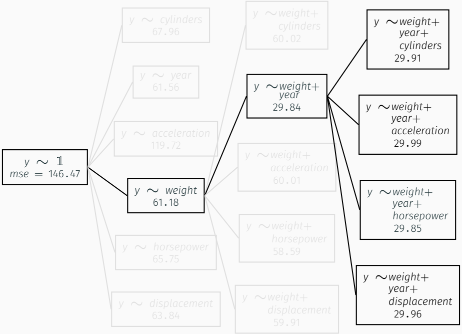

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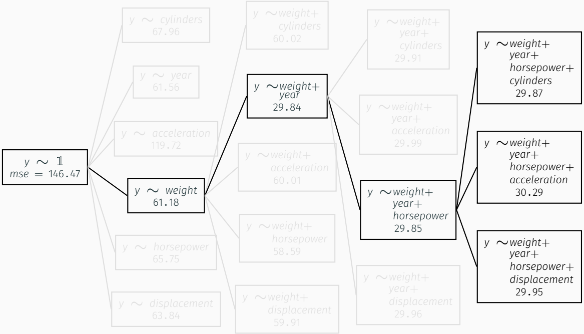
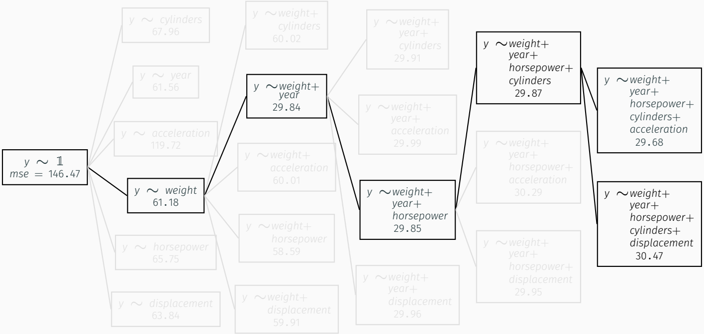


Variable selection: Forward stepwise selection

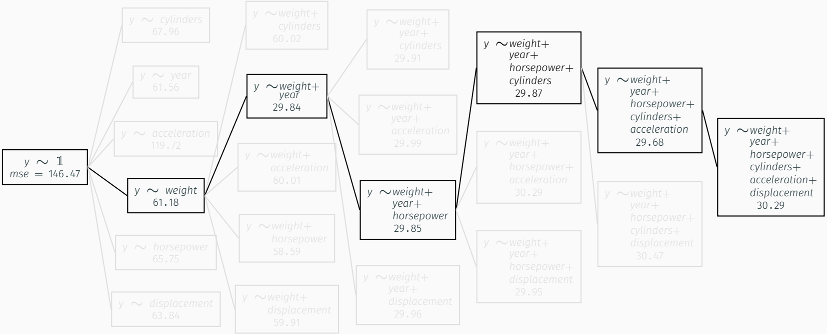
Problem
We have a set of predictors $P = \{x_0, x_1, ...\}$ and a target variable y, and we want to find the subset $p \subseteq P$ that yields the best (linear) model for predicting y.

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

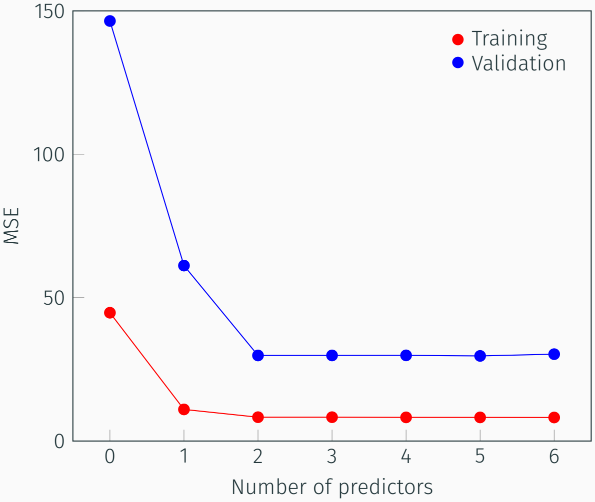


Problem
We have a set of predictors $P = \{x_0, x_1, \ldots\}$ and a target variable y, and we want to find the subset $p \subseteq P$ that yields the best (linear) model for predicting y.

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



Variable selection: Forward stepwise selection



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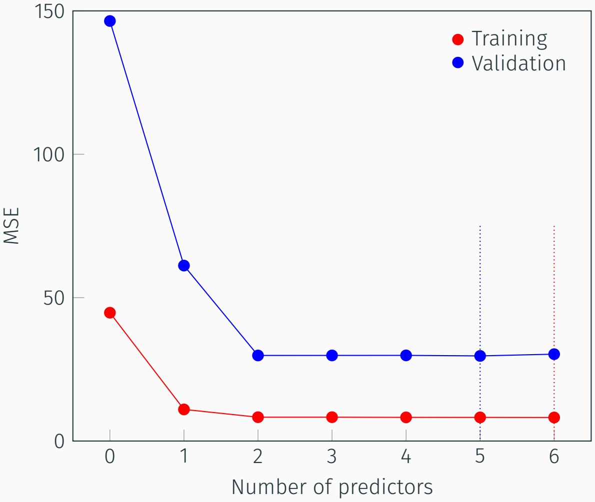

Problem

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

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

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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

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.

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Need to train fewer models.

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Not guaranteed to find the optimal solution.

Shrinkage

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

Shrinkage: Outline

Out[1]:

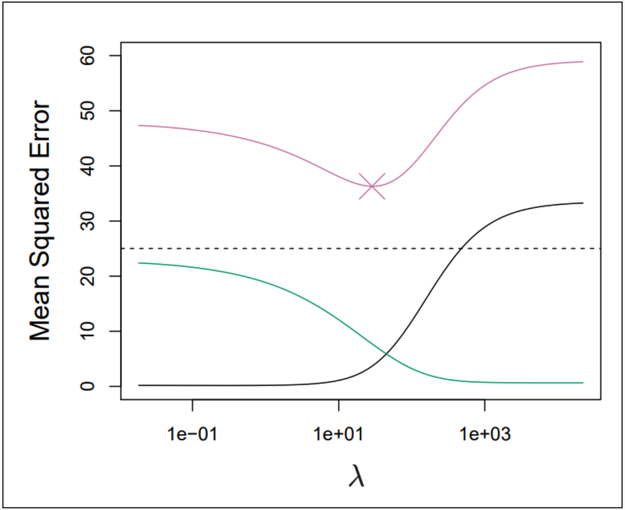
```
coef   std  err   P>|t|   [0.025  0.975]
---------------------------------------------
Intercept     -14.5353 4.764  0.002  -23.90  -5.16
cylinders      -0.3299  0.332  0.321   -0.98   0.32
displacement    0.0077  0.007  0.297   -0.00   0.02
horsepower     -0.0004  0.014  0.977   -0.02   0.02
weight         -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
=============================================
```

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

Shrinkage: Outline

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

Shrinkage: Outline



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

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

$$salary \sim 3000000 + 10000 * age \qquad salary \sim 6000000 + 0 * age$$

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

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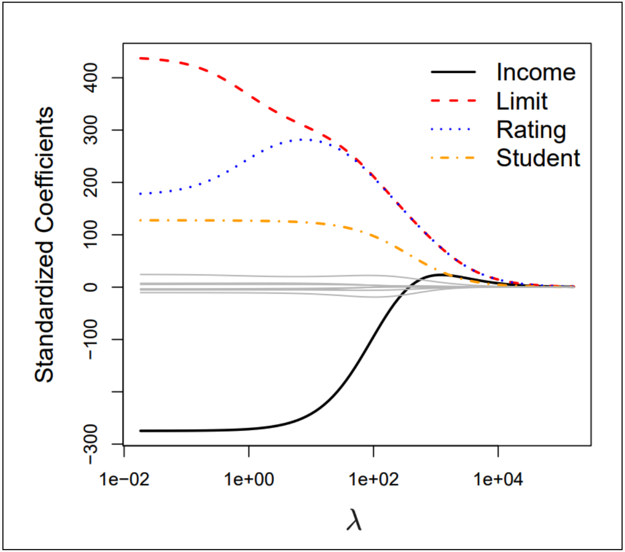
$$\Downarrow$$

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

Shrinkage

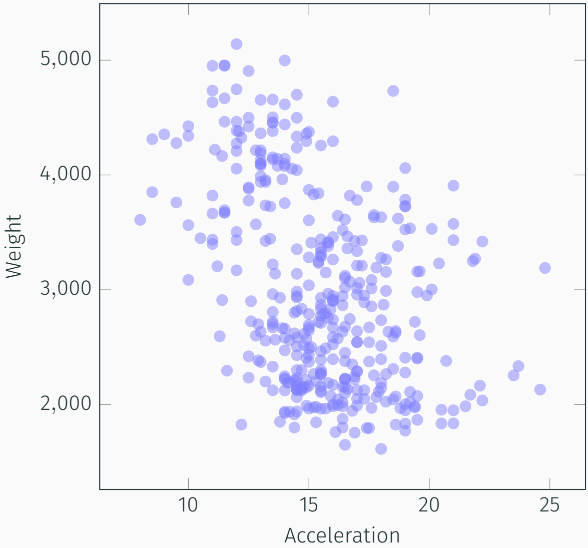


Income
Limit
Rating
Student
Standardized Coefficients
400
300
200
100
0
−100
−300
1e−02
1e+00
1e+02
1e+04
λ

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: Feature standardization



z-score standardization

Shrinkage: Feature standardization

z-score standardization

$$\mathsf{x} = \frac{\mathsf{x} - \mu_{\mathsf{x}}}{\sigma_{\mathsf{x}}^2}$$

Shrinkage: Feature standardization

z-score standardization

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

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})')
```

Shrinkage: Feature standardization

z-score standardization

$$x = \frac{x - \mu_x}{\sigma_x^2}$$

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```

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)
```

Shrinkage: Ridge regression

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 through shrinking the model covariates towards zero.

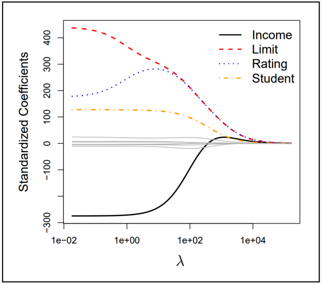
Shrinkage: LASSO

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

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

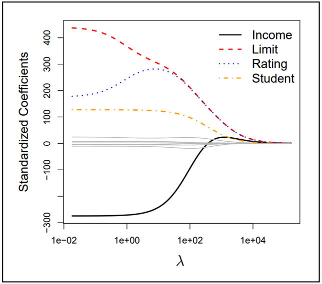
Shrinkage: LASSO

Ridge

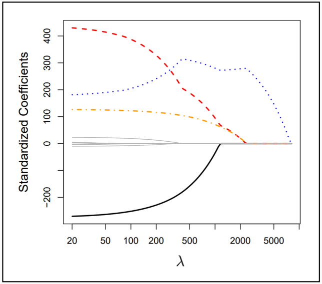


Shrinkage: LASSO

Ridge

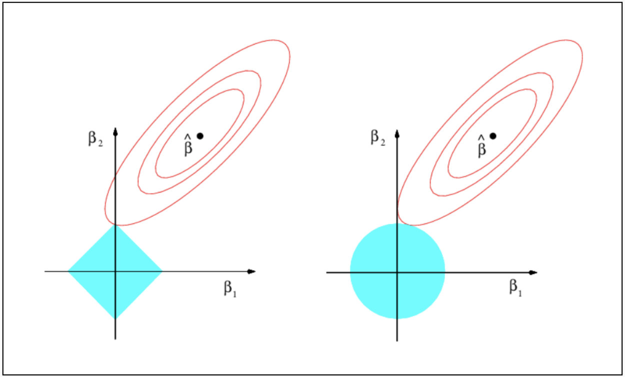


LASSO



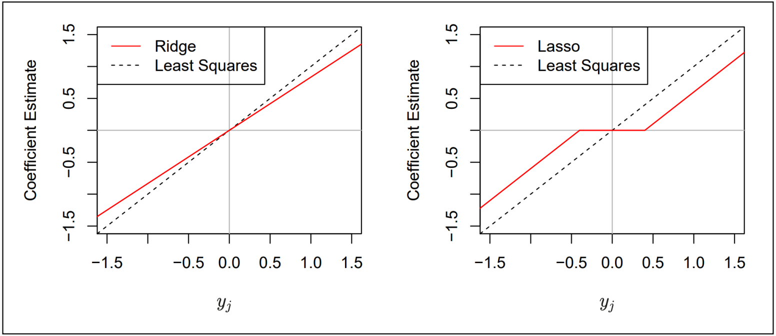
Predictor	Ridge	LASSO
Intercept	23.44	23.44
Weight	-5.59	-4.78
Year	2.75	2.00
Horsepower	-0.07	-0.09
Cylinders	-0.54	0
Acceleration	0.19	0
Displacement	0.66	0

Shrinkage: LASSO

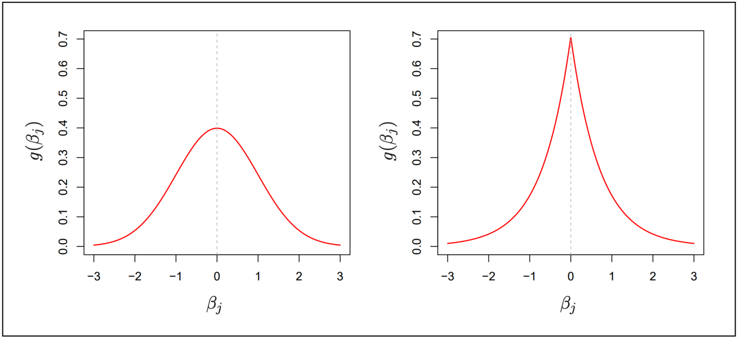


Whiteboard!

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.

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

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

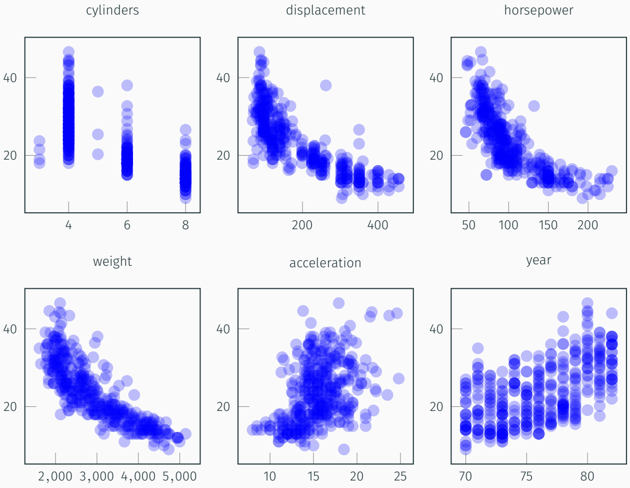
Fits the **best** model to the data while **shrinking** coefficients towards zero such that some variables are effectively **removed**.

Dimensionality reduction

Dimensionality reduction: Motivation

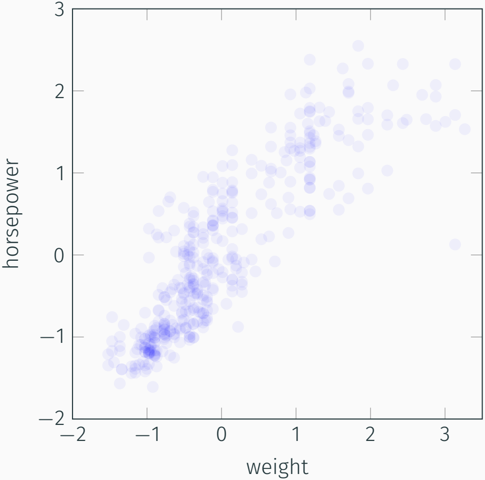
Although we have p predictors, there are actually $q < p$ dimensions of variability in our data, and using q instead of p is going to reduce model complexity.

Dimensionality reduction: Outline

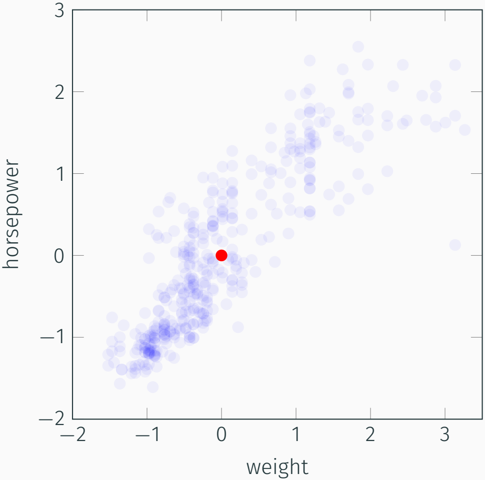


1	0.30	0.86	0.89	0.41	0.93
0.30	1	0.41	0.34	0.29	0.36
0.86	0.41	1	0.84	0.68	0.89
0.89	0.34	0.84	1	0.50	0.95
0.41	0.29	0.68	0.50	1	0.54
0.93	0.36	0.89	0.95	0.54	1

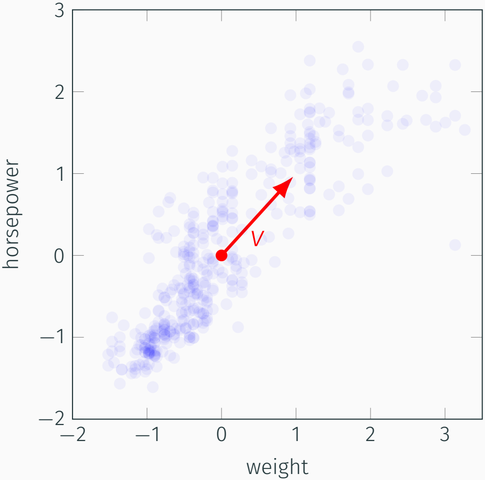
Dimensionality reduction: Principal component analysis



Dimensionality reduction: Principal component analysis

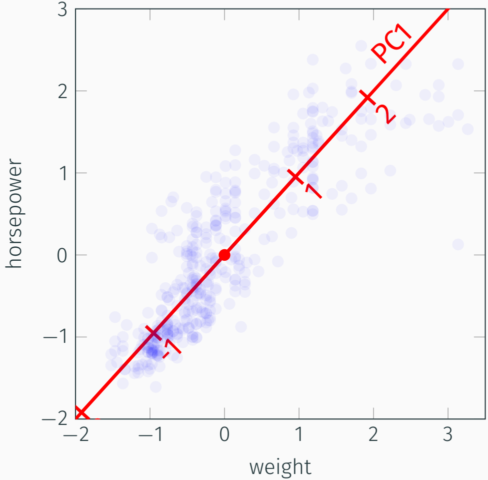


Dimensionality reduction: Principal component analysis

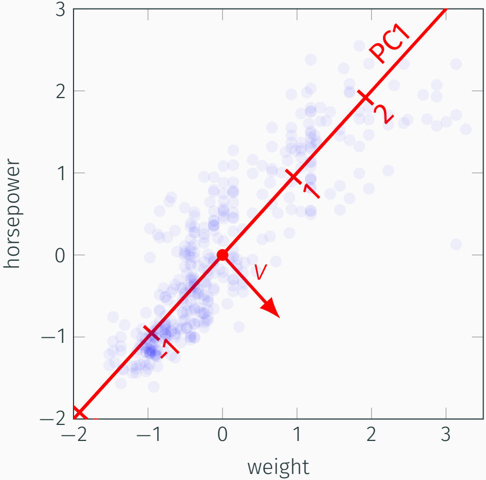


$v \implies$ direction of greatest variance in X

Dimensionality reduction: Principal component analysis

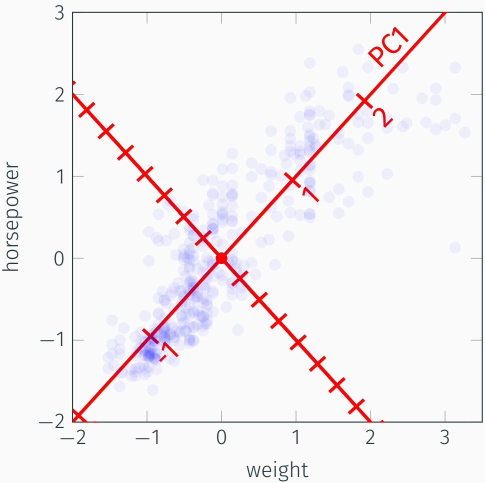


$$PC1 = 0.69 * horsepower + 0.71 * weight$$



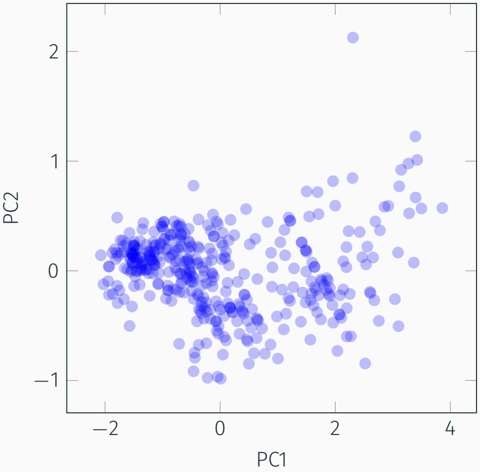
$v \implies$ direction of greatest variance in X **after regressing out PC1**

Dimensionality reduction: Principal component analysis



$$PC2 = 0.69 * horsepower + 0.71 * weight$$

Dimensionality reduction: Principal component analysis



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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$$mpg \sim \beta_0 + \beta_1 * horsepower + \beta_2 * weight$$

Dimensionality reduction: Principal component regression

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$$mpg \sim \beta_0 + \beta_1 * horsepower + \beta_2 * weight$$

$$mpg \sim \beta_0 + \beta_1 * PC1 + \beta_2 * PC2$$

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.

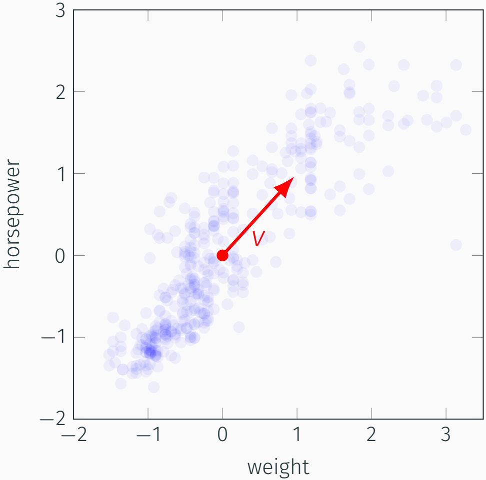
+ Positives

- 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 the early principal components are (probably) the best predictors.

- Drawbacks

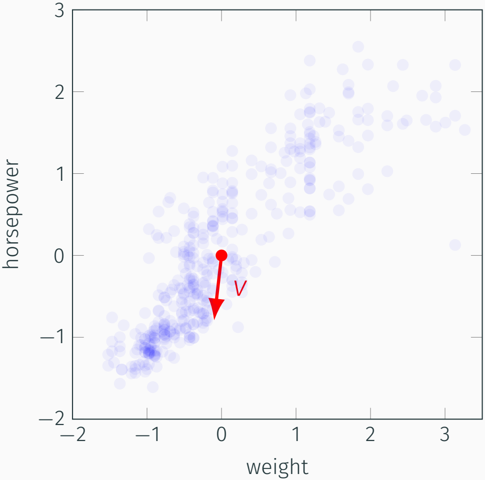
- Have to select number of principal components to use.
- What if the principal components that explain the largest amount of variance are not related to the outcome?

Dimensionality reduction: Partial least squares



$v \implies$ direction of greatest variance in X

Dimensionality reduction: Partial least squares



$v \implies$ direction of greatest covariance between X and Y