Overview

This tutorial will focus on Generalized Linear Models

We will include some additional topics, including:

- Attribute normalization to improve interpretability
- L1 regularization
- L2 regularization
- (Cross)-validation

The lecture relies on the the following proficiencies and tools:

- Python programming
- Vector computations via the numpy module
- Data handling using the pandas module
- Plotting using matplotlib
- Training and using Machine Learning model via scikit-learn

You will need them only if you plan to handle these tasks yourself

Normalization

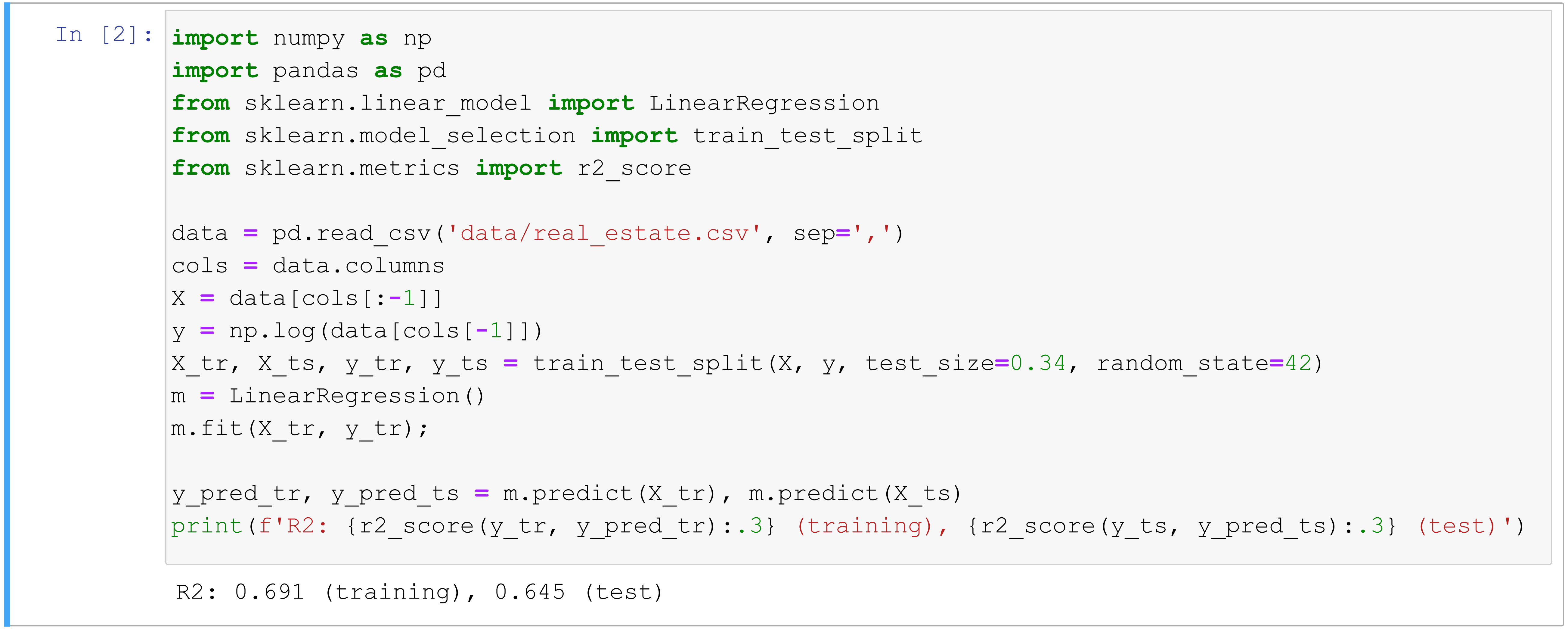
Impact of Individual Attributes

We may be interested in understanding the impact of individual attributes

- E.g. is the price more impacted by age, distance from MRT stations, or what?

A Straightforward Approach

Let's start by repeating our basic linear regression approach



In [2]:

```python
import numpy as np
import pandas as pd
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
from sklearn.metrics import r2_score

data = pd.read_csv('data/real_estate.csv', sep=',')
cols = data.columns
X = data[cols[:-1]]
y = np.log(data[cols[-1]])
X_tr, X_ts, y_tr, y_ts = train_test_split(X, y, test_size=0.34, random_state=42)
m = LinearRegression()
m.fit(X_tr, y_tr);

y_pred_tr, y_pred_ts = m.predict(X_tr), m.predict(X_ts)
print(f'R2: {r2_score(y_tr, y_pred_tr):.3} (training), {r2_score(y_ts, y_pred_ts):.3} (test)')
```

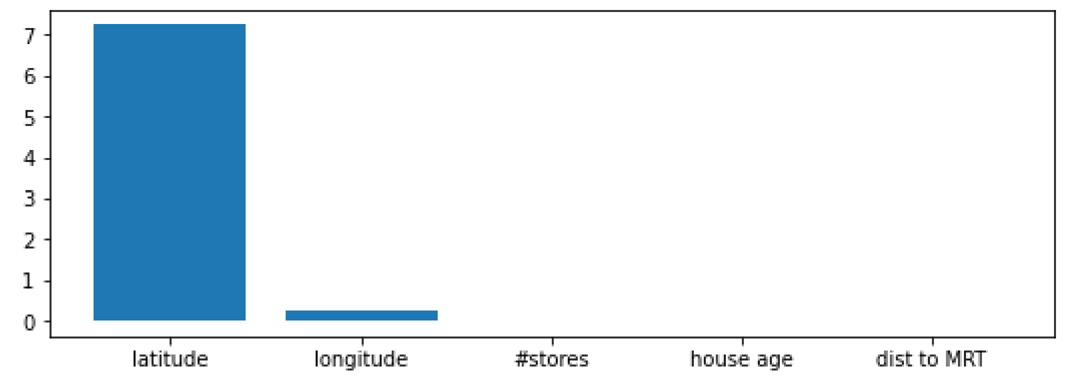
```
R2: 0.691 (training), 0.645 (test)
```

- We load the dataset, separate input & output, split the training and test set
- The we fit the model and evaluate the results

A Straightforward Approach

We can think of looking at the coefficients

```
In [3]: from matplotlib import pyplot as plt
        idx = np.argsort(-np.abs(m.coef_)) # Sort indexes by decreasing absolute coefficient
        scores = m.coef_[idx] # Coefficients, in the order defined by idx
        plt.figure(figsize=(9, 3))
        plt.bar(0.5 + np.arange(len(idx)), scores, tick_label=X.columns[idx]);
```



- Intuition: the higher the (absolute) weight, the more important the attribute
- Positive coefficient = price increase, negative coefficient = price decrease

A Straightforward Approach

There is a (huge) pitfall with this approach

- Each coefficient depends on the importance of an attribute
- ...But also on its scale!

An attribute with larger values may end up with a smaller coefficient

We can preprocess the data so that all attributes have similar scales

A couple of common approaches:

Normalization/Standardization

Scikit learn provides simple tools to take care of this step

The are called `MinMaxScaler` and `StandardScaler`:

```
In [4]: from sklearn.preprocessing import StandardScaler # for standardization

        scaler = StandardScaler()

        X_tr_s = scaler.fit_transform(X_tr)
```

On the training set:

- We calibrate the scaler (i.e. compute the mean and st. dev.)
- The we apply the transformation

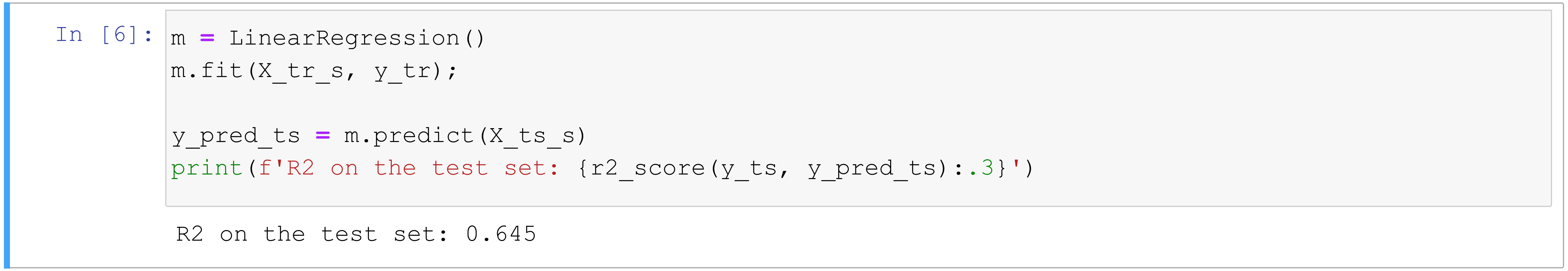
```
In [5]: X_ts_s = scaler.transform(X_ts)
```

On the test set we simply apply the transformation

- We do not want information about the test data to "leak" into the model

The Correct Approach

We can then repeat the process using the scaled data



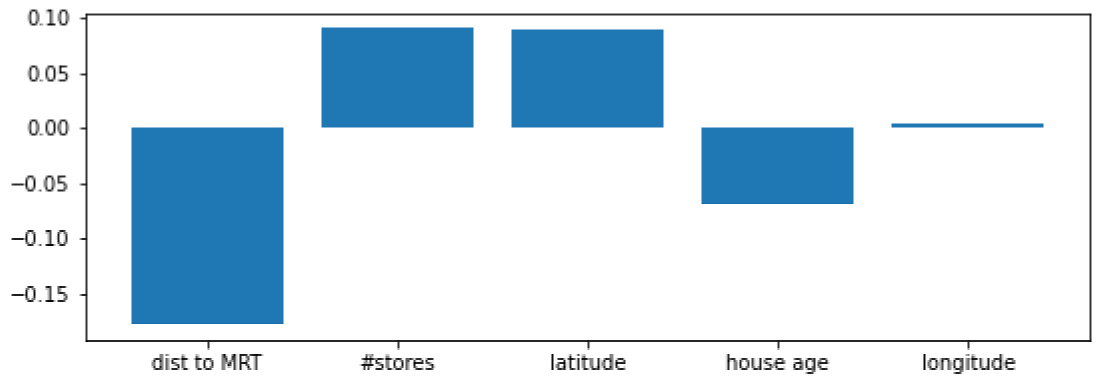
```
In [6]: m = LinearRegression()
        m.fit(X_tr_s, y_tr);

        y_pred_ts = m.predict(X_ts_s)
        print(f'R2 on the test set: {r2_score(y_ts, y_pred_ts):.3}')

        R2 on the test set: 0.645
```

- The quality of the predictions is the same as before
- ...Since we have applied only a linear transformation to the input

The Correct Approach

Now we can build and inspect the same plot as before

```
In [7]: idx = np.argsort(-np.abs(m.coef_)) # Sort indexes by decreasing absolute coefficient
        scores = m.coef_[idx] # Coefficients, in the order defined by idx
        plt.figure(figsize=(9, 3))
        plt.bar(0.5 + np.arange(len(idx)), scores, tick_label=X.columns[idx]);
```



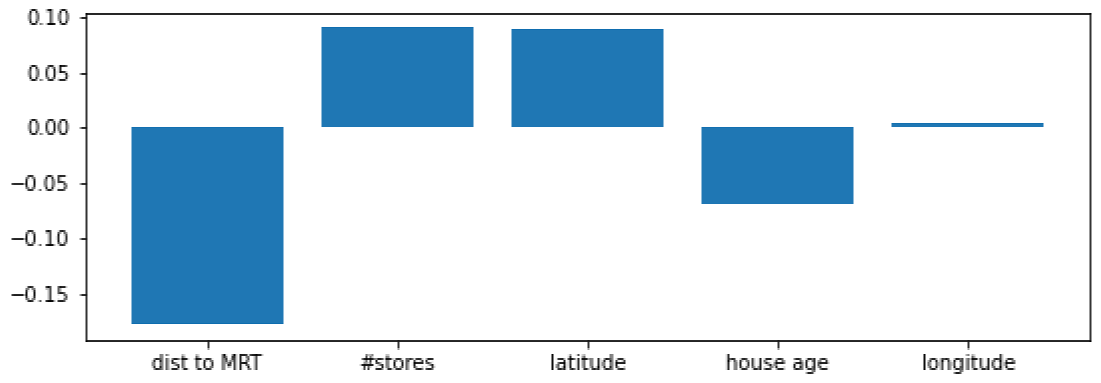
- The order of the attributes has changed!
- Positive/negative values = positive/negative effect if above average

LASSO

Attribute Selection

Let's look again at the last plot

```
In [8]: plt.figure(figsize=(9, 3))
        plt.bar(0.5 + np.arange(len(idx)), scores, tick_label=X.columns[idx]);
```



- The "longitude" attribute has very low importance
- Given that, is it worth keeping the attribute at all?
- Collecting useless attributes has still a cost

Attribute Selection

Choosing which attributes to keep is known as attribute selection

There are multiple solution approaches

- An exact (but costly) one: consider all possible sets and repeat training
- A cheap (but heuristic) one: remove attributes with small (abs.) coefficients

In the case of linear regression, we have a third option

We can act on the structure of the loss (error) function used during training:

$$L(w) = MSE(w) + \alpha \|w\|_1$$

- Where $\|w\|_1 = \sum_{j=1}^{n} |w_j|$
- The additional term $\|w\|$ is introduced to make mode model "well behaved"
- ...And for this reason it is called a reguralizer
- In particular, since we are using the L1 norm, we call it an L1 regularizer

LASSO

At training time, we will need to solve

$$\text{argmin}_w MSE(w) + \alpha \|w\|_1$$

For reasons not discussed in detail:

- If raising a coefficient does not provide enough error improvement
- ...Then the attribute will not be used at all
- What "enough" means in practice depends on the value of α

As a result, we naturally end-up doing attribute selection

The approach is known as Least Absolute Shrinkage and Selection Operator

- ...Or LASSO for short :-)

Using LASSO

Scikit-learn provides a convenient LASSO implementation

```
In [9]: from sklearn.linear_model import Lasso

        m2 = Lasso(alpha=1.0)
```

- When building the model, we need to pick a value for α
- Higher α values promote using fewer attributes
- ...Bu they also reduce the prediction quality

For now, we will fix α via trial-and-error approach:

```
In [10]: m2.fit(X_tr_s, y_tr);
         y_pred_tr2 = m2.predict(X_tr_s)
         print(f'R2 on the training set: {r2_score(y_tr, y_pred_tr2):.3}')

         R2 on the training set: 0.0
```

- This is too low, and therefore $\alpha = 1.0$ is too large

Choosing α

```
In [11]: m2 = Lasso(alpha=0.1)
         m2.fit(X_tr_s, y_tr);
         y_pred_tr2 = m2.predict(X_tr_s)
         print(f'R2 on the training set: {r2_score(y_tr, y_pred_tr2):.3}')
```

```
R2 on the training set: 0.549
```

- The prediction quality is still much lower than the original one

```
In [12]: m2 = Lasso(alpha=0.05)
         m2.fit(X_tr_s, y_tr);
         y_pred_tr2 = m2.predict(X_tr_s)
         print(f'R2 on the training set: {r2_score(y_tr, y_pred_tr2):.3}')
```

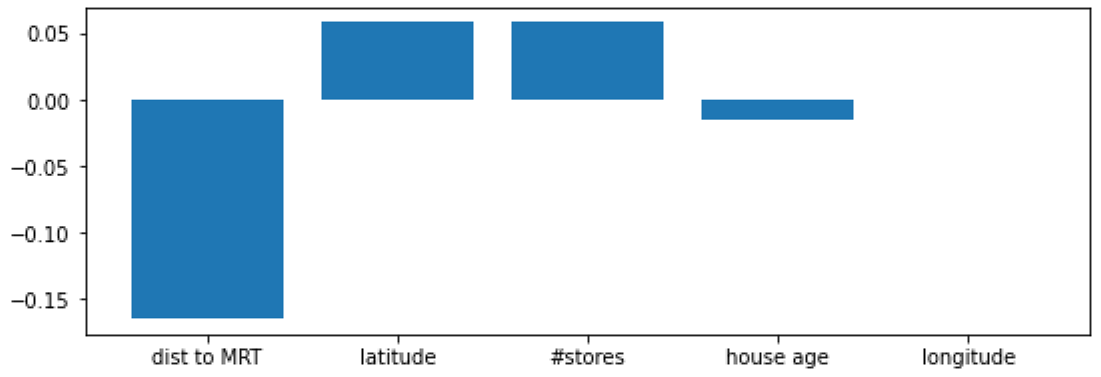
```
R2 on the training set: 0.643
```

- Now we are back to the original value (more or less)!

Impact of Each Attribute

Once we are satisfied with the α values, we can inspect the coefficients

In [13]:
```
idx = np.argsort(-np.abs(m2.coef_))
scores = m2.coef_[idx]
plt.figure(figsize=(9, 3))
plt.bar(0.5 + np.arange(len(idx)), scores, tick_label=X.columns[idx]);
```

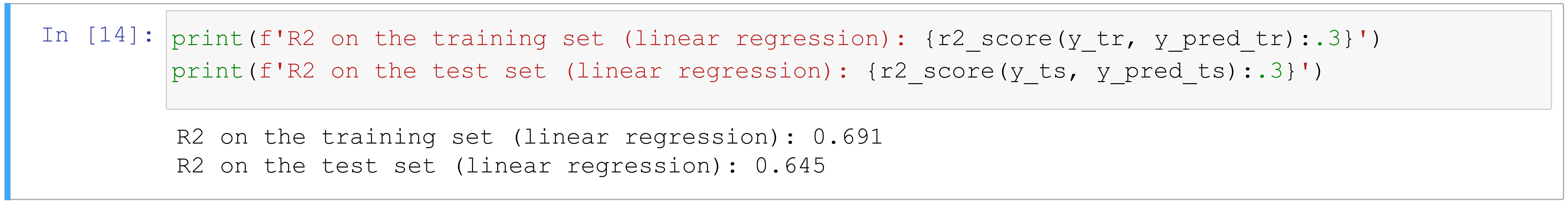


- The "longitude" attribute has been dropped
- When there are many attributes, the LASSO method can be extremely useful

Ridge Regression

Overfitting

We have already observed how our model has a modest degree of overfitting



```
In [14]: print(f'R2 on the training set (linear regression): {r2_score(y_tr, y_pred_tr):.3}')
         print(f'R2 on the test set (linear regression): {r2_score(y_ts, y_pred_ts):.3}')

R2 on the training set (linear regression): 0.691
R2 on the test set (linear regression): 0.645
```

Overfitting arises when:

- The model learns patterns in the training set
- ...That do not repeat on unseen data (e.g. since they due to random sampling)

This becomes more critical with many attributes and scarce data

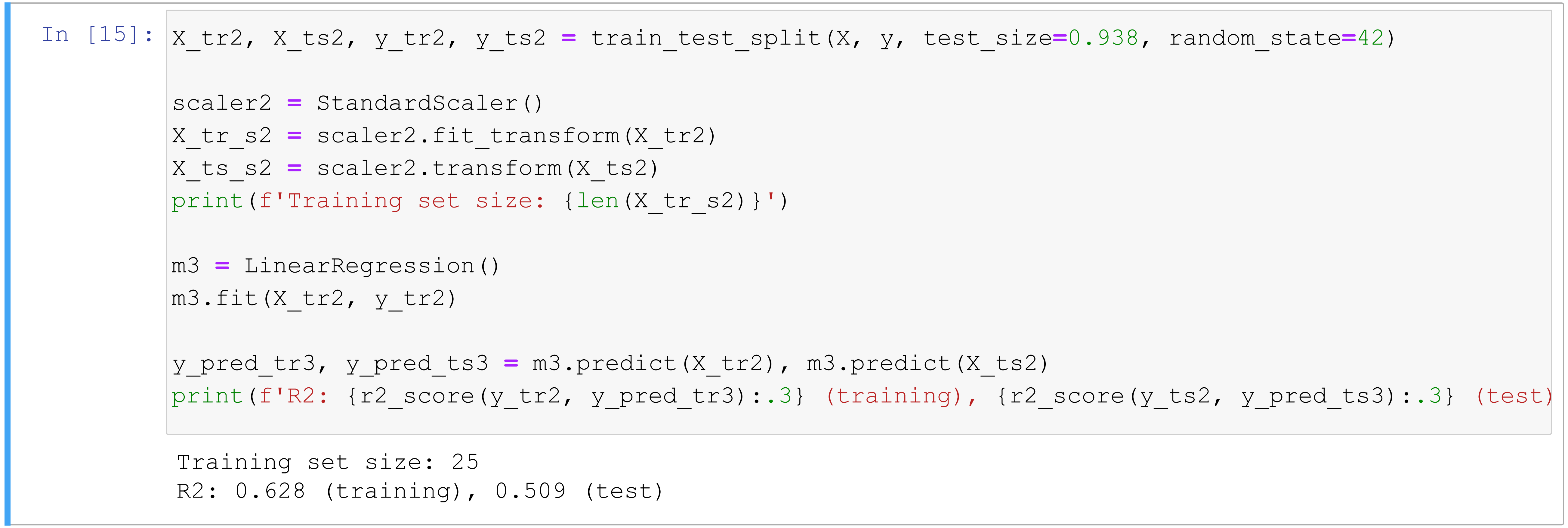
- A linear regression model with n coefficients
- ...Can interpolate perfectly any collections of n examples

...But typically, that means we learning noise

First, Let's Make It Worse

First, let's amplify the problem, so as to make any change more significant

In particular, we will reduce the amount of available training data



In [15]:

```python
X_tr2, X_ts2, y_tr2, y_ts2 = train_test_split(X, y, test_size=0.938, random_state=42)

scaler2 = StandardScaler()
X_tr_s2 = scaler2.fit_transform(X_tr2)
X_ts_s2 = scaler2.transform(X_ts2)
print(f'Training set size: {len(X_tr_s2)}')

m3 = LinearRegression()
m3.fit(X_tr2, y_tr2)

y_pred_tr3, y_pred_ts3 = m3.predict(X_tr2), m3.predict(X_ts2)
print(f'R2: {r2_score(y_tr2, y_pred_tr3):.3} (training), {r2_score(y_ts2, y_pred_ts3):.3} (test)
```

```
Training set size: 25
R2: 0.628 (training), 0.509 (test)
```

- Having access to little data is not uncommon
- Raw measurements are easy to obtain, but targets may be expensive to collect

Ridge Regression

We will show how to reduce overfitting by using ridge regression

...Which is obtained from linear regression by adding a quadratic reguralizer:

$$\text{argmin}_w MSE(w) + \alpha \|w\|_2^2$$

where $\|w\|_2^2 = \sum_{j=1}^{2} w_j^2$

- Since the $\|w\|_2$ is an L2 norm, this is called an L2 regularizer
- It looks similar to the L1 regularizer in the LASSO approach
- ...But it has a very different effect

This regularizer prevents weights from having a large absolute value

- Smaller (absolute) weights result in smoother behavior
- ...Which typically leads to better generalization

Using Ridge Regression

Scikit-learn provides an implementation for Ridge Regression

In [16]:
```
from sklearn.linear_model import Ridge
m4 = Ridge(alpha=1.0)
m4.fit(X_tr_s2, y_tr2);
```

It works similarly to the `Lasso` class

- When we build the model, we need to specify a value for α
- ...Then we train the model as usual

In [17]:
```
y_pred_tr4 = m4.predict(X_tr_s2)
y_pred_ts4 = m4.predict(X_ts_s2)
print(f'R2 on the training set: {r2_score(y_tr2, y_pred_tr4):.3}')
print(f'R2 on the test set: {r2_score(y_ts2, y_pred_ts4):.3}')
```

```
R2 on the training set: 0.627
R2 on the test set: 0.534
```

Cross-Validation and Hyper-Parameter Tuning

This time, we will follow a systematic approach to pick a value for α

- Our goal is to improve the model results on unseen examples
- So we can choose $\boldsymbol{\alpha}$ to minimize the error on examples not in the training set

It would be tempting to optimize α for the test set...

...But it would also be very wrong

- The test set is our ultimate approach to assess generalization
- For this, its content stay unseen whenever we calibrate parameters

We can however split yet another set on this purpose

- This would not be used to train the model
- ...But only for tuning the training parameters (also called hyper-parameters)

This is called a validation set

- But there is a drawback: we have even less data available for training

Cross-Validation and Hyper-Parameter Tuning

As an alternative, we can use k-fold cross-validation:

- We partition the training data in k sets, called folds
- For $i = 1..k$:
  - We separate the i-th fold
  - We train a model on the remaining data
  - We evaluate the prediction quality on the separated fold
  - Then we put the fold back

During each iteration, the examples in the i-th folder are effectively unseen

At the end of the process we have:

- k models (that typically we don't use)
- k prediction quality evaluations (of which we can take the mean)

We can use cross validation to assess how good a model is with unseen data

Applying Cross-Validation and Hyper-Parameter Tuning

Scikit learn allows us to automate this process with a few lines of code

- First we specify which parameters we want to tune
- ...And which range we want to investigate

We do so by building a dictionary:

```
In [18]: param_ranges = {'alpha': np.logspace(0, 2, 100)}
```

- The dictionary keys are the parameters to be tuned
- The entries are the values to be tested

Then we build a `GridSearchCV` object:

```
In [19]: from sklearn.model_selection import GridSearchCV

         gscv = GridSearchCV(estimator=Ridge(), param_grid=param_ranges, cv=5)
```

Applying Cross-Validation and Hyper-Parameter Tuning

The we can "train" the `GridSearchCV` object

- This will try all combinations of the values in parameter ranges
- ...And pick the parameters leading to the best cross-validation score

```
In [20]: gscv.fit(X_tr_s2, y_tr2);
```

The best parameters can be accessed via the `best_params_` field:

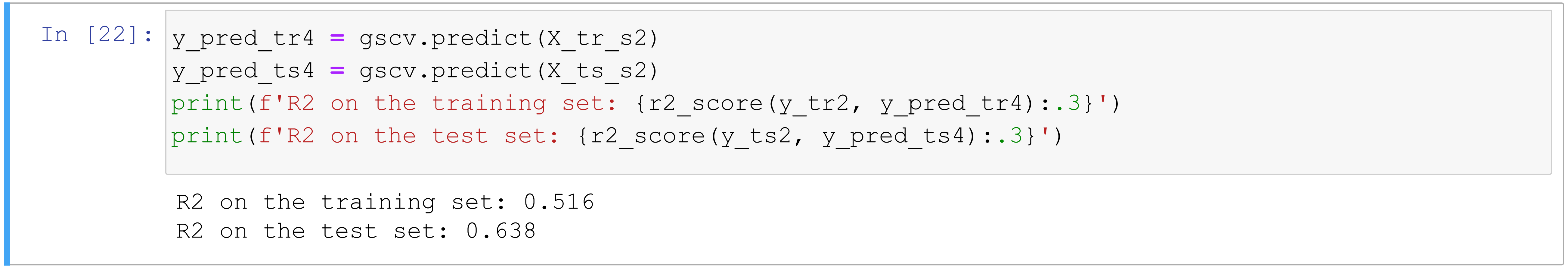
```
In [21]: gscv.best_params_

Out[21]: {'alpha': 27.185882427329414}
```

Applying Cross-Validation and Hyper-Parameter Tuning

By default, the `GridSearchCV` object:

- Trains an estimator with the best parameters on all data
- This is the model that we are going to use

Calling `predict` on `GridSearchCV` calls the same method on the best estimator:



```
In [22]: y_pred_tr4 = gscv.predict(X_tr_s2)
         y_pred_ts4 = gscv.predict(X_ts_s2)
         print(f'R2 on the training set: {r2_score(y_tr2, y_pred_tr4):.3}')
         print(f'R2 on the test set: {r2_score(y_ts2, y_pred_ts4):.3}')

         R2 on the training set: 0.516
         R2 on the test set: 0.638
```

- This is close to our original approach on unseen data
- ...Even if we using only 25 data points!

Conclusions and Take-Home Messages

- Attribute normalization to improve interpretability
  - Linear Regression is a rather interpretable ML model...
  - ...Provided that attributes are processed to have a similar scale
- L1 regularization
  - L1 regularization can be employed for automatic attribute selection
  - ...And it also helps reducing overfitting
- L2 regularization
  - L2 regularization is mostly about reducing overfitting
  - ...But for that it works better than L1 regularization
- (Cross)-validation
  - Validation data can be used to calibrate hyper-parameters
  - ...Such as the regularization weights
  - Cross-validation enables a more efficient use of data