More Machine Learning

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Overview

- 3 data sets
    - randomly generated sine curve with noise
    - randomly generated irrelevant features
    - Boston housing prices (kaggle)
- 4 models
    - random forest
    - neural network
    - linear regression
    - LASSO
- Main topic: overfitting and how to avoid it

Tuning hyperparameters

- In a random forest, max_depth is a hyperparameter (specified in advance, not fitted by the algorithm).
- In a neural network, hidden_layer_sizes is a hyperparameter.
- There are ways to use the data to select the best hyperparameter, called tuning the hyperparameter.

Overfitting

- In general, we want to choose a hyperparameter to get the best fit to the data without overfitting.
- More complex models may overfit the data and not work well on new data.
- We have to assess how well the model and hyperparameter work on data not used in the training.

Train-test split

- We'll use scikit-learn's train-test-split function.
- Randomly select a subset of the data for training. The rest is used for testing.
- Can specify test size as a fraction of the whole.

Dataset 1

In [2]:

```
# sine curve
def curve(x):
    return 2 * np.sin(2 * x)

# Generate data
np.random.seed(0)
X1 = np.random.uniform(low=-5, high=5, size=(1000, 1))
y1 = curve(X1) + np.random.normal(scale=2, size=(1000, 1))
y1 = y1.flatten()
```

Train-test split

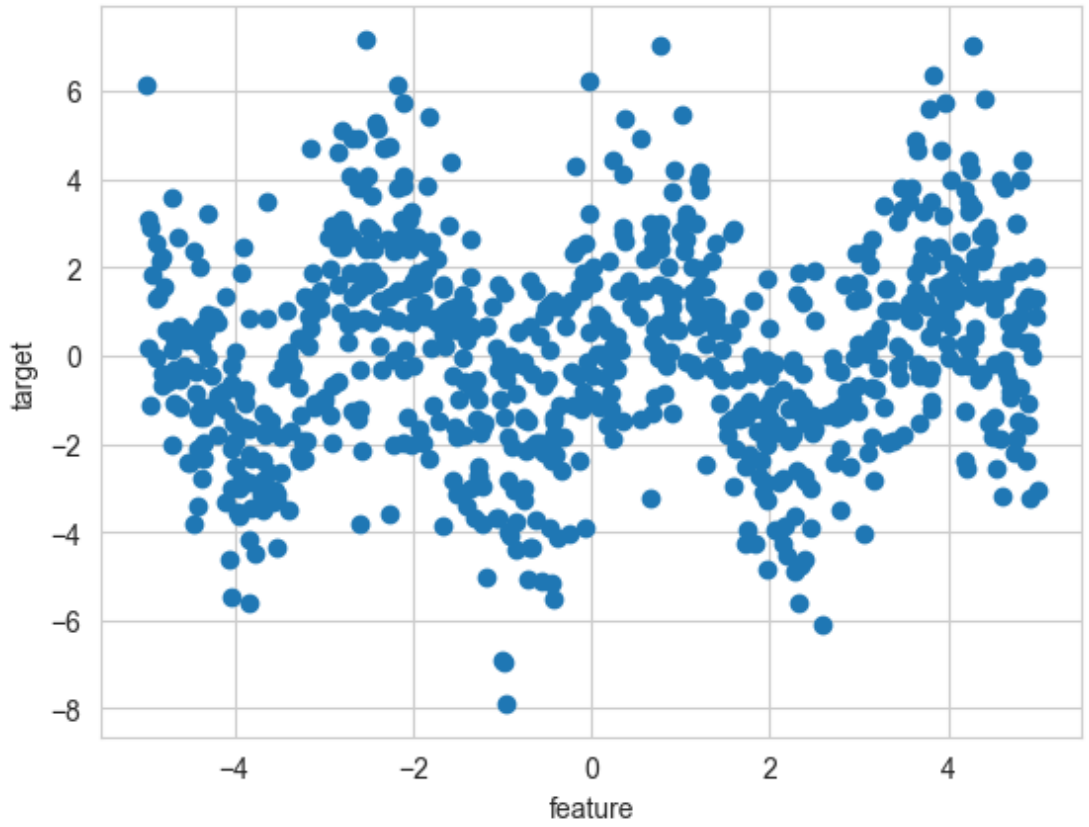
In [3]:

```
from sklearn.model_selection import train_test_split

X1_train, X1_test, y1_train, y1_test = train_test_split(
    X1, y1, test_size=0.2, random_state=0
)
```

View

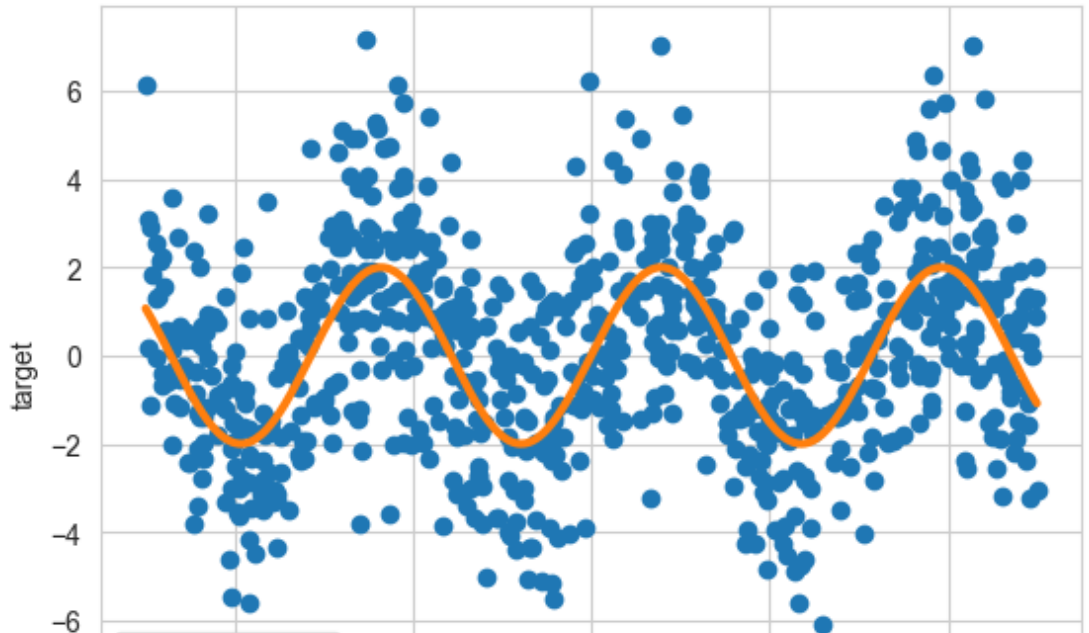
In [4]:

```
# View training data
plt.scatter(X1_train, y1_train, label="noisy data")
plt.xlabel("feature")
plt.ylabel("target")
plt.show()
```



In [5]:

```
# Training data and true curve
plt.scatter(X1_train, y1_train, label="noisy data")
plt.xlabel("feature")
plt.ylabel("target")
plt.plot(
    np.sort(X1.flatten()),
    curve(np.sort(X1.flatten())),
    label="true curve",
    c=colors[1],
    lw=3
)
plt.legend()
plt.show()
```



Dataset 2

In [6]:

```
# Generate 100 features (predictors) and 1000 data points

np.random.seed(0)
X2 = np.random.normal(size=(1000, 100))

# only the first feature will matter
y2 = X2[:, 0] + np.random.normal(size=1000)
```

Train-test split

In [7]:

```
from sklearn.model_selection import train_test_split

X2_train, X2_test, y2_train, y2_test = train_test_split(
    X2, y2, test_size=0.2, random_state=0
)
```

Random forests

Shallow and deep forests for dataset 1

In [8]:
```
from sklearn.ensemble import RandomForestRegressor

# shallow forest
forest1a = RandomForestRegressor(max_depth=4, random_state=0)
forest1a.fit(X=X1_train, y=y1_train)

# deep forest
forest1b = RandomForestRegressor(max_depth=50, random_state=0)
forest1b.fit(X=X1_train, y=y1_train)
```

Out[8]:

▼ RandomForestRegressor

```
RandomForestRegressor(max_depth=50, random_sta
te=0)
```

R^2's of shallow and deep forests for dataset 1

In [9]:

```
# training data
train1a = forest1a.score(X=X1_train, y=y1_train)
train1b = forest1b.score(X=X1_train, y=y1_train)

# test data
test1a = forest1a.score(X=X1_test, y=y1_test)
test1b = forest1b.score(X=X1_test, y=y1_test)
```

In [10]:

```
print(f"R-squared of shallow forest on training data = {train1a:.2%}")
print(f"R-squared of deep forest on training data = {train1b:.2%}")
print("\n")
print(f"R-squared of shallow forest on test data = {test1a:.2%}")
print(f"R-squared of deep forest on test data = {test1b:.2%}")
```

```
R-squared of shallow forest on training data = 35.23%
R-squared of deep forest on training data = 86.87%


R-squared of shallow forest on test data = 23.72%
R-squared of deep forest on test data = -4.33%
```

Avoid overfitting by cross validation

Cross validation

- The following can be done by usng GridSearchCV on the training data:
    - Split the training data into five sets (could make more or fewer sets).
    - Combine four sets for training and compute the score on the fifth ("validation") set.
    - Then choose a different one of the five sets for validation and repeat.
    - End up with five validation scores. Average them.
    - Choose hyperparameter value with highest average validation score.
- To forecast performance on new data, compute the R^2 on the test data.

Cross validation explained again

- Split the training data into 5 randomly chosen subsets A, B, C, D, and E.
- Use $A \cup B \cup C \cup D$ as training data and validate on E.
- Then use $B \cup C \cup D \cup E$ as training data and validate on A.
- Then, ..., until we have trained and validated 5 times.
- Average the 5 validation scores for each model.
- Choose the hyperparameter value that gives the highest average validation score.
- Then test on the testing data to estimate performance on new data.

Cross validate random forest on dataset 1

In [11]:

```
from sklearn.model_selection import GridSearchCV

param_grid = {"max_depth": range(2, 22, 2)}
forest_cv1 = GridSearchCV(
    RandomForestRegressor(random_state=0),
    param_grid=param_grid,
)
forest_cv1.fit(X=X1_train, y=y1_train)
print(f"best hyperparameter is {forest_cv1.best_params_}")
print(f"R-squared on the test data is {forest_cv1.score(X=X1_test, y=y1_test)
```

```
best hyperparameter is {'max_depth': 6}
R-squared on the test data is  24.80%
```

See the full cross-validation results if we want

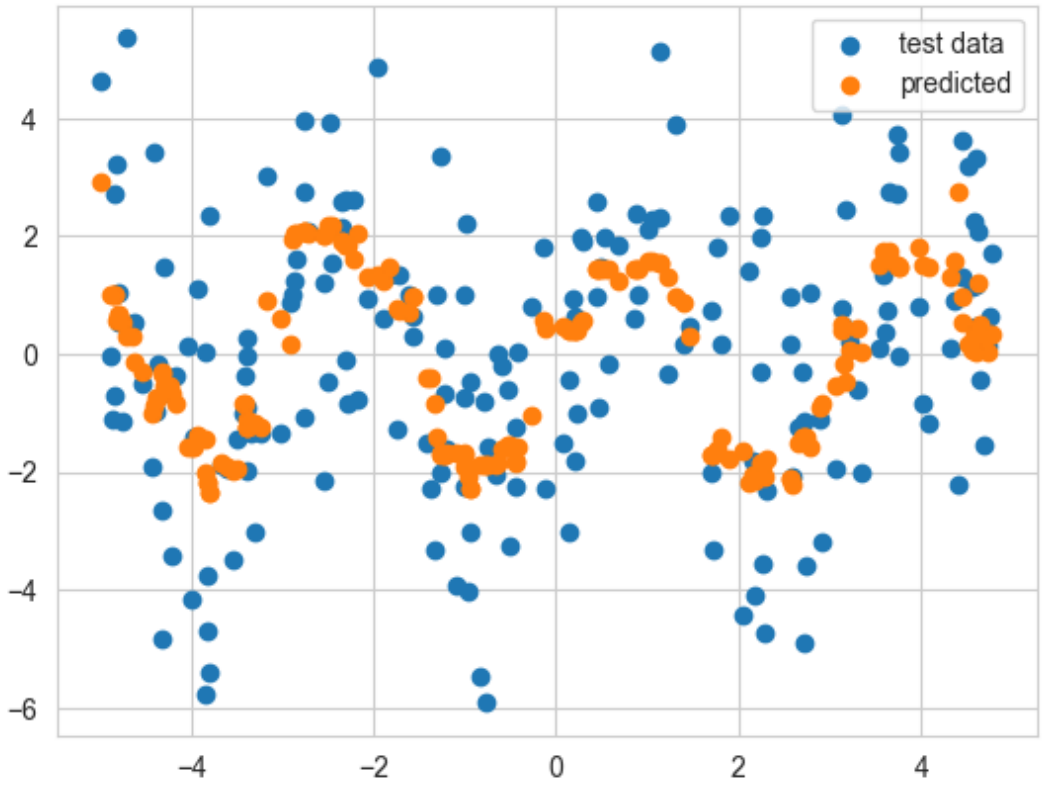
In [12]:
```
forest_cv1.cv_results_
```

Out[12]:
```
{'mean_fit_time': array([0.07377267, 0.08717914, 0.09889469, 0.112524
27, 0.12421117,
        0.12569208, 0.1228476 , 0.1191843 , 0.12329407, 0.12679143]),
 'std_fit_time': array([0.00582796, 0.00928541, 0.00741403, 0.0092549
5, 0.00805558,
        0.00675253, 0.00531868, 0.0084519 , 0.00760523, 0.00612412]),
 'mean_score_time': array([0.00211639, 0.00513015, 0.00760536, 0.0062
7818, 0.0107892 ,
        0.00312495, 0.00312672, 0.00828857, 0.0067699 , 0.0001091 ]),
 'std_score_time': array([0.00423279, 0.00559281, 0.00619265, 0.00680
234, 0.00666072,
        0.0062499 , 0.00625343, 0.00738377, 0.00833234, 0.0002182 ]),
 'param_max_depth': masked_array(data=[2, 4, 6, 8, 10, 12, 14, 16, 1
8, 20],
              mask=[False, False, False, False, False, False, False,
False,
                    False, False],
        fill_value='?',
             dtype=object),
 'params': [{'max_depth': 2},
  {'max_depth': 4},
  {'max_depth': 6},
  {'max_depth': 8},
  {'max_depth': 10},
  {'max_depth': 12},
  {'max_depth': 14},
  {'max_depth': 16},
```

View fit on the best forest on the test data if we want

In [13]:

```
predict1 = forest_cv1.predict(X=X1_test)
plt.scatter(X1_test, y1_test, label="test data")
plt.scatter(X1_test, predict1, label="predicted")
plt.legend()
plt.show()
```



Cross validate random forest on dataset 2

In [14]:

```
param_grid = {"max_depth": range(2, 22, 2)}
forest_cv2 = GridSearchCV(
    RandomForestRegressor(random_state=0),
    param_grid=param_grid,
)
forest_cv2.fit(X=X2_train, y=y2_train)
print(f"best hyperparameter is {forest_cv2.best_params_}")
print(f"R-squared on the test data is {forest_cv2.score(X=X2_test, y=y2_test)
```

```
best hyperparameter is {'max_depth': 4}
R-squared on the test data is 51.19%
```

Cross validate neural network on dataset 1

In [15]:

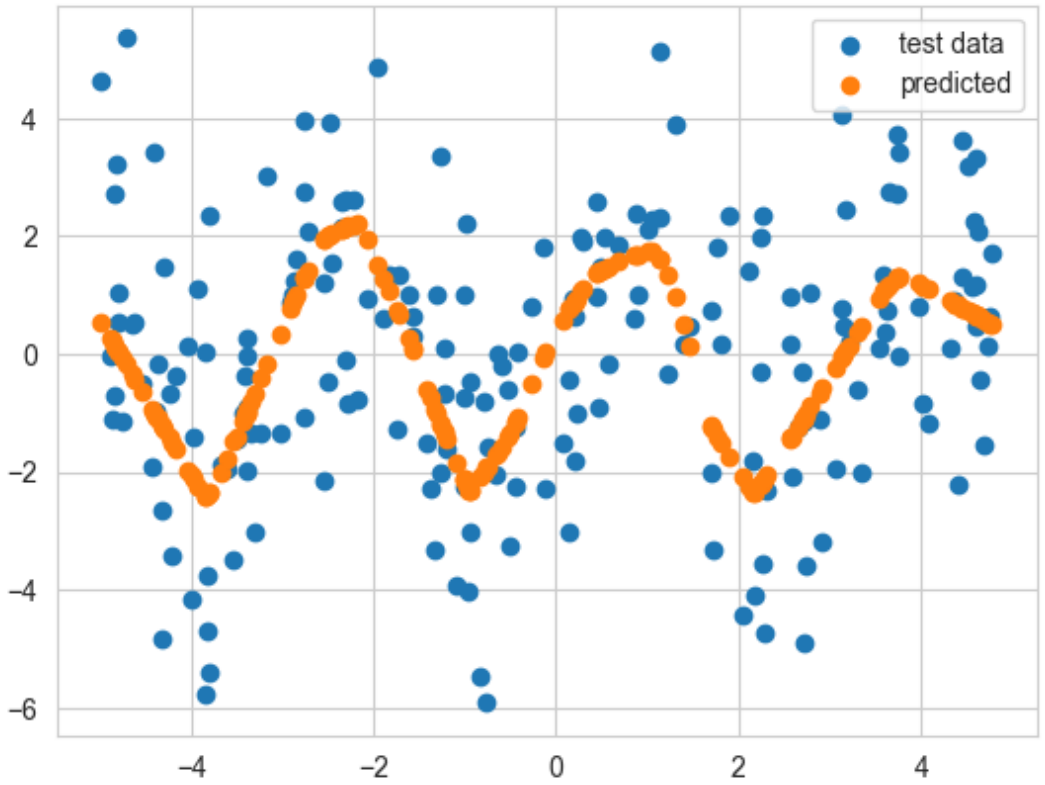
```
from sklearn.neural_network import MLPRegressor

param_grid = {"hidden_layer_sizes": [[100], [100, 100], [100, 100, 100]]}

net_cv1 = GridSearchCV(
    MLPRegressor(random_state=0, max_iter=1000),
    param_grid=param_grid,
)
net_cv1.fit(X=X1_train, y=y1_train)

print(f"best hyperparameter is {net_cv1.best_params_}")
print(f"R-squared on the test data is {net_cv1.score(X=X1_test, y=y1_test):.2
```

```
best hyperparameter is {'hidden_layer_sizes': [100, 100, 100]}
R-squared on the test data is 25.75%
```

View fit of the best neural network on the test data if we want

In [16]:

```
predict1 = net_cv1.predict(X=X1_test)
plt.scatter(X1_test, y1_test, label="test data")
plt.scatter(X1_test, predict1, label="predicted")
plt.legend()
plt.show()
```



Cross-validate neural network on dataset 2

In [17]:

```
param_grid = {"hidden_layer_sizes": [[100], [100, 100], [100, 100, 100]]}

net_cv2 = GridSearchCV(
    MLPRegressor(random_state=0, max_iter=1000),
    param_grid=param_grid,
)
net_cv2.fit(X=X2_train, y=y2_train)

print(f"best hyperparameter is {net_cv2.best_params_}")
print(f"R-squared on the test data is {net_cv2.score(X=X2_test, y=y2_test):.2
```

```
best hyperparameter is {'hidden_layer_sizes': [100, 100]}
R-squared on the test data is 5.55%
```

Linear regression

- No hyperparameters
- Train on the training data (instead of cross-validating)
- Test on the test data

Linear regression on both datasets

In [18]:

```
from sklearn.linear_model import LinearRegression

linear1 = LinearRegression()
linear1.fit(X=X1_train, y=y1_train)
test1 = linear1.score(X=X1_test, y=y1_test)

linear2 = LinearRegression()
linear2.fit(X=X2_train, y=y2_train)
test2 = linear2.score(X=X2_test, y=y2_test)

print(f"R-squared for dataset 1 test data is {test1:.2%}")
print(f"R-squared for dataset 2 test data is {test2:.2%}")
```

```
R-squared for dataset 1 test data is 1.18%
R-squared for dataset 2 test data is 40.97%
```

View regression coefficients if we want

In [19]:
```
np.round(linear2.coef_, 3)
```

Out[19]:
```
array([ 0.993,  0.058, -0.032, -0.037,  0.014,  0.033, -0.002,  0.01
4,
       -0.032,  0.015,  0.035, -0.004, -0.07 , -0.038,  0.03 , -0.04
,
       -0.007,  0.045,  0.002, -0.012, -0.014, -0.089, -0.007,  0.00
2,
       -0.052,  0.01 ,  0.012, -0.111, -0.003, -0.038,  0.01 , -0.04
9,
        0.115,  0.054,  0.053,  0.032, -0.027, -0.022, -0.033, -0.00
3,
       -0.047, -0.03 ,  0.005, -0.034, -0.004, -0.041, -0.083,  0.05
4,
        0.031, -0.007,  0.021,  0.049, -0.027, -0.073,  0.033,  0.02
3,
        0.038,  0.035,  0.004,  0.05 , -0.018,  0.003, -0.078,  0.02
1,
        0.008, -0.016, -0.003, -0.014, -0.028, -0.037, -0.022,  0.07
5,
        0.003, -0.021, -0.111,  0.023, -0.015,  0.02 ,  0.015,  0.01
8,
       -0.01 , -0.043, -0.091,  0.044, -0.014, -0.03 ,  0.017, -0.02
5,
        0.095, -0.001, -0.022, -0.043, -0.072, -0.019,  0.052,  0.02
8,
        0.006,  0.016, -0.046, -0.036])
```

Lasso

- OLS minimizes the mean squared error. Lasso is an example of penalized linear regression. It chooses coefficients to minimize

$$\frac{1}{2}\text{MSE} + \text{penalty} \times \sum_{i=1}^{n} |\beta_i|$$

- The penalty is a hyperparameter. It is called "alpha" (not the regression intercept).
- The larger the penalty, the smaller the estimated betas will be. For large alpha, the estimated betas will be zeros.
- Penalizing is a way to reduce model complexity and avoid overfitting.

Cross-validation for lasso on dataset 1

In [20]:

```
from sklearn.linear_model import Lasso

param_grid = {"alpha": np.arange(0.1, 2.1, 0.1)}

lasso_cv1 = GridSearchCV(Lasso(), param_grid=param_grid)
lasso_cv1.fit(X1_train, y1_train)

print(f"best hyperparameter is {lasso_cv1.best_params_}")
print(f"R-squared on the test data is {lasso_cv1.score(X1_test, y1_test):.2%}")
```

```
best hyperparameter is {'alpha': 0.1}
R-squared on the test data is 1.12%
```

Cross-validation for lasso on dataset 2

In [21]:

```
param_grid = {"alpha": np.arange(0.1, 2.1, 0.1)}

lasso_cv2 = GridSearchCV(Lasso(), param_grid=param_grid)
lasso_cv2.fit(X2_train, y2_train)

print(f"best hyperparameter is {lasso_cv2.best_params_}")
print(f"R-squared on the test data is {lasso_cv2.score(X2_test, y2_test):.2%}")
```

```
best hyperparameter is {'alpha': 0.1}
R-squared on the test data is 51.76%
```

View the regression coefficients if we want

In [22]:
```
lasso = Lasso(alpha=0.1)
lasso.fit(X2_train, y2_train)
np.round(lasso.coef_, 3)
```

Out[22]:
```
array([ 0.898,  0.   , -0.   , -0.   ,  0.   ,  0.   , -0.   ,  0.
,
       -0.   ,  0.   ,  0.   ,  0.   , -0.   , -0.   ,  0.   , -0.
,
       -0.   ,  0.   , -0.   ,  0.   , -0.   , -0.   , -0.   ,  0.
,
       -0.   , -0.   ,  0.   , -0.   ,  0.   , -0.   ,  0.   , -0.
,
        0.   ,  0.   ,  0.   ,  0.   , -0.   , -0.   , -0.   , -0.
,
       -0.   ,  0.   , -0.   , -0.   , -0.   , -0.   , -0.   ,  0.
,
        0.   , -0.   ,  0.   ,  0.   , -0.   , -0.   ,  0.   ,  0.
,
        0.   ,  0.   ,  0.   ,  0.   ,  0.   ,  0.   , -0.   ,  0.
,
        0.   , -0.   , -0.   , -0.   , -0.   , -0.   , -0.   ,  0.
,
        0.   , -0.   , -0.   ,  0.   ,  0.   ,  0.   ,  0.   ,  0.
,
       -0.   , -0.   , -0.009,  0.   ,  0.   , -0.   , -0.   , -0.
,
        0.   , -0.   , -0.   , -0.   , -0.   , -0.   ,  0.   ,  0.
,
        0.   ,  0.   , -0.   , -0.   ])
```

Some real data

- Boston house prices
- Try to predict median house price in different neighborhoods of Boston based on characteristics of the houses and characteristics of the residents
- University of California-Irvine Machine Learning Repository and Kaggle
- See https://www.kaggle.com/datasets/fedesoriano/the-boston-houseprice-data for a description of the data.

In [23]:
```
url = "https://www.dropbox.com/scl/fi/g9uzsntv93waniyw9pkc2/boston.csv?rlkey=
df = pd.read_csv(url)
df.head(3)
```

Out[23]:

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	DIS	RAD	TAX	PTRATI
0	0.00632	18.0	2.31	0	0.538	6.575	65.2	4.0900	1	296.0	15.
1	0.02731	0.0	7.07	0	0.469	6.421	78.9	4.9671	2	242.0	17.
2	0.02729	0.0	7.07	0	0.469	7.185	61.1	4.9671	2	242.0	17.

In [24]:

```
X = df.drop(columns=["MEDV"])
y = df.MEDV

X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=0
)
```

Tasks

1. Run GridSearchCV on training data to find best hyperparameter
2. Test the model on the test data

Do this for

1. Random forest with

```
param_grid = {"max_depth": range(2, 22, 2)}
```

2. Neural network with

```
param_grid = {"hidden_layer_sizes": [[100], [100, 100], [100, 100,
100]]}
```

Can chatGPT help?