



SUPERVISED LEARNING WITH SCIKIT-LEARN

# **Introduction to regression**



# Boston housing data

```
In [1]: boston = pd.read_csv('boston.csv')
```

```
In [2]: print(boston.head())
```

|   | CRIM    | ZN   | INDUS | CHAS | NX    | RM    | AGE  | DIS    | RAD | TAX   | \ |
|---|---------|------|-------|------|-------|-------|------|--------|-----|-------|---|
| 0 | 0.00632 | 18.0 | 2.31  | 0    | 0.538 | 6.575 | 65.2 | 4.0900 | 1   | 296.0 |   |
| 1 | 0.02731 | 0.0  | 7.07  | 0    | 0.469 | 6.421 | 78.9 | 4.9671 | 2   | 242.0 |   |
| 2 | 0.02729 | 0.0  | 7.07  | 0    | 0.469 | 7.185 | 61.1 | 4.9671 | 2   | 242.0 |   |
| 3 | 0.03237 | 0.0  | 2.18  | 0    | 0.458 | 6.998 | 45.8 | 6.0622 | 3   | 222.0 |   |
| 4 | 0.06905 | 0.0  | 2.18  | 0    | 0.458 | 7.147 | 54.2 | 6.0622 | 3   | 222.0 |   |

|   | PTRATIO | B      | LSTAT | MEDV |
|---|---------|--------|-------|------|
| 0 | 15.3    | 396.90 | 4.98  | 24.0 |
| 1 | 17.8    | 396.90 | 9.14  | 21.6 |
| 2 | 17.8    | 392.83 | 4.03  | 34.7 |
| 3 | 18.7    | 394.63 | 2.94  | 33.4 |
| 4 | 18.7    | 396.90 | 5.33  | 36.2 |



# Creating feature and target arrays

```
In [3]: X = boston.drop('MEDV', axis=1).values
```

```
In [4]: y = boston['MEDV'].values
```



# Predicting house value from a single feature

```
In [5]: X_rooms = X[:,5]
```

```
In [6]: type(X_rooms), type(y)
```

```
Out[6]: (numpy.ndarray, numpy.ndarray)
```

```
In [7]: y = y.reshape(-1, 1)
```

```
In [8]: X_rooms = X_rooms.reshape(-1, 1)
```



# Plotting house value vs. number of rooms

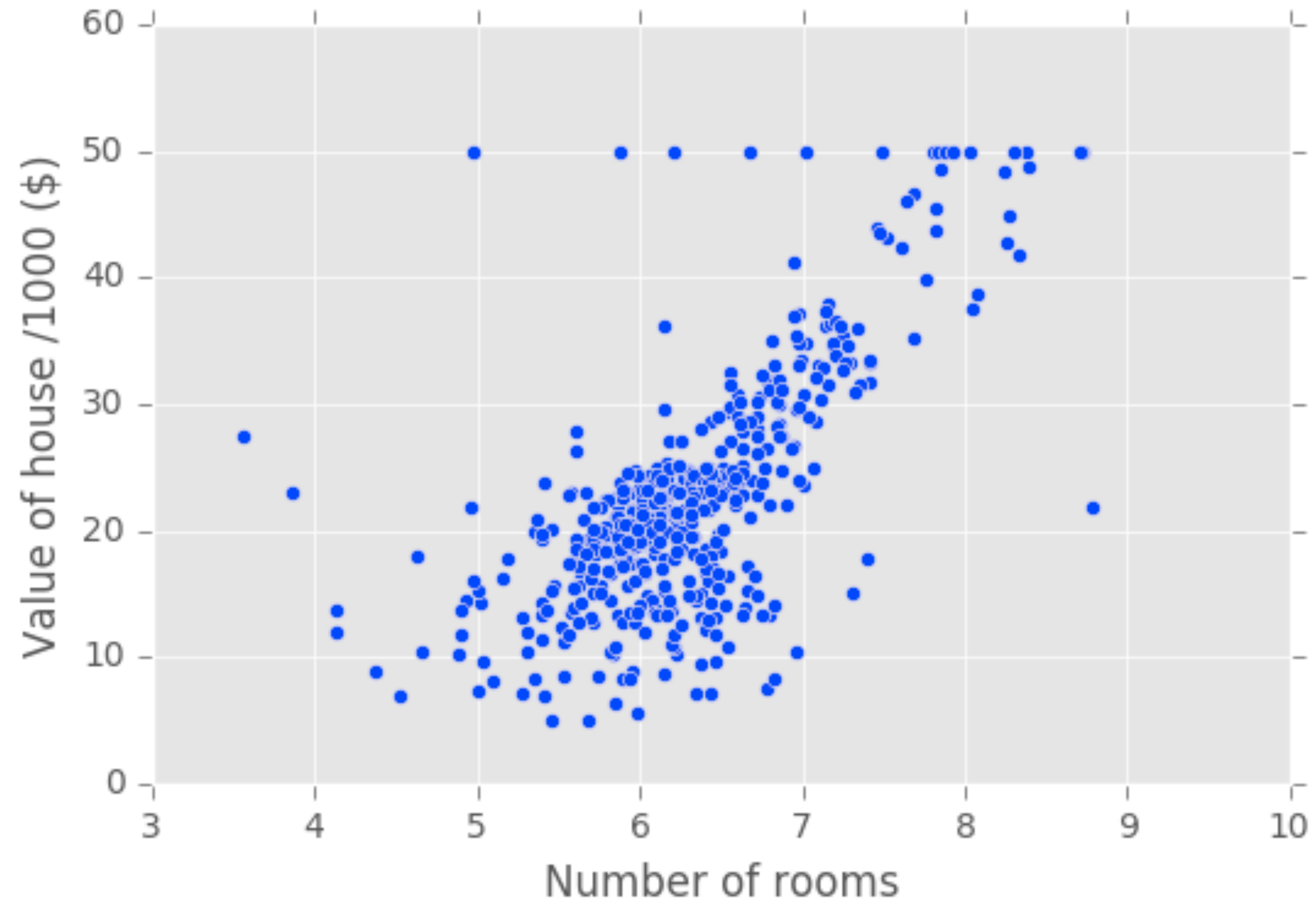
```
In [9]: plt.scatter(X_rooms, y)
```

```
In [10]: plt.ylabel('Value of house /1000 ($)')
```

```
In [11]: plt.xlabel('Number of rooms')
```

```
In [12]: plt.show();
```

# Plotting house value vs. number of rooms





# Fitting a regression model

```
In [13]: import numpy as np
```

```
In [14]: from sklearn import linear_model
```

```
In [15]: reg = linear_model.LinearRegression()
```

```
In [16]: reg.fit(X_rooms, y)
```

```
In [17]: prediction_space = np.linspace(min(X_rooms),  
....:                                   max(X_rooms)).reshape(-1, 1)
```

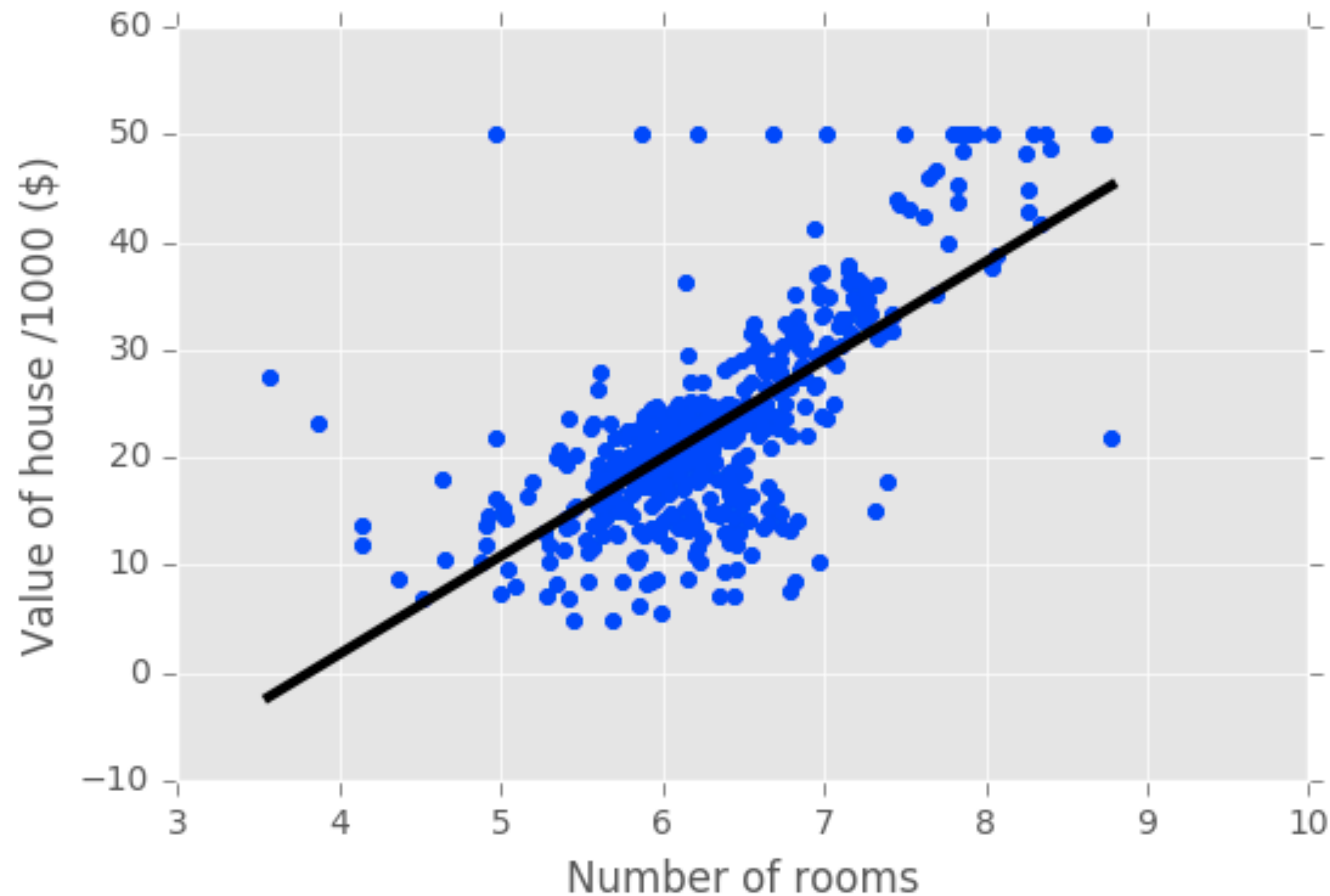
```
In [18]: plt.scatter(X_rooms, y, color='blue')
```

```
In [19]: plt.plot(prediction_space, reg.predict(prediction_space),  
....:              color='black', linewidth=3)
```

```
In [20]: plt.show()
```



# Fitting a regression model







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# **The basics of linear regression**

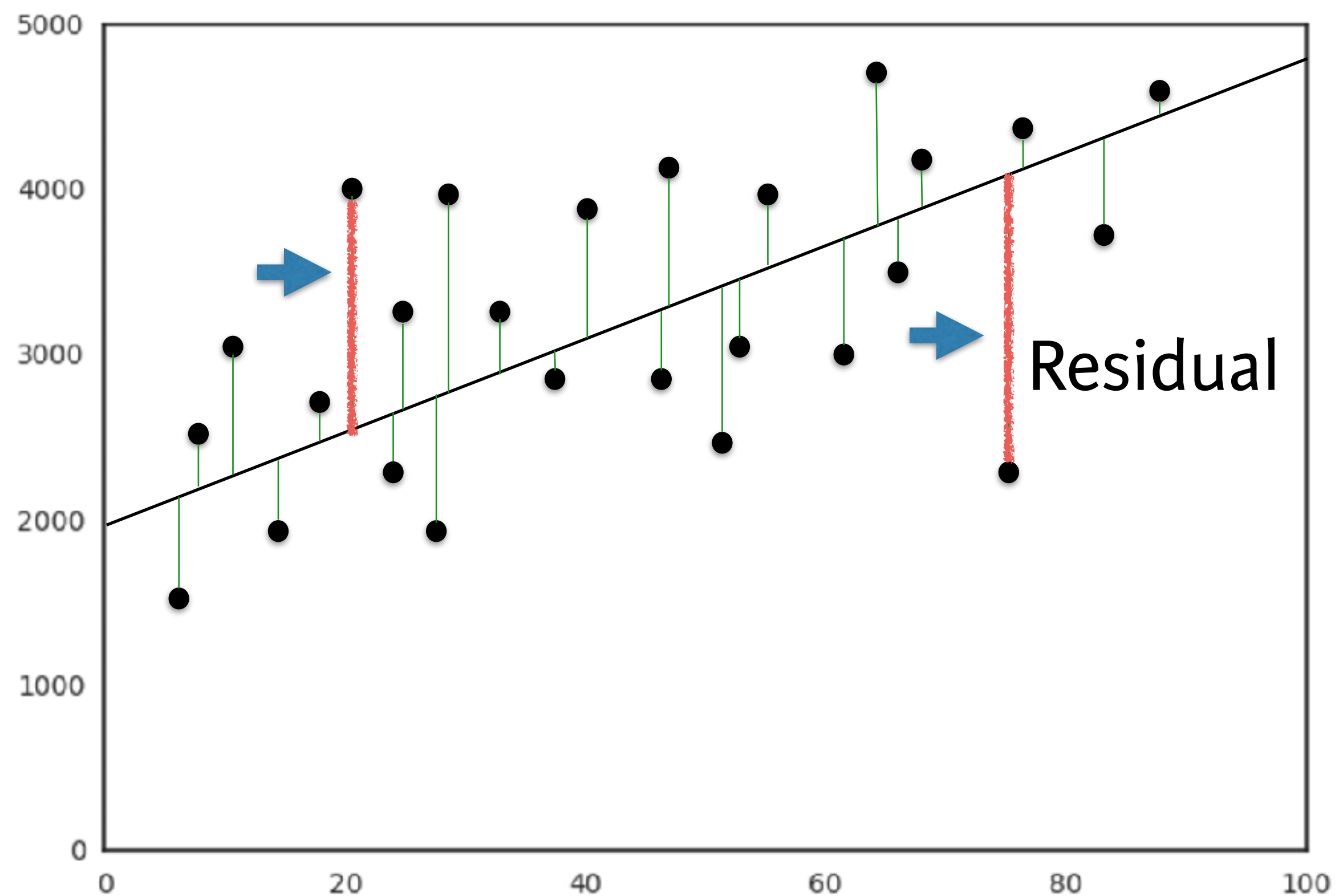


# Regression mechanics

- $y = ax + b$ 
  - $y = \text{target}$
  - $x = \text{single feature}$
  - $a, b = \text{parameters of model}$
- How do we choose  $a$  and  $b$ ?
- Define an error function for any given line
  - Choose the line that minimizes the error function

# The loss function

- Ordinary least squares (OLS): Minimize sum of squares of residuals





# Linear regression in higher dimensions

$$y = a_1x_1 + a_2x_2 + b$$

- To fit a linear regression model here:
  - Need to specify 3 variables

- In higher dimensions:

$$y = a_1x_1 + a_2x_2 + a_3x_3 + a_nx_n + b$$

- Must specify coefficient for each feature and the variable  $b$
- Scikit-learn API works exactly the same way:
  - Pass two arrays: Features, and target



# Linear regression on all features

```
In [1]: from sklearn.model_selection import train_test_split

In [2]: X_train, X_test, y_train, y_test = train_test_split(X, y,
...: test_size = 0.3, random_state=42)

In [3]: reg_all = linear_model.LinearRegression()

In [4]: reg_all.fit(X_train, y_train)

In [5]: y_pred = reg_all.predict(X_test)

In [6]: reg_all.score(X_test, y_test)
Out[6]: 0.71122600574849526
```



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# Cross-validation



# Cross-validation motivation

- Model performance is dependent on way the data is split
- Not representative of the model's ability to generalize
- Solution: Cross-validation!



# Cross-validation basics

|         |        |        |        |        |        |          |
|---------|--------|--------|--------|--------|--------|----------|
| Split 1 | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5 | Metric 1 |
| Split 2 | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5 | Metric 2 |
| Split 3 | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5 | Metric 3 |
| Split 4 | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5 | Metric 4 |
| Split 5 | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5 | Metric 5 |

Training data

Test data

# Cross-validation and model performance

- 5 folds = 5-fold CV
- 10 folds = 10-fold CV
- k folds = k-fold CV
- More folds = More computationally expensive



# Cross-validation in scikit-learn

```
In [1]: from sklearn.model_selection import cross_val_score
```

```
In [2]: reg = linear_model.LinearRegression()
```

```
In [3]: cv_results = cross_val_score(reg, X, y, cv=5)
```

```
In [4]: print(cv_results)
```

```
[ 0.63919994  0.71386698  0.58702344  0.07923081 -0.25294154]
```

```
In [5]: np.mean(cv_results)
```

```
Out[5]: 0.35327592439587058
```



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# Regularized regression



# Why regularize?

- Recall: Linear regression minimizes a loss function
- It chooses a coefficient for each feature variable
- Large coefficients can lead to overfitting
- Penalizing large coefficients: Regularization



# Ridge regression

- Loss function = OLS loss function +  $\alpha * \sum_{i=1}^n a_i^2$
- Alpha: Parameter we need to choose
- Picking alpha here is similar to picking k in k-NN
- Hyperparameter tuning (More in Chapter 3)
- Alpha controls model complexity
  - Alpha = 0: We get back OLS (Can lead to overfitting)
  - Very high alpha: Can lead to underfitting





# Ridge regression in scikit-learn

```
In [1]: from sklearn.linear_model import Ridge
```

```
In [2]: X_train, X_test, y_train, y_test = train_test_split(X, y,  
...: test_size = 0.3, random_state=42)
```

```
In [3]: ridge = Ridge(alpha=0.1, normalize=True)
```

```
In [4]: ridge.fit(X_train, y_train)
```

```
In [5]: ridge_pred = ridge.predict(X_test)
```

```
In [6]: ridge.score(X_test, y_test)
```

```
Out[6]: 0.69969382751273179
```



# Lasso regression

- Loss function = OLS loss function +  $\alpha * \sum_{i=1}^n |a_i|$



# Lasso regression in scikit-learn

```
In [1]: from sklearn.linear_model import Lasso
```

```
In [2]: X_train, X_test, y_train, y_test = train_test_split(X, y,  
...: test_size = 0.3, random_state=42)
```

```
In [3]: lasso = Lasso(alpha=0.1, normalize=True)
```

```
In [4]: lasso.fit(X_train, y_train)
```

```
In [5]: lasso_pred = lasso.predict(X_test)
```

```
In [6]: lasso.score(X_test, y_test)
```

```
Out[6]: 0.59502295353285506
```

# Lasso regression for feature selection

- Can be used to select important features of a dataset
- Shrinks the coefficients of less important features to exactly 0



# Lasso for feature selection in scikit-learn

```
In [1]: from sklearn.linear_model import Lasso

In [2]: names = boston.drop('MEDV', axis=1).columns

In [3]: lasso = Lasso(alpha=0.1)

In [4]: lasso_coef = lasso.fit(X, y).coef_

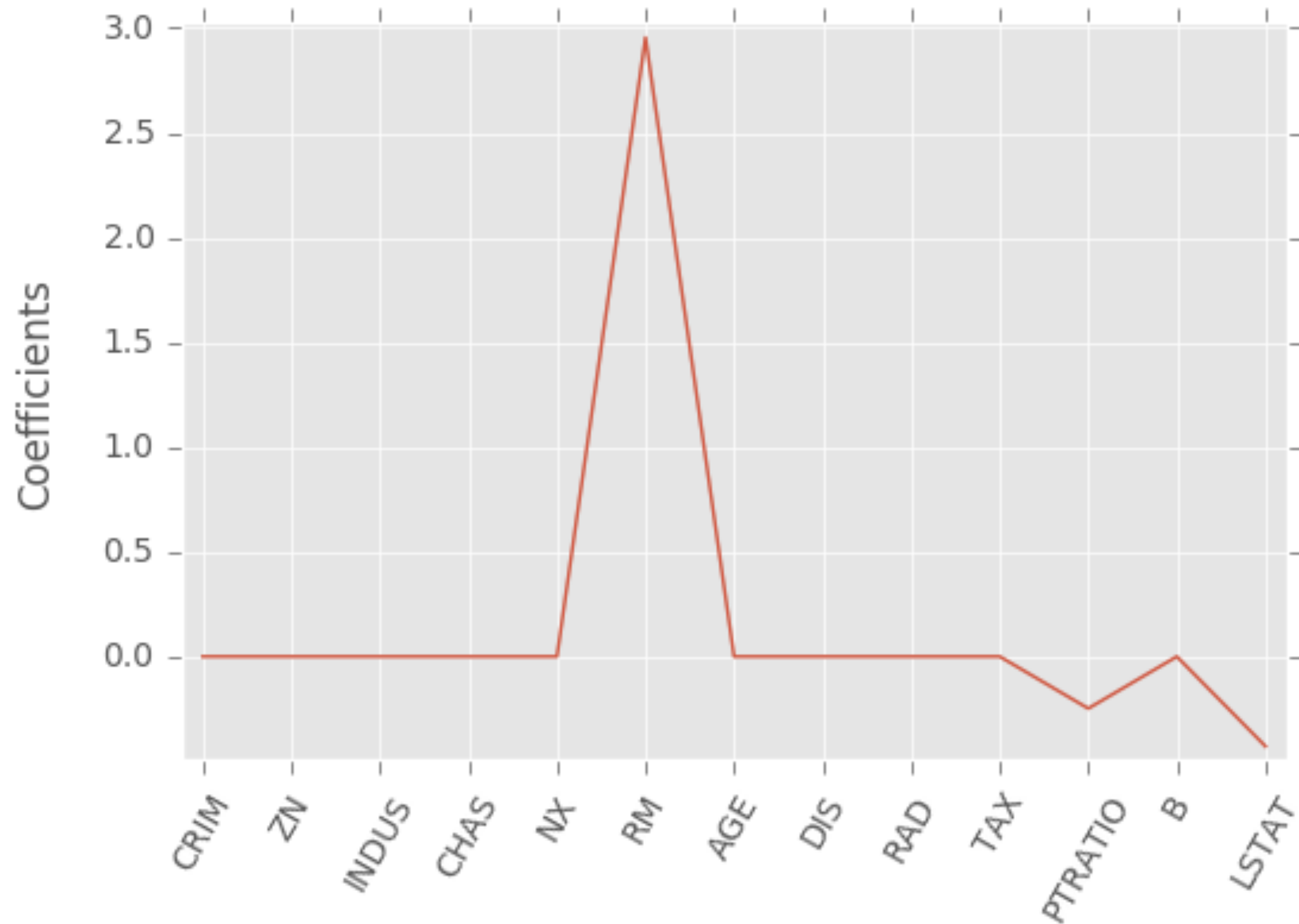
In [5]: _ = plt.plot(range(len(names)), lasso_coef)

In [6]: _ = plt.xticks(range(len(names)), names, rotation=60)

In [7]: _ = plt.ylabel('Coefficients')

In [8]: plt.show()
```

# Lasso for feature selection in scikit-learn





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