

Introduction to regression

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Core developer, scikit-learn

Boston housing data

```
boston = pd.read_csv('boston.csv')  
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

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

Predicting house value from a single feature

```
X_rooms = X[:, 5]  
  
type(X_rooms), type(y)
```

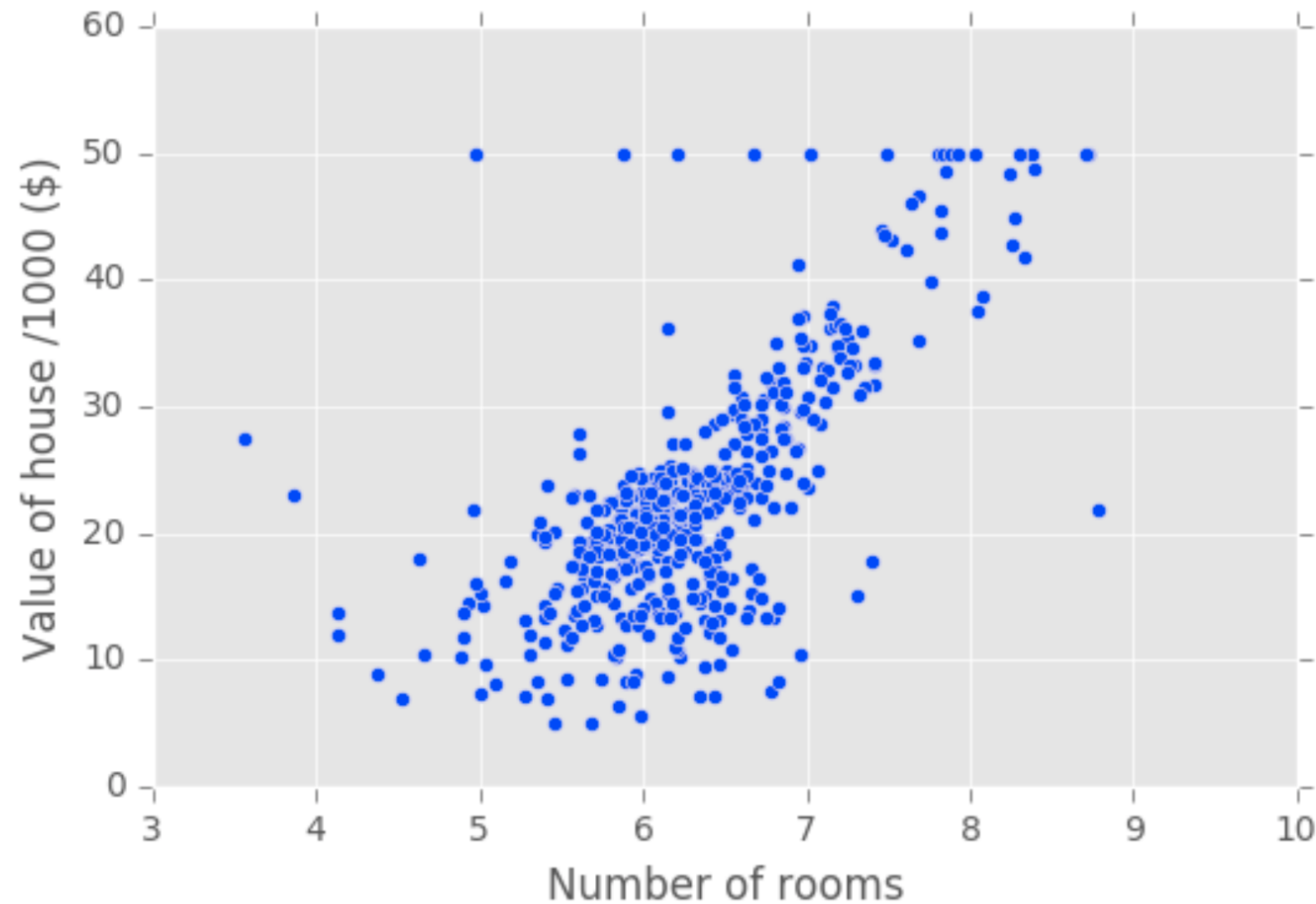
```
(numpy.ndarray, numpy.ndarray)
```

```
y = y.reshape(-1, 1)  
X_rooms = X_rooms.reshape(-1, 1)
```

Plotting house value vs. number of rooms

```
plt.scatter(X_rooms, y)
plt.ylabel('Value of house /1000 ($)')
plt.xlabel('Number of rooms')
plt.show();
```

Plotting house value vs. number of rooms



Fitting a regression model

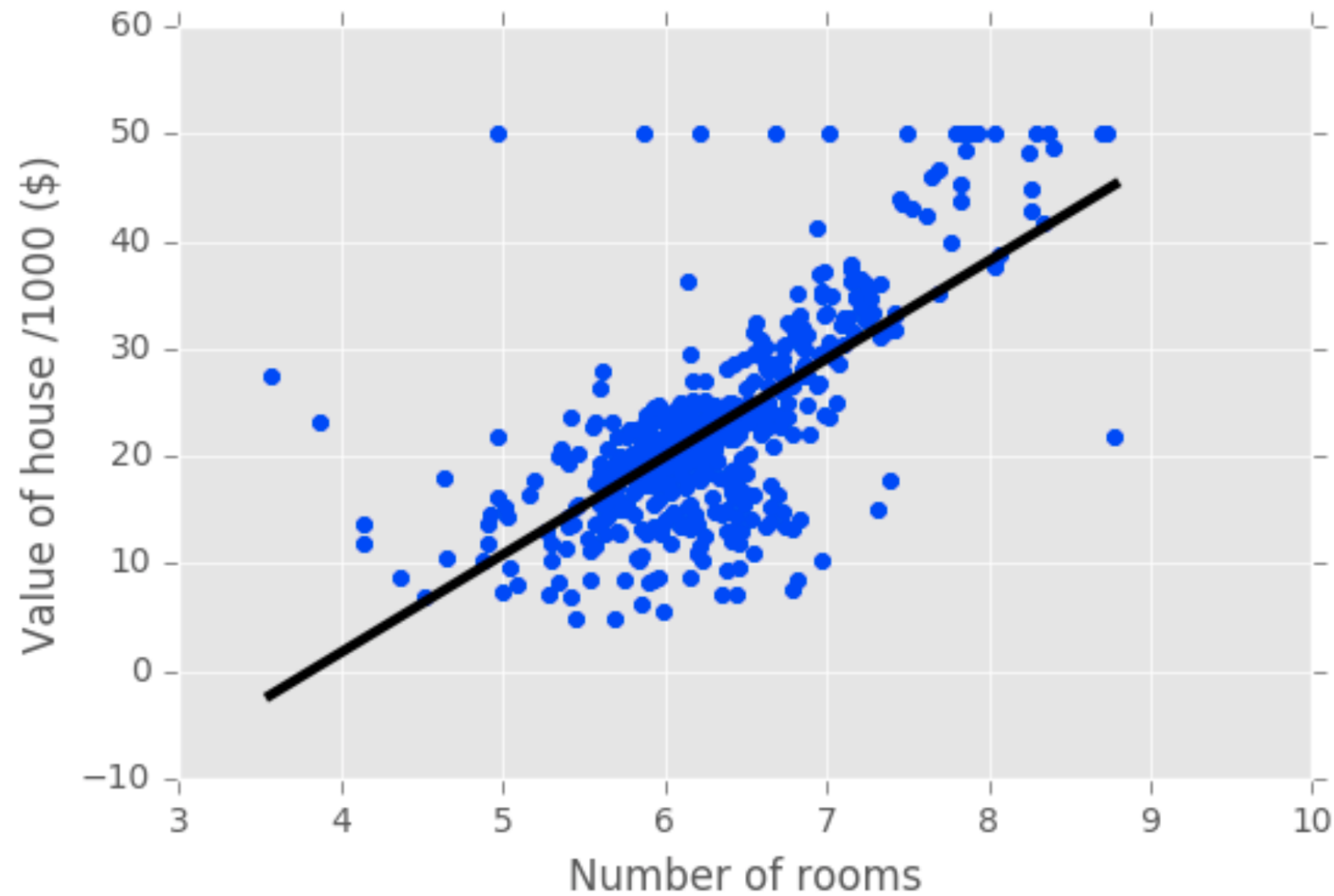
```
import numpy as np
from sklearn.linear_model import LinearRegression

reg = LinearRegression()
reg.fit(X_rooms, y)
prediction_space = np.linspace(min(X_rooms),
                                max(X_rooms)).reshape(-1, 1)

plt.scatter(X_rooms, y, color='blue')
plt.plot(prediction_space, reg.predict(prediction_space),
         color='black', linewidth=3)

plt.show()
```

Fitting a regression model



Let's practice!

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The basics of linear regression

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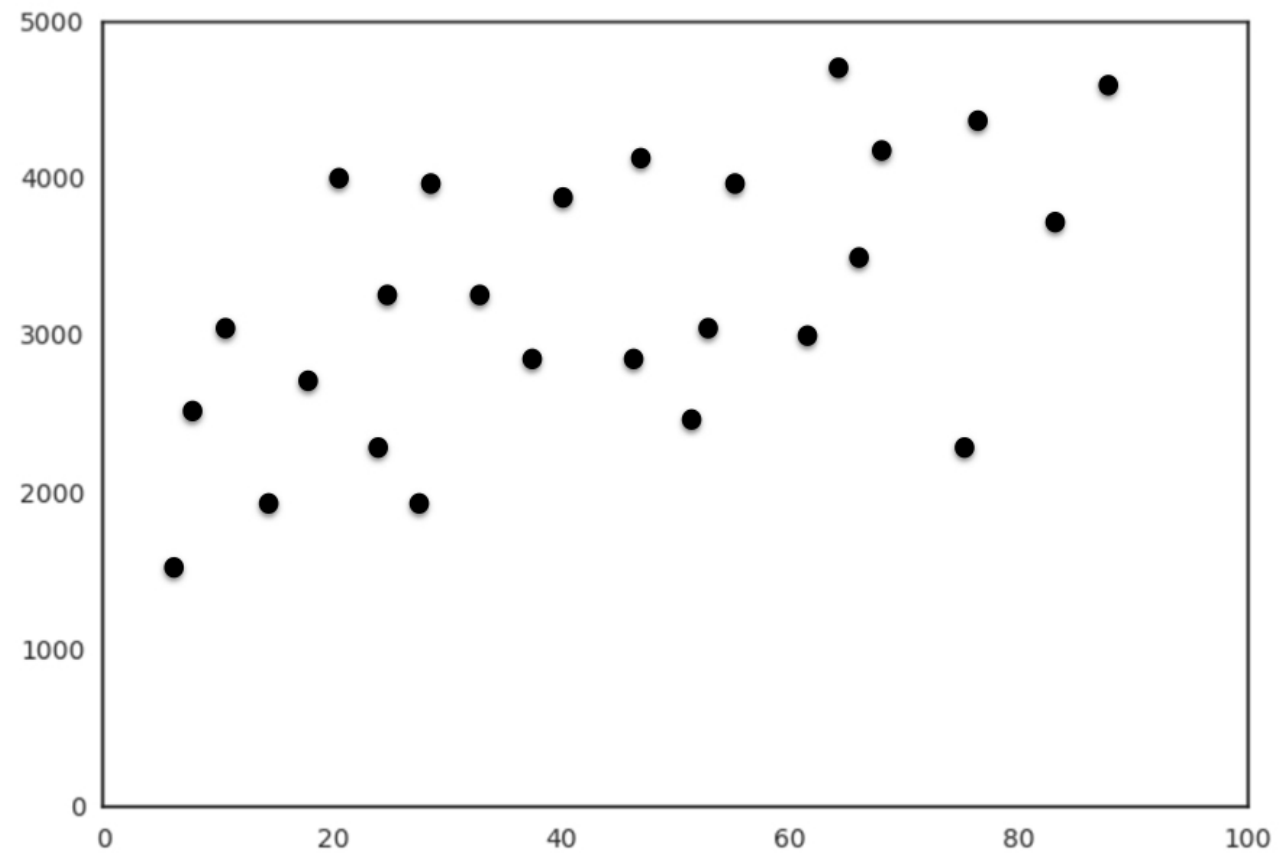


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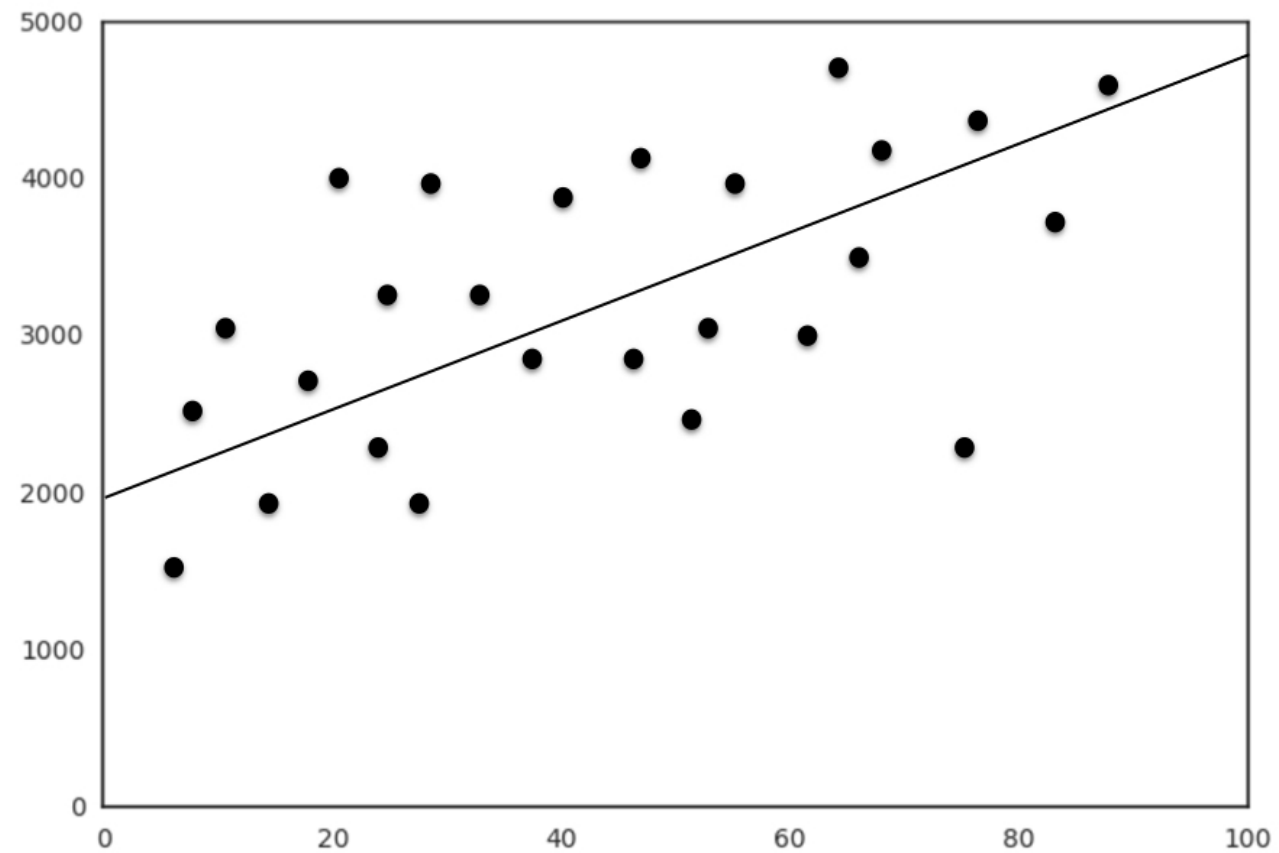
Regression mechanics

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

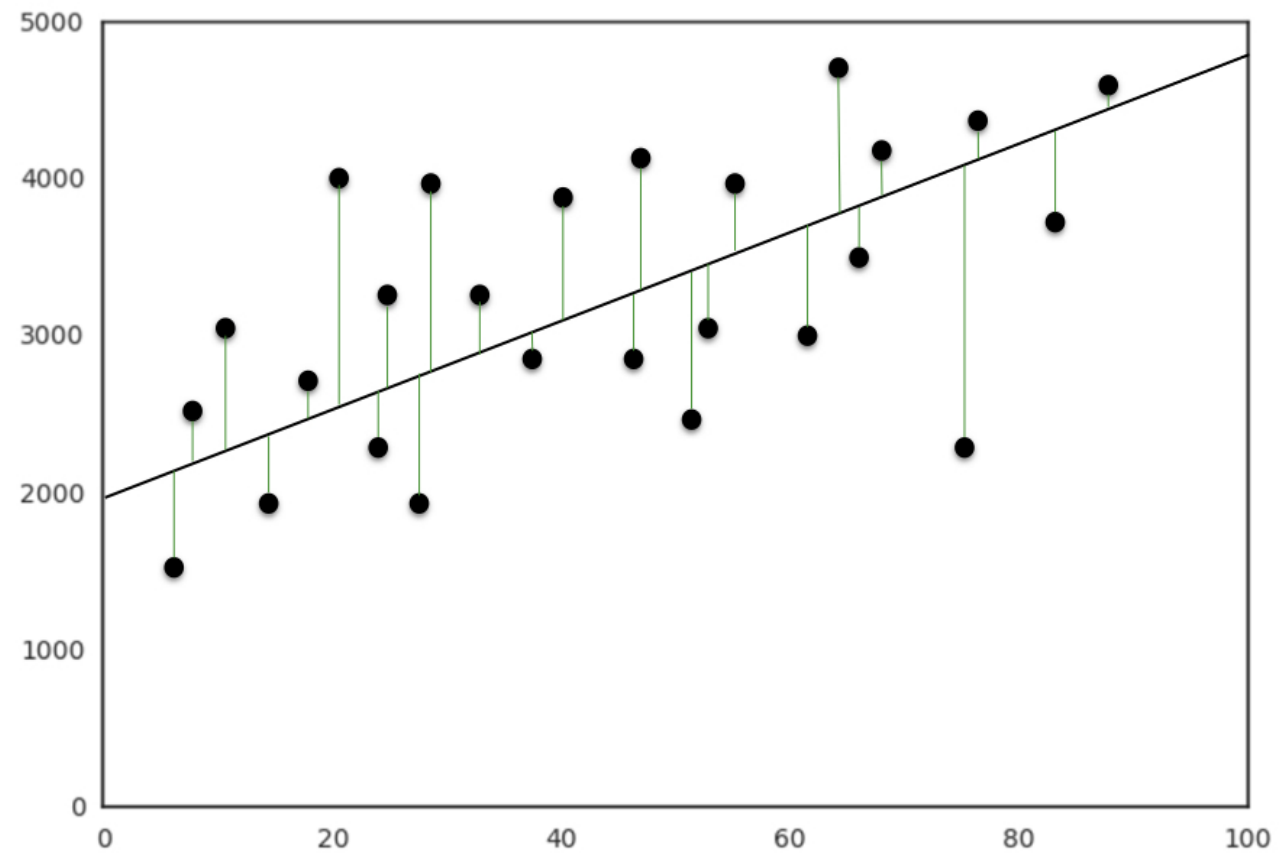
The loss function



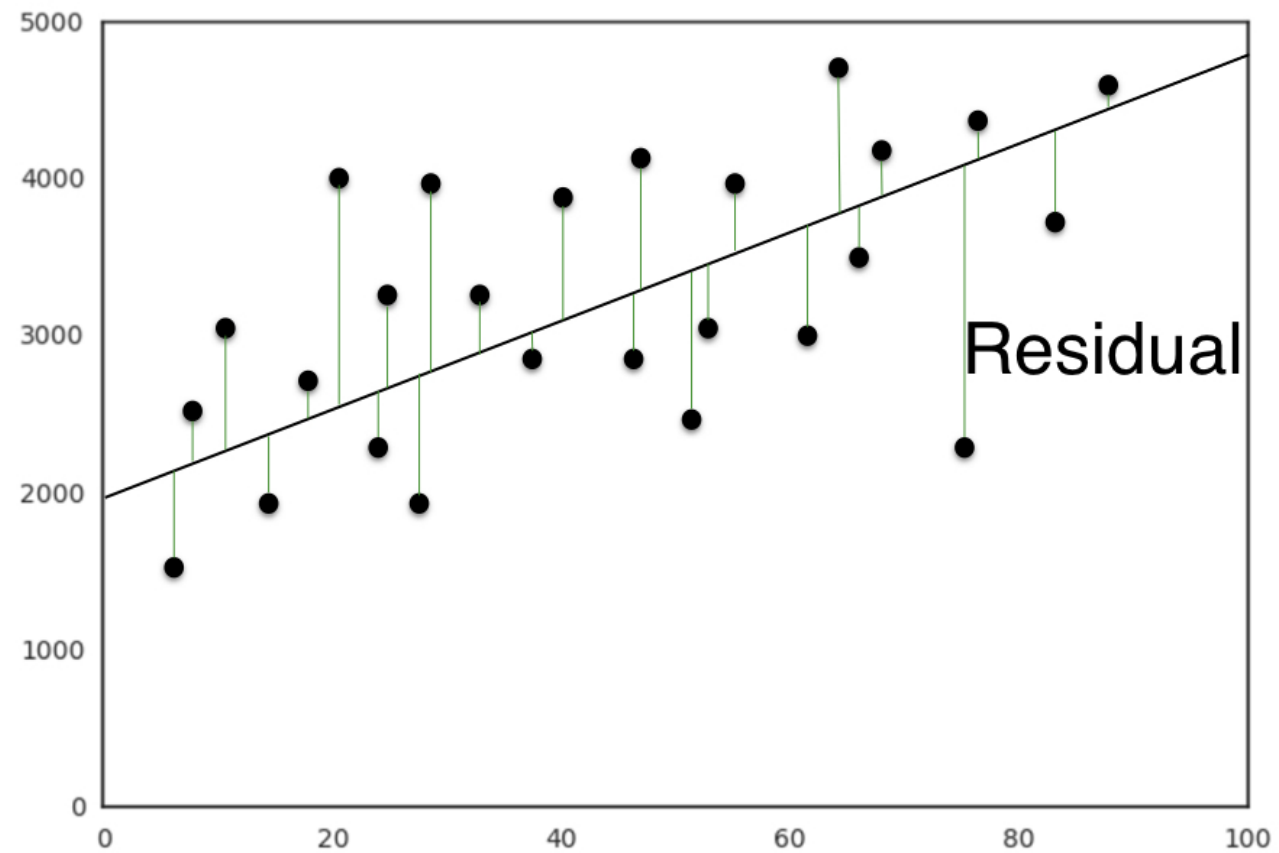
The loss function



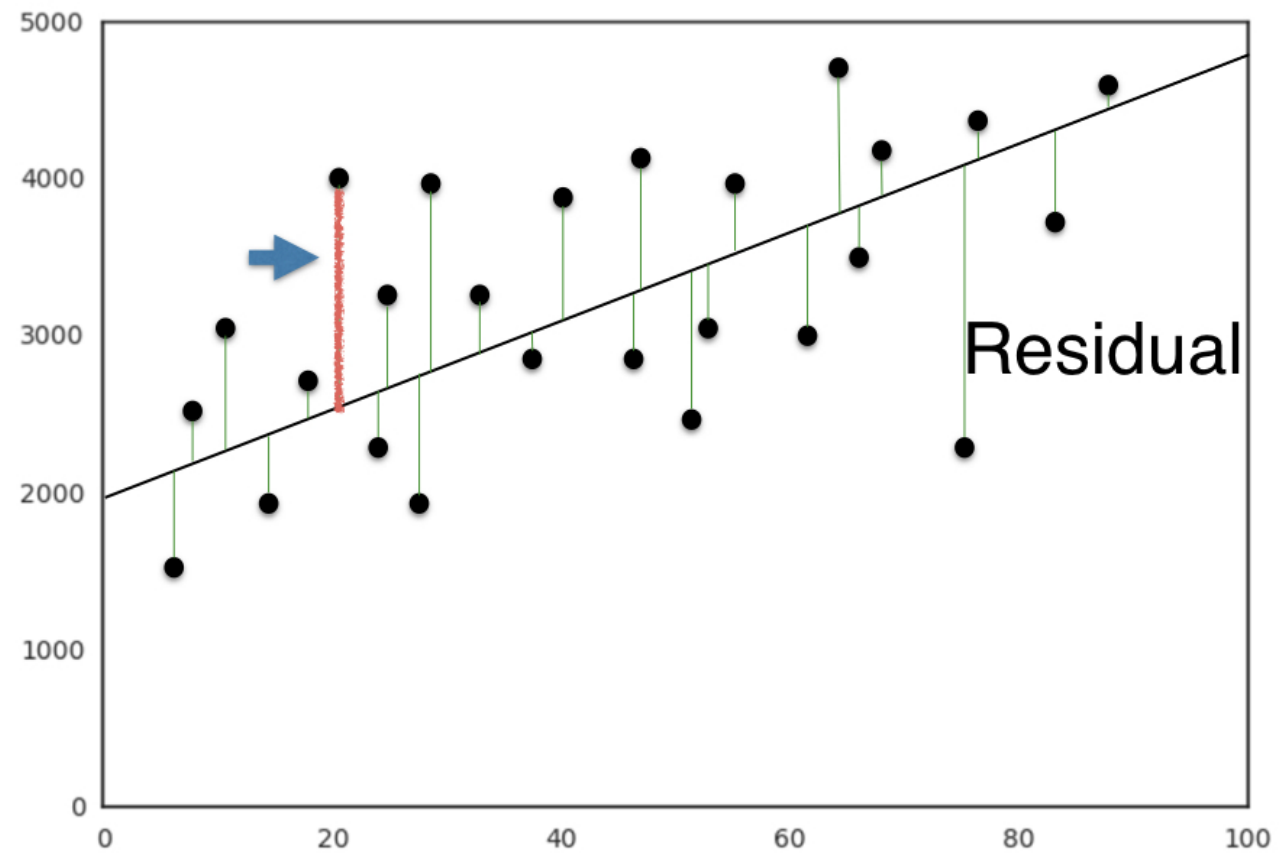
The loss function



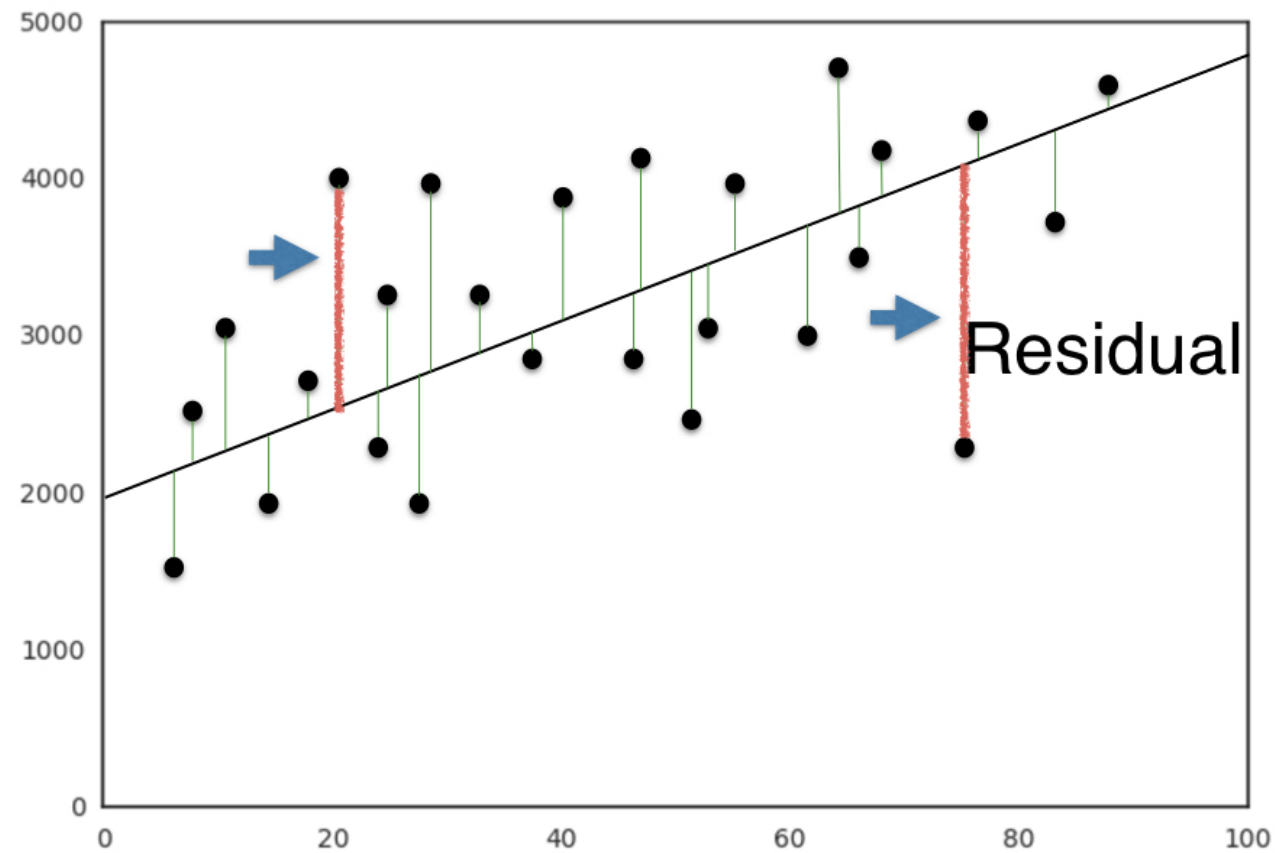
The loss function



The loss 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:
 - Must specify coefficient for each feature and the variable b

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

- Scikit-learn API works exactly the same way:
 - Pass two arrays: Features, and target

Linear regression on all features

```
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression

X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size = 0.3, random_state=42)

reg_all = LinearRegression()
reg_all.fit(X_train, y_train)
y_pred = reg_all.predict(X_test)
reg_all.score(X_test, y_test)
```

```
0.71122600574849526
```

Let's practice!

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Cross-validation

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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!

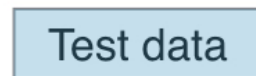
Cross-validation basics

Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
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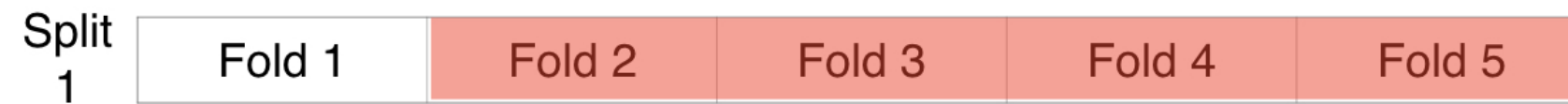
Cross-validation basics



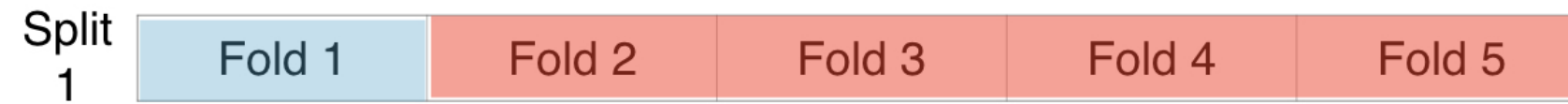
Test data

A single light blue rectangular box containing the text 'Test data'.

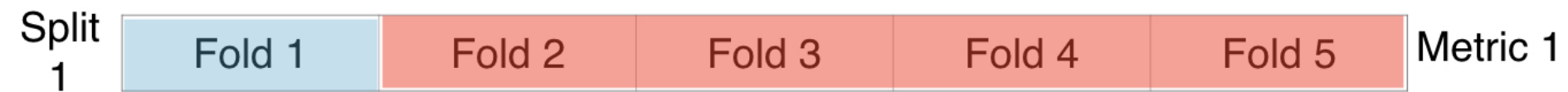
Cross-validation basics



Cross-validation basics



Cross-validation basics



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	



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	



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	



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	



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



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



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



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 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

```
from sklearn.model_selection import cross_val_score
from sklearn.linear_model import LinearRegression
reg = LinearRegression()
cv_results = cross_val_score(reg, X, y, cv=5)
print(cv_results)
```

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

```
np.mean(cv_results)
```

```
0.35327592439587058
```

Let's practice!

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Regularized regression

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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

```
from sklearn.linear_model import Ridge
X_train, X_test, y_train, y_test = train_test_split(X, y,
    test_size = 0.3, random_state=42)
ridge = Ridge(alpha=0.1, normalize=True)
ridge.fit(X_train, y_train)
ridge_pred = ridge.predict(X_test)
ridge.score(X_test, y_test)
```

```
0.69969382751273179
```

Lasso regression

- Loss function = OLS loss function +

$$\alpha * \sum_{i=1}^n |a_i|$$

Lasso regression in scikit-learn

```
from sklearn.linear_model import Lasso
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size = 0.3, random_state=42)

lasso = Lasso(alpha=0.1, normalize=True)
lasso.fit(X_train, y_train)
lasso_pred = lasso.predict(X_test)
lasso.score(X_test, y_test)
```

```
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

```
from sklearn.linear_model import Lasso

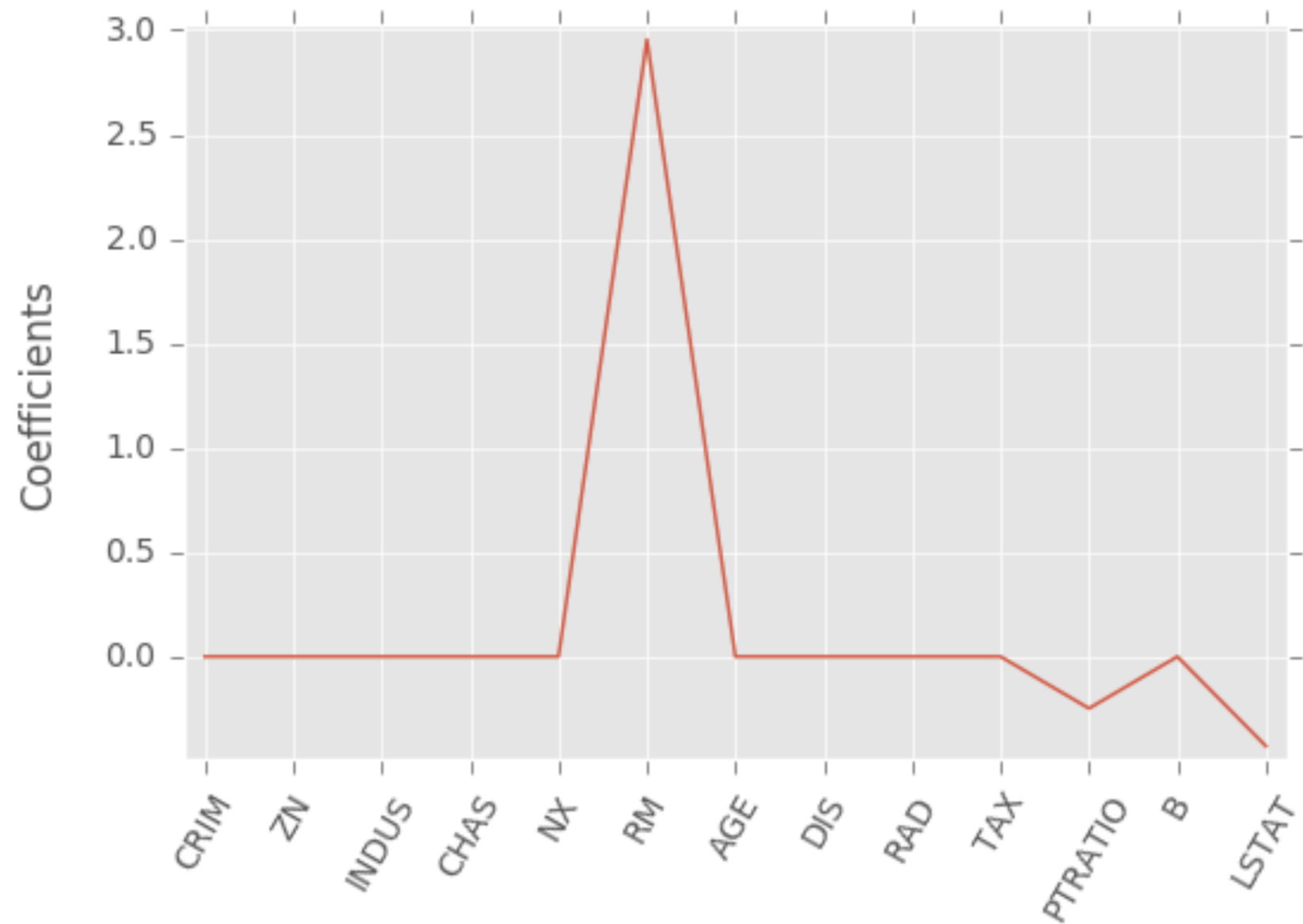
names = boston.drop('MEDV', axis=1).columns

lasso = Lasso(alpha=0.1)

lasso_coef = lasso.fit(X, y).coef_

_ = plt.plot(range(len(names)), lasso_coef)
_ = plt.xticks(range(len(names)), names, rotation=60)
_ = plt.ylabel('Coefficients')
plt.show()
```

Lasso for feature selection in scikit-learn



Let's practice!

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