Introduction to regression

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Core developer, scikit-learn



Boston housing data

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

```
CRIM
                                                          TAX \\
          ZN INDUS
                    CHAS
                            NX
                                   RM
                                       AGE
                                               DIS RAD
0.00632
        18.0
               2.31
                       0 0.538 6.575 65.2 4.0900
                                                     1 296.0
0.02731
                       0 0.469 6.421 78.9 4.9671
         0.0
               7.07
                                                     2 242.0
0.02729
               7.07
                      0 0.469 7.185 61.1 4.9671
                                                     2 242.0
         0.0
0.03237
                       0 0.458 6.998 45.8 6.0622
                                                     3 222.0
         0.0
               2.18
0.06905
         0.0
               2.18
                       0 0.458 7.147 54.2 6.0622
                                                     3 222.0
PTRATIO
             B LSTAT
                      MEDV
   15.3 396.90
                4.98 24.0
   17.8 396.90
                9.14 21.6
                4.03 34.7
   17.8 392.83
   18.7 394.63
                2.94 33.4
   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)

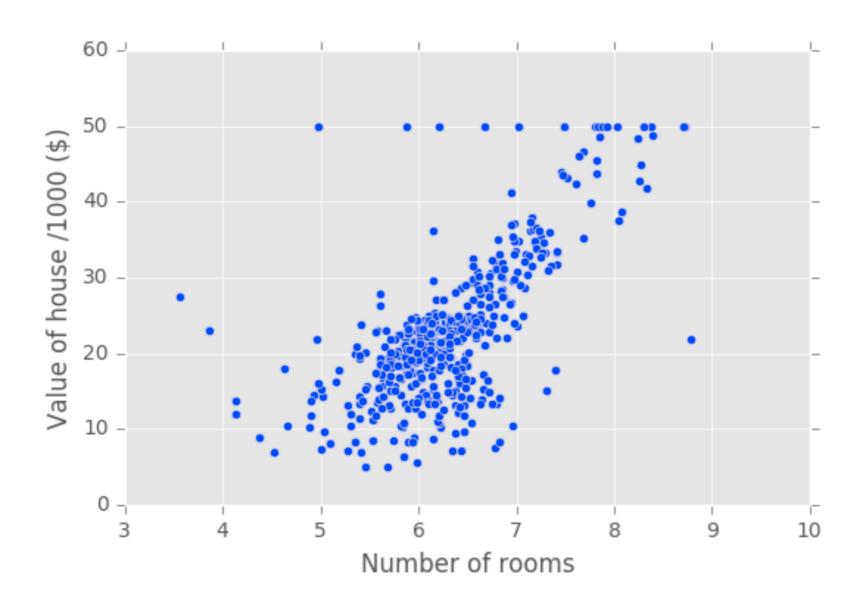
(numpy.ndarray, numpy.ndarray)

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

Plotting house value vs. number of rooms

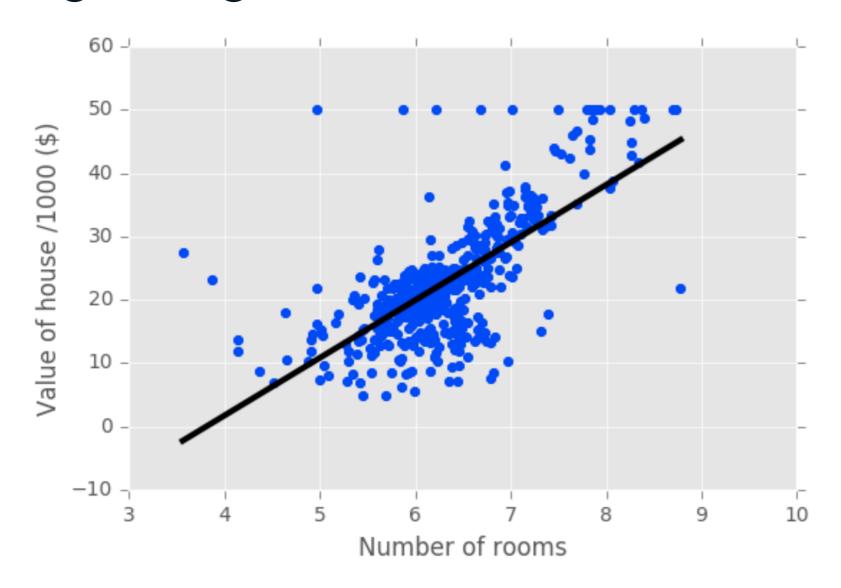
```
plt.scatter(X_rooms, y)
plt.ylabel('Value of house /1000 ($)')
plt.xlabel('Number of rooms')
plt.show();
```

Plotting house value vs. number of rooms



Fitting a regression model

Fitting a regression model





Let's practice!

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The basics of linear regression

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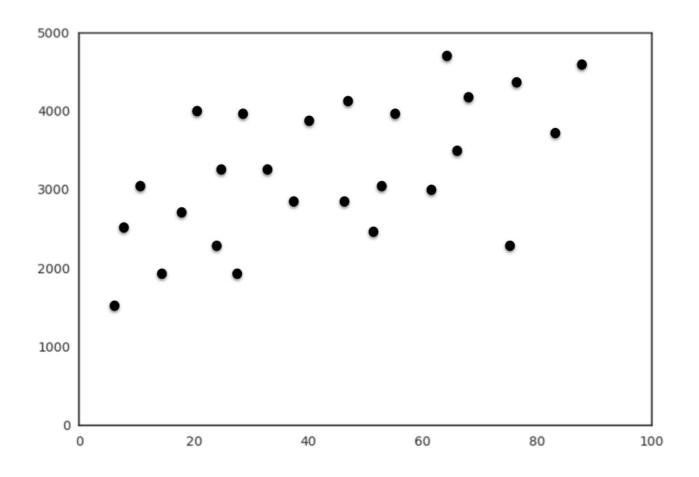


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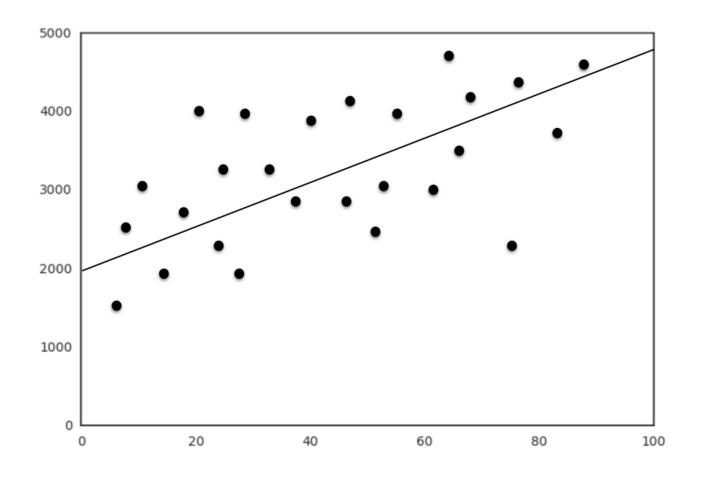


Regression mechanics

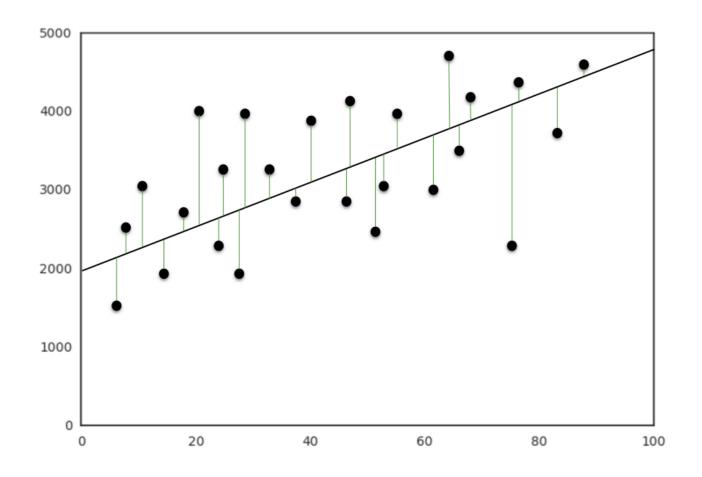
- y = ax + b
 - \circ y = target
 - x = single feature
 - o a, b = parameters of model
- How do we choose a and b?
- Define an error functions for any given line
 - Choose the line that minimizes the error function



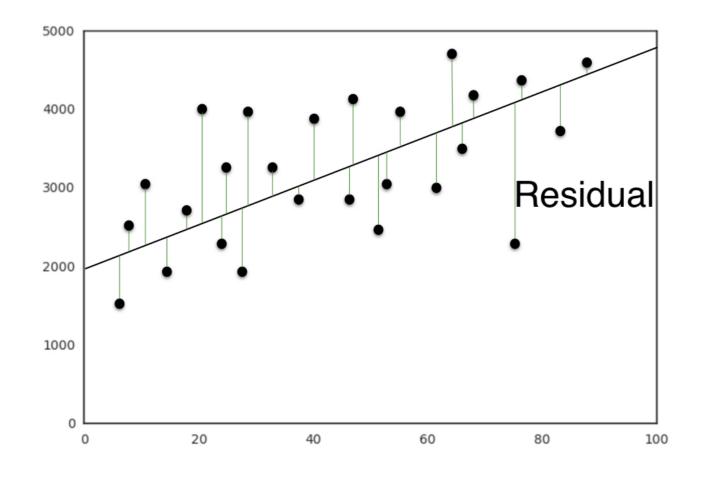




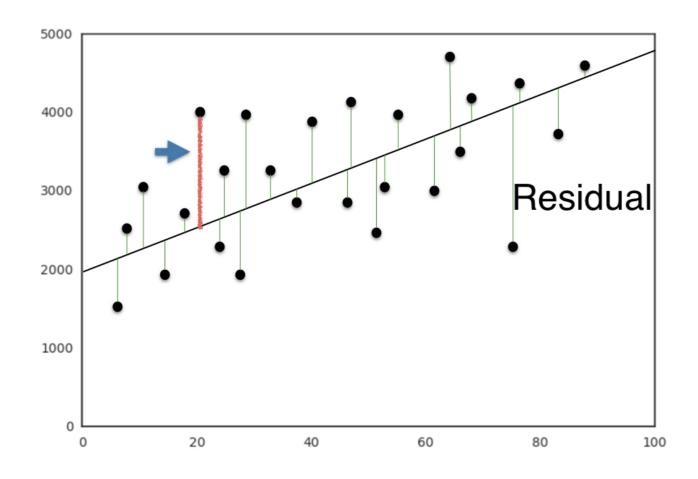




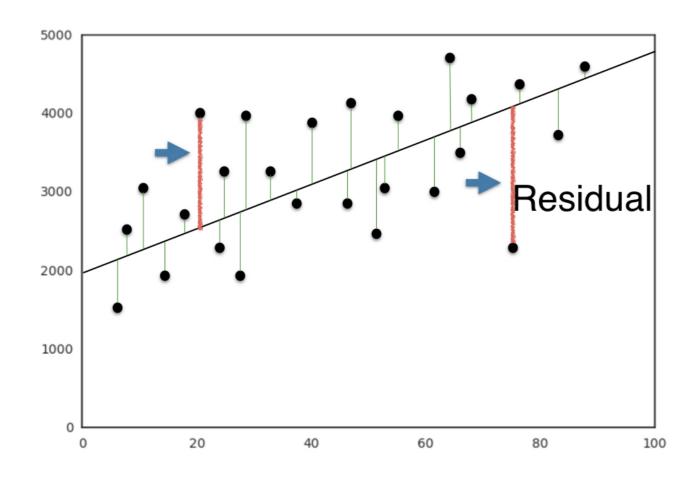












Ordinary least squares(OLS): Minimize sum of squares of residuals



Linear regression in higher dimensions

$$y = a_1 x_1 + a_2 x_2 + b$$

- 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

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

- 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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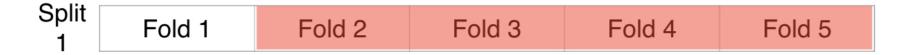
Cross-validation motivation

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

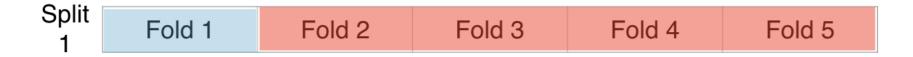
Split Fold 1 Fold 2 Fold 3 Fold 4 Fold 5



Split Fold 1 Fold 2 Fold 3 Fold 4 Fold 5



Training data



Training data



Training data

Split [Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 1
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	

Training data

Split [Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 1
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	

Training data

Split [Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 1
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	

Training data

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	

Training data

Split [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

Training data

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

Training data

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

Training data

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

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

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 +

$$lpha * \sum_{i=1}^n {a_i}^2$$

- 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 +

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

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

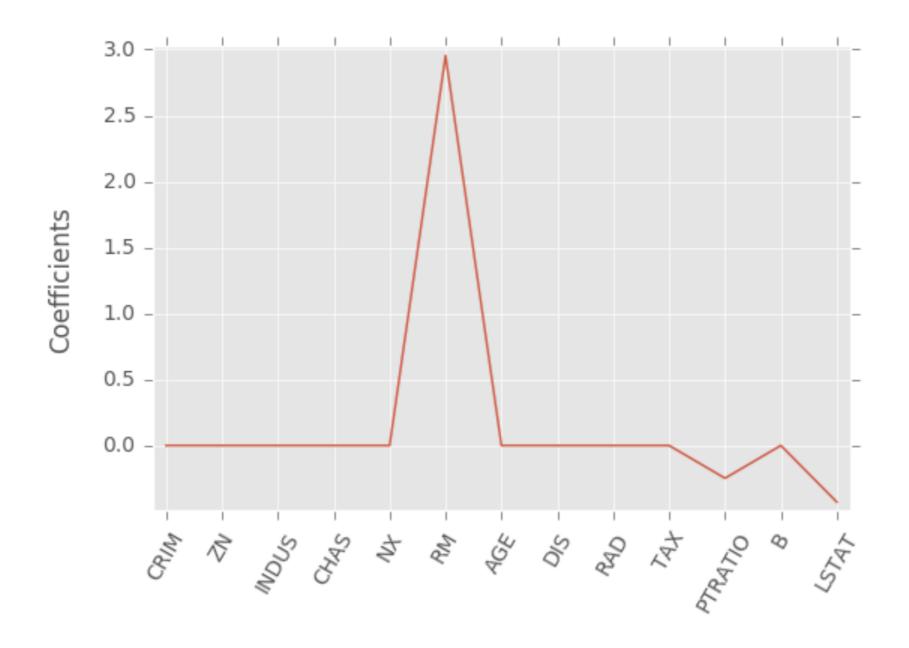


Lasso regression for feature selection

- 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

Lasso for feature selection in scikit-learn



Let's practice!

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