06_linear_regression

February 28, 2024

1 Data science pipeline: pandas, seaborn, scikit-learn

Lesson 6 from Introduction to Machine Learning with scikit-learn

Note: This notebook uses Python 3.9.1 and scikit-learn 0.23.2. The original notebook (shown in the video) used Python 2.7 and scikit-learn 0.16.

1.1 Agenda

- How do I use the **pandas library** to read data into Python?
- How do I use the **seaborn library** to visualize data?
- What is **linear regression**, and how does it work?
- How do I **train and interpret** a linear regression model in scikit-learn?
- What are some **evaluation metrics** for regression problems?
- How do I choose **which features to include** in my model?

1.2 Types of supervised learning

- **Classification:** Predict a categorical response
- **Regression:** Predict a continuous response

1.3 Reading data using pandas

Pandas: popular Python library for data exploration, manipulation, and analysis

- Anaconda users: pandas is already installed
- Other users: installation instructions

[1]:
```
# added empty cell so that the cell numbering matches the video
```

[2]:
```
# conventional way to import pandas
import pandas as pd
```

[3]:
```
# read CSV file from the 'data' subdirectory using a relative path
data = pd.read_csv('data/Advertising.csv', index_col=0)

# display the first 5 rows
data.head()
```

[3]:

	TV	Radio	Newspaper	Sales
1	230.1	37.8	69.2	22.1
2	44.5	39.3	45.1	10.4
3	17.2	45.9	69.3	9.3
4	151.5	41.3	58.5	18.5
5	180.8	10.8	58.4	12.9

Primary object types:

- **DataFrame:** rows and columns (like a spreadsheet)
- **Series:** a single column

[4]:
```
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```

[5]:
```
# display the last 5 rows
data.tail()
```

[5]:

	TV	Radio	Newspaper	Sales
196	38.2	3.7	13.8	7.6
197	94.2	4.9	8.1	9.7
198	177.0	9.3	6.4	12.8
199	283.6	42.0	66.2	25.5
200	232.1	8.6	8.7	13.4

[6]:
```
# check the shape of the DataFrame (rows, columns)
data.shape
```

[6]: (200, 4)

What are the features? - **TV:** advertising dollars spent on TV for a single product in a given market (in thousands of dollars) - **Radio:** advertising dollars spent on Radio - **Newspaper:** advertising dollars spent on Newspaper

What is the response? - **Sales:** sales of a single product in a given market (in thousands of items)

What else do we know? - Because the response variable is continuous, this is a **regression** problem. - There are 200 **observations** (represented by the rows), and each observation is a single market.

1.4 Visualizing data using seaborn

Seaborn: Python library for statistical data visualization built on top of Matplotlib

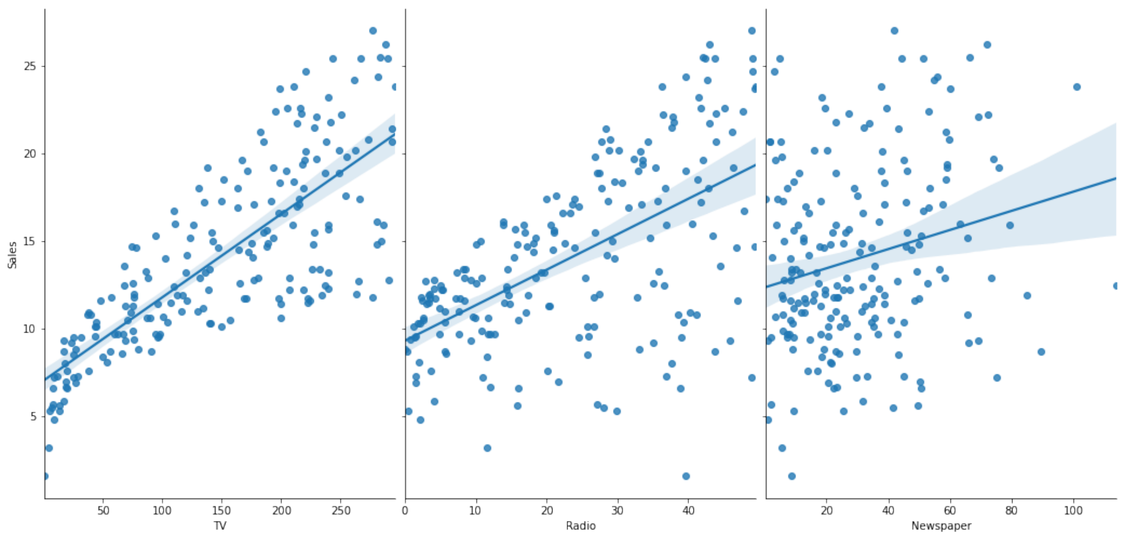
- Anaconda users: run **`conda install seaborn`** from the command line
- Other users: installation instructions

[7]:
```
# conventional way to import seaborn
import seaborn as sns

# allow plots to appear within the notebook
%matplotlib inline
```

[8]:
```python
# visualize the relationship between the features and the response using␣
↪scatterplots
sns.pairplot(data, x_vars=['TV','Radio','Newspaper'], y_vars='Sales', height=7,␣
↪aspect=0.7, kind='reg')
```

[8]: <seaborn.axisgrid.PairGrid at 0x7fb0288ec550>



1.5 Linear regression

Pros: fast, no tuning required, highly interpretable, well-understood

Cons: unlikely to produce the best predictive accuracy (presumes a linear relationship between the features and response)

1.5.1 Form of linear regression

$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \beta_n x_n$

- y is the response
- β_0 is the intercept
- β_1 is the coefficient for x_1 (the first feature)
- β_n is the coefficient for x_n (the nth feature)

In this case:

$y = \beta_0 + \beta_1 \times TV + \beta_2 \times Radio + \beta_3 \times Newspaper$

The β values are called the **model coefficients**. These values are "learned" during the model fitting step using the "least squares" criterion. Then, the fitted model can be used to make predictions!

1.6 Preparing X and y using pandas

- scikit-learn expects X (feature matrix) and y (response vector) to be NumPy arrays.

- However, pandas is built on top of NumPy.
- Thus, X can be a pandas DataFrame and y can be a pandas Series!

[9]:
```python
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```

[10]:
```python
# added empty cell so that the cell numbering matches the video
```

[11]:
```python
# create a Python list of feature names
feature_cols = ['TV', 'Radio', 'Newspaper']

# use the list to select a subset of the original DataFrame
X = data[feature_cols]

# equivalent command to do this in one line
X = data[['TV', 'Radio', 'Newspaper']]

# print the first 5 rows
X.head()
```

[11]:

	TV	Radio	Newspaper
1	230.1	37.8	69.2
2	44.5	39.3	45.1
3	17.2	45.9	69.3
4	151.5	41.3	58.5
5	180.8	10.8	58.4

[12]:
```python
# check the type and shape of X
print(type(X))
print(X.shape)
```

```
<class 'pandas.core.frame.DataFrame'>
(200, 3)
```

[13]:
```python
# select a Series from the DataFrame
y = data['Sales']

# equivalent command that works if there are no spaces in the column name
y = data.Sales

# print the first 5 values
y.head()
```

[13]:
```
1    22.1
2    10.4
3     9.3
4    18.5
5    12.9
Name: Sales, dtype: float64
```

[14]:
```
# check the type and shape of y
print(type(y))
print(y.shape)
```

```
<class 'pandas.core.series.Series'>
(200,)
```

1.7 Splitting X and y into training and testing sets

[15]:
```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)
```

[16]:
```
# default split is 75% for training and 25% for testing
print(X_train.shape)
print(y_train.shape)
print(X_test.shape)
print(y_test.shape)
```

```
(150, 3)
(150,)
(50, 3)
(50,)
```

1.8 Linear regression in scikit-learn

[17]:
```
# import model
from sklearn.linear_model import LinearRegression

# instantiate
linreg = LinearRegression()

# fit the model to the training data (learn the coefficients)
linreg.fit(X_train, y_train)
```

[17]:
```
LinearRegression()
```

1.8.1 Interpreting model coefficients

[18]:
```
# print the intercept and coefficients
print(linreg.intercept_)
print(linreg.coef_)
```

```
2.8769666223179318
[0.04656457 0.17915812 0.00345046]
```

[19]:
```
# pair the feature names with the coefficients
list(zip(feature_cols, linreg.coef_))
```

[19]: [('TV', 0.046564567874150289),
 ('Radio', 0.17915812245088839),
 ('Newspaper', 0.0034504647111803788)]

$$y = 2.88 + 0.0466 \times TV + 0.179 \times Radio + 0.00345 \times Newspaper$$

How do we interpret the **TV coefficient** (0.0466)?

- For a given amount of Radio and Newspaper ad spending, **a "unit" increase in TV ad spending** is associated with a **0.0466 "unit" increase in Sales**.
- Or more clearly: For a given amount of Radio and Newspaper ad spending, **an additional $1,000 spent on TV ads** is associated with an **increase in sales of 46.6 items**.

Important notes:

- This is a statement of **association**, not **causation**.
- If an increase in TV ad spending was associated with a **decrease** in sales, β_1 would be **negative**.

1.8.2 Making predictions

[20]:
```
# make predictions on the testing set
y_pred = linreg.predict(X_test)
```

We need an **evaluation metric** in order to compare our predictions with the actual values!

1.9 Model evaluation metrics for regression

Evaluation metrics for classification problems, such as **accuracy**, are not useful for regression problems. Instead, we need evaluation metrics designed for comparing continuous values.

Let's create some example numeric predictions, and calculate **three common evaluation metrics** for regression problems:

[21]:
```
# define true and predicted response values
true = [100, 50, 30, 20]
pred = [90, 50, 50, 30]
```

Mean Absolute Error (MAE) is the mean of the absolute value of the errors:

$$\frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

[22]:
```
# calculate MAE by hand
print((10 + 0 + 20 + 10)/4.)

# calculate MAE using scikit-learn
from sklearn import metrics
print(metrics.mean_absolute_error(true, pred))
```

```
10.0
10.0
```

Mean Squared Error (MSE) is the mean of the squared errors:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

[23]:
```
# calculate MSE by hand
print((10**2 + 0**2 + 20**2 + 10**2)/4.)

# calculate MSE using scikit-learn
print(metrics.mean_squared_error(true, pred))
```

```
150.0
150.0
```

Root Mean Squared Error (RMSE) is the square root of the mean of the squared errors:

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

[24]:
```
# calculate RMSE by hand
import numpy as np
print(np.sqrt((10**2 + 0**2 + 20**2 + 10**2)/4.))

# calculate RMSE using scikit-learn
print(np.sqrt(metrics.mean_squared_error(true, pred)))
```

```
12.24744871391589
12.24744871391589
```

Comparing these metrics:

- **MAE** is the easiest to understand, because it's the average error.
- **MSE** is more popular than MAE, because MSE "punishes" larger errors.
- **RMSE** is even more popular than MSE, because RMSE is interpretable in the "y" units.

1.9.1 Computing the RMSE for our Sales predictions

[25]:
```
print(np.sqrt(metrics.mean_squared_error(y_test, y_pred)))
```

```
1.404651423032895
```

1.10 Feature selection

Does **Newspaper** "belong" in our model? In other words, does it improve the quality of our predictions?

Let's **remove it** from the model and check the RMSE!

[26]:
```
# create a Python list of feature names
feature_cols = ['TV', 'Radio']

# use the list to select a subset of the original DataFrame
X = data[feature_cols]

# select a Series from the DataFrame
y = data.Sales

# split into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)

# fit the model to the training data (learn the coefficients)
linreg.fit(X_train, y_train)

# make predictions on the testing set
y_pred = linreg.predict(X_test)

# compute the RMSE of our predictions
print(np.sqrt(metrics.mean_squared_error(y_test, y_pred)))
```

```
1.3879034699382886
```

The RMSE **decreased** when we removed Newspaper from the model. (Error is something we want to minimize, so **a lower number for RMSE is better**.) Thus, it is unlikely that this feature is useful for predicting Sales, and should be removed from the model.

1.11 Resources

Linear regression:

- Longer notebook on linear regression by me
- Chapter 3 of An Introduction to Statistical Learning and related videos by Hastie and Tibshirani (Stanford)
- Quick reference guide to applying and interpreting linear regression by me
- Introduction to linear regression by Robert Nau (Duke)

Pandas:

- pandas Q&A video series by me
- Three-part pandas tutorial by Greg Reda
- read_csv and read_table documentation

Seaborn:

- Official seaborn tutorial
- Example gallery

1.12 Comments or Questions?

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