Machine Learning Notebook

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Contents

※ Chapter 3 (3/31)

1.1 Scalar-Vector Equation Derivatives

1.1.1 Scalar Equation

$\vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$, where$f(\vec{y})$ is a 1×1 scalar, $\vec{y}$ is an $m \times 1$ vector.

Denominator Layout. Number of rows is the same as the denominator.

$$\frac{\partial f(\vec{y})}{\partial \vec{y}} = \begin{bmatrix} \frac{\partial f(\vec{y})}{\partial y_1} \\ \frac{\partial f(\vec{y})}{\partial y_2} \\ \vdots \\ \frac{\partial f(\vec{y})}{\partial y_m} \end{bmatrix}_{m\times 1} \tag{1}$$

Numerator Layout. Number of columns is the same as the numerator.

$$\frac{\partial f(\vec{y})}{\partial \vec{y}} = \begin{bmatrix} \frac{\partial f(\vec{y})}{\partial y_1} & \frac{\partial f(\vec{y})}{\partial y_2} & \dots & \frac{\partial f(\vec{y})}{\partial y_m} \end{bmatrix}_{1\times m} \tag{2}$$

1.1.2 Vector Equation

$$\vec{f}(\vec{y}) = \begin{bmatrix} f_1(\vec{y}) \\ f_2(\vec{y}) \\ \vdots \\ f_n(\vec{y}) \end{bmatrix}_{n\times 1}, \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}_{m\times 1} \tag{3}$$

$$\frac{\partial \vec{f}(\vec{y})_{n\times 1}}{\partial \vec{y}_{m\times 1}} = \begin{bmatrix} \frac{\partial f(\vec{y})}{\partial y_1} \\ \frac{\partial f(\vec{y})}{\partial y_2} \\ \vdots \\ \frac{\partial f(\vec{y})}{\partial y_m} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1(\vec{y})}{\partial y_1} & \frac{\partial f_2(\vec{y})}{\partial y_1} & \dots & \frac{\partial f_n(\vec{y})}{\partial y_1} \\ \frac{\partial f_1(\vec{y})}{\partial y_2} & \frac{\partial f_2(\vec{y})}{\partial y_2} & \dots & \frac{\partial f_n(\vec{y})}{\partial y_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_1(\vec{y})}{\partial y_m} & \frac{\partial f_2(\vec{y})}{\partial y_m} & \dots & \frac{\partial f_n(\vec{y})}{\partial y_m} \end{bmatrix} \tag{4}$$

$$\text{eg.} \quad \vec{f}(\vec{y}) = \begin{bmatrix} f_1(\vec{y}) \\ f_2(\vec{y}) \end{bmatrix} = \begin{bmatrix} y_1^2 + y_2^2 + y_3 \\ y_3^2 + 2y_1 \end{bmatrix}_{2\times 1}, \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}_{3\times 1} \tag{5}$$

$$\frac{\partial \vec{f}(\vec{y})_{n\times 1}}{\partial \vec{y}_{m\times 1}} = \begin{bmatrix} \frac{\partial f(\vec{y})}{\partial y_1} \\ \frac{\partial f(\vec{y})}{\partial y_2} \\ \frac{\partial f(\vec{y})}{\partial y_3} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1(\vec{y})}{\partial y_1} & \frac{\partial f_2(\vec{y})}{\partial y_1} \\ \frac{\partial f_1(\vec{y})}{\partial y_2} & \frac{\partial f_2(\vec{y})}{\partial y_2} \\ \frac{\partial f_1(\vec{y})}{\partial y_3} & \frac{\partial f_2(\vec{y})}{\partial y_3} \end{bmatrix} = \begin{bmatrix} 2y_1 & 2 \\ 2y_2 & 0 \\ 1 & 2y_3 \end{bmatrix}_{3\times 2} \tag{6}$$

1.1.3 Special Cases

Common special cases in matrix differentiation.

$\frac{\partial A\vec{y}}{\partial \vec{y}} = A^T$

$\frac{\partial \vec{y}^T A\vec{y}}{\partial \vec{y}} = A\vec{y} + A^T\vec{y} = 2A\vec{y} \quad$ (if A is symmetric.)

1.2 Linear Regression

Find y_1, y_2 to minimize the cost function J.

$$J = \sum_{i=1}^{n} [z_i - (y_1 + y_2 x_i)]^2$$

$$\vec{z} = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix}, \vec{x} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}, \vec{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$\text{Least Squares Estimation} \quad \vec{\hat{z}} = \vec{x}\vec{y} = \begin{bmatrix} y_1 + y_2 x_1 \\ y_1 + y_2 x_2 \\ \vdots \\ y_1 + y_2 x_n \end{bmatrix}$$

$$\begin{aligned} \therefore J &= (\vec{z} - \vec{\hat{z}})^T \cdot (\vec{z} - \vec{\hat{z}}) \\ &= (\vec{z} - \vec{x} \cdot \vec{y})^T \cdot (\vec{z} - \vec{x} \cdot \vec{y}) \\ &= (\vec{z}^T - (\vec{x} \cdot \vec{y})^T) \cdot (\vec{z} - \vec{x} \cdot \vec{y}) \\ &= \vec{z}^T \cdot \vec{z} - 2 \cdot (\vec{x} \cdot \vec{y})^T \cdot \vec{z} + (\vec{x} \cdot \vec{y})^T \cdot (\vec{x} \cdot \vec{y}) \end{aligned}$$

Now, taking the derivative of J with respect to $\vec{y}$ and setting it to zero:

$$\frac{\partial J}{\partial \vec{y}} = -2 \cdot \vec{x}^T \cdot \vec{z} + 2 \cdot \vec{x}^T \cdot (\vec{x} \cdot \vec{y}) = 0$$

Solving for $\vec{y}$:

$$\vec{y} = (\vec{x}^T \cdot \vec{x})^{-1} \cdot \vec{x}^T \cdot \vec{z}$$

1.3 Chain Rule

For the scalar function $J = f(y(u))$:

$$\frac{\partial J}{\partial u} = \frac{\partial f}{\partial y} \cdot \frac{\partial y}{\partial u}$$

When taking the derivative of a scalar with respect to a vector $J = f(\vec{y}(\vec{u}))$:

$$\frac{\partial J}{\partial \vec{u}} = \frac{\partial \vec{y}}{\partial \vec{u}} \cdot \frac{\partial f}{\partial \vec{y}}$$

❊ Chapter 4 (4/31)

2.1 Gradient Descent Principles

Gradient descent aims to iteratively minimize a given loss or cost function.

2.1.1 Algorithm Steps:

1. Define a loss function $J(x_0)$.
2. Choose an initial point x_0 with any precision.
3. Calculate the gradient at the starting point: $\nabla J(x_0) = \frac{\partial J(x_0)}{\partial x_0}$.
4. Set a learning rate η.
5. Compute the next point $x_1 = x_0 - \eta \nabla J(x_0)$.
6. Iterate the process.
7. Choose a very small number ε.
8. Stop the iteration when the condition $|J(x_1) - J(x_0)| < \varepsilon$ is satisfied.
9. The stopping point $J(x_1)$ is the minimum value.

Key Considerations

1. The gradient is a vector pointing in a direction where moving along that direction increases $J(x)$ the fastest, and moving in the opposite direction decreases it the fastest.
2. In problems aiming to find the minimum value, the objective is to make $J(x)$ decrease rapidly.
3. The absolute value of the gradient diminishes, and the distance between adjacent x values decreases.

2.1.2 Mathematical derivation

Using Taylor expansion, expand $J(x)$ at any point x_0:

$$J(x_1) = J(x_0) + (x_1 - x_0)\frac{\partial J(x_0)}{\partial x_0}$$

How to make $J(x_1) - J(x_0) \leq 0$? One simple approach is: $x_1 - x_0 = -\frac{\partial J(x_0)}{\partial x_0}$. In practical applications, it is necessary to introduce a step size adjustment:

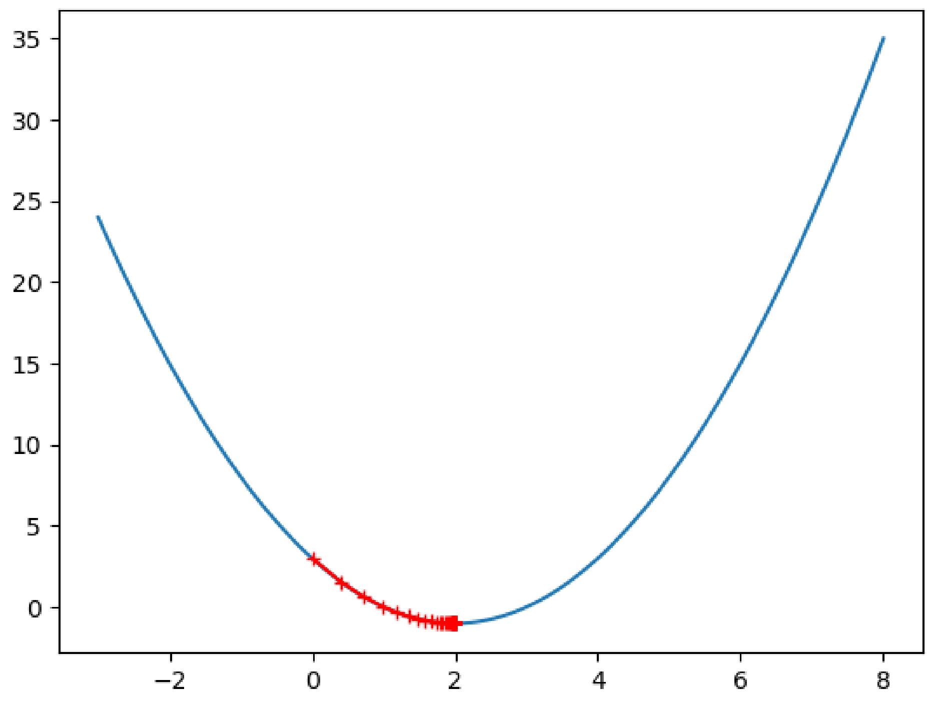
$x_1 - x_0 = -\eta \frac{\partial J(x_0)}{\partial x_0}$

2.2 Programming Implementation in PyCharm

2.2.1 Bivariate Function

The code implementation of gradient descent for the function $y = (x - 2)^2 + 1$ is as follows:

```
import numpy as np
import matplotlib.pyplot as plt

def dJ(theta):
    return 2 * (theta - 2)  # Calculate the gradient

def J(theta):
    try:
        return (theta - 2) ** 2 - 1
    except:
        return float('inf')

def gradient_descent(initial_theta, eta, theta_history=[],
   n_iters=1000, epsilon=1e-8):
    theta = initial_theta  # Initialize theta
    theta_history.append(initial_theta)
    i_iter = 0
    while i_iter < n_iters:
        gradient = dJ(theta)
        last_theta = theta
        theta = theta - eta * gradient
        theta_history.append(theta)
        # Termination condition
        if abs(J(theta) - J(last_theta)) < epsilon:
            break
        i_iter += 1
    return theta_history

def plot_theta_history(x, theta_history=[]):
    plt.plot(x, J(x))
    plt.plot(np.array(theta_history), J(np.array(theta_history)
   ), color='red', marker="+")
    plt.show()

# This is an example of a univariate function.
plot_x = np.linspace(-3, 8, 201)  # Prepare data
plot_y = (plot_x - 2) ** 2 - 1  # Define the function form
theta = 0.0
eta = 1
theta_history = []
theta_history = gradient_descent(0, eta)  # Call the gradient
   descent method
print("The function achieves the minimum value at x = %s!" %
   theta_history[-1])
print("The minimum value of the function is: %s" % J(
   theta_history[-1]))
plot_theta_history(plot_x, theta_history)
```



※ Chapter 5 (5/31)

The main contents of this chapter are as follows:

(1) The principle of linear regression, i.e., why minimize the sum of squared residuals?

(2) Matrix representation formula for the sum of squared residuals in linear regression.

(3) Matrix representation formula for the derivative (or gradient) of the sum of squared residuals.

(4) Based on the above two matrices, one can write code for gradient descent to solve regression coefficients. The focus is on the iterative formula for coefficients.

(5) We validate the diversity of data used in the code. If the absolute differences of variables in X (including the intercept term) are not significant, the results are relatively accurate. However, if the differences are large, there may be cases where the absolute values of the sum of squared residuals are too large. This is because it is a sum of squares. Generally, the approach is to divide it by the length of the data. If the absolute value of the sum of squared residuals is too large, the absolute value of the gradient may also be relatively large. The general approach is to divide the gradient by the length of the data. Additionally, adjusting the learning rate to be very small may be necessary. After making these adjustments, it may lead to less accurate estimates of the intercept coefficient.

(6) Through the analysis in (5), we can understand why in future machine learning, data normalization is generally performed.

Below is my assignment code.

```
import numpy as np
from sklearn.model_selection import train_test_split

class LinearRegression:
    def __init__(self):
        self._theta = None
        self.intercept_ = None
        self.coef_ = None

    def fit_gd(self, X_train, y_train, eta=0.01, n_iters=10000)
   :
        X_b = np.c_[np.ones((len(X_train), 1)), X_train]
        initial_theta = np.zeros(X_b.shape[1])
        def J(theta, X_b, y):
            return ((y - X_b.dot(theta)).T @ (y - X_b.dot(theta
))) / len(X_b)

        def DJ(theta, X_b, y):
            return X_b.T.dot(X_b.dot(theta) - y) * 2 / len(X_b)

        def gradient_descent(X_b, y, initial_theta, eta,
n_iters, epsilon=1e-8):
            theta = initial_theta
            for _ in range(n_iters):
                last_theta = theta
                theta = theta - eta * DJ(theta, X_b, y)

                if abs(J(theta, X_b, y) - J(last_theta, X_b, y)
) < epsilon:
                    break

            return theta

        self._theta = gradient_descent(X_b, y_train,
initial_theta, eta, n_iters)
        self.intercept_ = self._theta[0]
        self.coef_ = self._theta[1:]

        return self

    def predict(self, X_predict):
        assert self._theta is not None
        assert X_predict.shape[1] == len(self._theta) - 1

        X_b = np.c_[np.ones((len(X_predict), 1)), X_predict]
        return X_b.dot(self._theta)

# Generate simulated data
np.random.seed(666)
x = 2 * np.random.random(size=100)
y = 4.0 + 3.0 * x + np.random.normal(size=100)
X = x.reshape(-1, 1)
```

```
# Split the dataset
X_train, X_test, y_train, y_test = train_test_split(X, y)

# Fit using gradient descent
reg = LinearRegression()
reg.fit_gd(X_train, y_train)
print("Coefficients:", reg.coef_)
print("Intercept:", reg.intercept_)
```

❊ Chapter 6 (6/31)

Let y be a random variable with a probability density function dependent on parameters θ (a vector, possibly with multiple parameters, e.g., mean μ and variance σ). Then, the probability of observing a sequence of numbers $y_1, y_2, y_3, \ldots, y_n$ is given by:

$$L(y|\theta) = \prod_{i=1}^{n} f(y_i, \theta)$$

Here, the expression $L(\theta)$ is called the likelihood function. Given a specific set of parameters θ, it becomes a concrete numerical value. Now, consider the inverse problem where we lack information about θ but possess information about f. How can we infer θ using this information?

- We can express the likelihood function mentioned above as a function of θ:

$$L(\theta|y, f) = \prod_{i=1}^{n} f(y_i|\theta)$$

- A natural idea is that θ, which maximizes the above function, is the one we seek. Denote this optimal θ as $\hat{\theta}_{MLE}$:

$$\hat{\theta}_{MLE} = \arg\max_{\theta} L(\theta|y, f)$$

Solution Approach:

- To find the solution, the following equation is commonly employed:

$$\frac{\partial}{\partial\theta} L(\theta, y) = 0$$

- Another common form is expressed using the logarithm:

$$\frac{\partial}{\partial\theta} \ln(L(\theta, y)) = g(\theta) = 0$$

  This expression is often referred to as the likelihood equation and is typically expressed in the form of a summation.

$$g(\theta) = \sum_{i=1}^{n} g_i(\theta)$$

  where $g(\theta)$ and $g_i(\theta)$ are random vectors.

※ Chapter 7 (7/31)

5.1 Linear Probability Model

Disregarding the characteristics of binary classification data, we still employ the conventional linear regression for estimation. The advantages of the linear probability model include:

- The coefficients have clear interpretations.
- At the population level:

$$E(y|x) = \beta_0 + \beta_1 x \quad \beta_1 = \frac{dE(y|x)}{dx}$$

$$E(y|x) = pr(y = x) \quad \beta_1 = \frac{dpr(y = x)}{dx}$$

  – If x increases by 1, how much does the probability $y = 1$ increase?

However, the drawback of the linear probability model lies in the emergence of meaningless probabilities and negative variances. To tackle this issue:

- Fundamental Problem:

$$E(y|x) = \mathrm{pr}(y = 1|x) = \beta_0 + \beta_1 x$$

  – The root of the problem lies in the quest for a function $G(x)$ that consistently yields values within the [0, 1] interval.

$$E(y|x) = \mathrm{pr}(y = 1|x) = G(\beta_0 + \beta_1 x)$$

- Approach:
  – Random variable distribution functions, such as the normal distribution and logistic distribution, can serve as potential solutions.

5.2 Logistic regression

Logistic Regression Sufficiency:

Latent Regression:

$$y^* = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_k x_k + u$$

where u follows a logistic distribution.

Density Function:

$$f(y|x) = \frac{e^{-x}}{(1+e^{-x})^2}$$

Distribution Function:

$$F(y|x) = \frac{1}{1+e^{-x}}$$

From Latent Regression to Observed Values y:

$$y = \begin{cases} 1 & \text{if } y^* \geq 0 \\ 0 & \text{if } y^* < 0 \end{cases}$$

- **A Simple Derivation:**

$$\begin{aligned} pr(y=1) &= pr(y^* \geq 0) \\ &= pr(u \geq -(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots \beta_k x_k)) \\ &= 1 - \phi(-(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots \beta_k x_k)) \\ &= \phi(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots \beta_k x_k) \end{aligned}$$

  This is the distribution function of logistic regression. By using logistic regression, we can ensure that the predicted values fall within the interval (0, 1).

- **How to Estimate Coefficients?**

  - Maximum Likelihood Estimation. The coefficients should maximize the probability of observing our dataset. Given a set of coefficients $\beta_0, \beta_1, \beta_2, \ldots, \beta_k$,
    $$y = \begin{cases} 1 & \text{if } x = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_k X_k \geq 0 \\ 0 & \text{if } x = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_k X_k < 0 \end{cases}$$
  - Probability of y

    $$P(y=1) = \phi(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots \beta_k x_k)$$

    $$P(y=0) = 1 - P(y=1)$$

    Probability of an Observation:

    $$\phi^{y_i}(1-\phi)^{(1-y_i)}$$

  - **Probability of All n Observations Simultaneously Occurring:**

    $$\prod_{i=1}^{n} \phi^{y_i}(1-\phi)^{(1-y_i)}$$

The problem of maximizing the above probability is equivalent to maximizing its logarithm:

$$\sum_{i=1}^{n}(y_i \log \phi + (1 - y_i) \log(1 - \phi))]$$

– In machine learning, the relationship with the loss function is exactly opposite: one seeks to maximize, while the other seeks to minimize. Both lack closed-form solutions.

5.3 Multi-nominal Logit

※ Chapter 8 (8/31)

Econometrics is also a modeling method. Their connection is simple: all are based on existing data information to create models, aiming to find the functional relationship between the dependent variable Y and independent variables $X_1, X_2, \ldots, X_n$. The differences are more complex, primarily in the following aspects:

- Econometrics uses known functional forms, such as linear functions. Machine learning's functional form is unknown, somewhat resembling non-parametric econometrics. In deep learning, what influences Y are not the original independent variables. In mathematical terms, their differences can be roughly represented as:

  Econometrics:$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_k X_n$

  Machine Learning:$Y = f(X_1, X_2, \ldots, X_n)$

  Deep Learning:

  $Y = f[g_1(X_1, X_2, \ldots, X_n), g_2(X_1, X_2, \ldots, X_n), \ldots, g_k(X_1, X_2, \ldots, X_n)]$

- Econometrics emphasizes "testing theories" and causal relationship identification. It usually starts with a theoretical judgment that a certain independent variable X_k affects Y in a particular direction. Econometrics then verifies whether this directional judgment is correct. Contrarily, econometrics does not focus much on whether X_k is the most important factor influencing Y. Machine learning and deep learning emphasize "predictive accuracy," without explicitly emphasizing the importance of specific independent variables. All variables are treated equally, and determining the most important variable relies on the results. In this sense, machine learning and deep learning are more likely to discover the variables with significant impact, facilitating the discovery of new theories and aligning with the principle that "practice is the sole criterion for testing truth."

- Machine learning and deep learning emphasize practicality. They build models based on training sets and use test sets to check predictive accuracy. Traditional econometrics does not make a clear distinction between training and test sets. It builds and tests models within the same dataset, acting both as an athlete and a referee. High goodness of fit in econometrics usually corresponds to the situation of "overfitting" in machine learning and deep learning, which is not a good thing.

- Econometrics has better interpretability; variable coefficients can usually be interpreted as "if X changes by one unit, Y changes by how many units (or percentage)." Machine learning and deep learning lack interpretability. This is also a reason why they are not widely used in academic research.

- Due to the unavailability of population data, econometrics emphasizes "inferring the population from the sample" and the significance of coefficients. Machine learning and deep learning sometimes have access to population data (such as the access control system of a certain unit), and even if they don't, they don't emphasize the significance of coefficients.

※ Chapter 9 (9/31)

Econometrics Concepts

In econometrics, we deal with the following concepts:

- **Sample:** A subset of the population used for analysis.
- **Population:** The entire set of individuals or instances about which information is sought.
- **Variable:** A characteristic or property that can take different values.
- **Observation:** A single instance or data point in a dataset.
- **Explanatory Variable (X):** Independent variables used to explain or predict the dependent variable.
- **Dependent Variable (y):** The variable being predicted or explained.

Machine Learning Concepts

In machine learning, the corresponding concepts are as follows:

- **Data Set:** Corresponds to the econometric "sample," a collection of instances used for training and testing.
- **Feature:** Corresponds to the econometric "variable," a measurable property or characteristic.
- **Instance, Sample, Feature Vector:** Correspond to the econometric "observation" – individual data points or records.
- **Label:** Corresponds to the econometric "dependent variable," the variable to be predicted.

Machine Learning Classification

Machine learning can be classified based on different criteria:

- **Supervised Learning and Unsupervised Learning:**
  - **Supervised Learning:** Involves using labeled data for training.

  - **Unsupervised Learning:** Utilizes unlabeled data for training.

- **Batch Learning (Offline Learning) and Online Learning:**
  - **Batch Learning:** The training set remains unchanged during the learning process.
  - **Online Learning:** The training set changes, and new examples continuously enter the training set.

- **Parametric Learning and Nonparametric Learning:**
  - **Parametric Learning:** Assumes specific parameterized forms for the model.
  - **Nonparametric Learning:** Makes no assumptions about the model parameters.

※ Chapter 11 (11/31)

Steps for Using Scikit-Learn Module:

1. Prepare the data.
2. Split the data into training and testing sets.
3. Train the model using the training data.
4. Make predictions based on the testing data.
5. Evaluate the model.

```
from sklearn import datasets
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler

# (1) Create an instance based on the class
LR1 = LinearRegression()
print("Type of the instance:")
print(type(LR1))
print("Attributes and methods of the instance:")
print(dir(LR1))

# (2) Import data
X, y = datasets.load_diabetes(return_X_y=True)
print("Shape of X:")
print(X.shape)

# (3) Split the data into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(X, y,
   test_size=0.3, random_state=666)

# (4) Standardize the data using the training set
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)

# (5) Train the model using the training set
LR1.fit(X_train_scaled, y_train)
```

```
print("Attributes and methods of the trained model:")
print(dir(LR1))

# (6) Results of the training
print("Coefficients obtained from training:")
print(LR1.coef_)
print("Intercept obtained from training:")
print(LR1.intercept_)

# (7) Predictions based on the test set using the trained model
X_test_scaled = scaler.transform(X_test)
print(LR1.predict(X_test_scaled))

# (8) Compare predictions with actual results and provide model
    accuracy assessment
print("Model score:", LR1.score(X_test_scaled, y_test))
```

References

[1] Chapter 3. DRCAN. *Matrix Differentiation*. Link.

[2] Chapter 4. gyhccer. *Gradient Descent*. Link.

[3] Chapter 11. Hector. *Master Scikit-learn*. Link.