Multiple Liear Regression

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## Multiple Linear Regression

The multiple linear regression takes the form

with constants or parameters of the model. In vector notation, ,

$$
\vec{\beta}=\begin{pmatrix}\beta\_0\\ \beta\_1\\ \vdots \\ \beta\_d \end{pmatrix};\hspace{4mm}\vec{x}=\begin{pmatrix}1\\ x\_1\\ x\_2\\ \vdots\\ x\_d\end{pmatrix}
$$

For data points, in matrix algebra notation, we can write where and with

$$
X=\begin{pmatrix}1&x\_{11}&x\_{12}&\cdots&x\_{1d}\\1&x\_{21}&x\_{22}&\cdots&x\_{2d}\\ \vdots& \vdots &\vdots&\ddots &\vdots\\1&x\_{n1}&x\_{n2}&\cdots&x\_{nd} \end{pmatrix};\hspace{4mm} y=\begin{pmatrix}y\_1\\y\_2\\ \vdots\\ y\_n\end{pmatrix};\hspace{4mm} \xi=\begin{pmatrix}\xi\_1\\ \xi\_2\\ \vdots\\ \xi\_n\end{pmatrix}
$$

We fit the data points with the objective to minimize the loss function, mean squared error

## Ordinary Least Square Method

The scikit-learn library uses ***Ordinary Least Squares (OLS)*** method to find the parameters. This method is good for a simple and relatively smaller dataset. Here is a short note on this method. However, when the dimension is very high and the dataset is bigger, scikit-learn uses another method called ***Stochastic Gradient Descent*** for optimization which is discussed in the next section.

The goal of OLS is to find the parameter vector that minimizes the sum of squared errors (SSE) between the observed target values and the predicted values :

This can be expressed in matrix form as:

To minimize the SSE, let’s first expand the expression:

Since is a scalar (a 1x1 matrix), it is equal to its transpose. That is

and therefore,

To find the minimum of the SSE, we take the derivative with respect to and set it to zero:

Now, solve for :

To isolate , we multiply both sides by (assuming is invertible):

The vector gives the estimated coefficients that minimize the sum of squared errors between the observed target values and the predicted values . This method is exact and works well when is invertible and the dataset size is manageable. This method is very efficient for small to medium-sized datasets but can become computationally expensive for very large datasets due to the inversion of the matrix .

## Iterative Method

### Gradient Descent

GIF Credit: gbhat.com  
 Gradient Descent is an optimization algorithm used to minimize the cost function. The cost function measures how well a model with parameters fits the data. The goal is to find the values of that minimize this cost function. In terms of the iterative method, we want to find and such that . For a small change in , we can approximate using Taylor series expansion

The update rule for vanilla gradient descent is given by:

Where:

* is the current estimate of the parameters at iteration .
* is the learning rate, a small positive scalar that controls the step size.
* is the gradient of the cost function with respect to at the current point .

The update rule comes from the idea of moving the parameter vector in the direction that decreases the cost function the most.

1. **Gradient**: The gradient represents the direction and magnitude of the steepest ascent of the function at the point . Since we want to minimize the function, we move in the opposite direction of the gradient.
2. **Step Size**: The term scales the gradient by the learning rate , determining how far we move in that direction. If is too large, the algorithm may overshoot the minimum; if it’s too small, the convergence will be slow.
3. **Iterative Update**: Starting from an initial guess , we repeatedly apply the update rule until the algorithm converges, meaning that the changes in become negligible, and is close to the optimal value .

### Stochastic Gradient Descent (SGD)

Stochastic Gradient Descent is a variation of the vanilla gradient descent. Instead of computing the gradient using the entire dataset, SGD updates the parameters using only a single data point or a small batch of data points at each iteration. The later one we call it mini batch SGD.

Suppose our cost function is defined as the average over a dataset of size :

Where represents the contribution of the -th data point to the total cost function. The gradient of the cost function with respect to is:

Vanilla gradient descent would update the parameters as:

Instead of using the entire dataset to compute the gradient, SGD approximates the gradient by using only a single data point (or a small batch). The update rule for SGD is:

Where:

* is the index of a randomly selected data point at iteration .
* is the gradient of the cost function with respect to the parameter , evaluated only at the data point indexed by .

## Python Execution

### Synthetic Data

import numpy as np  
from sklearn.linear\_model import LinearRegression  
X=np.random.randn(1000,2)  
y=3\*X[:,0]+2\*X[:,1]+1+np.random.randn(1000)

So for this project, our known relationship is .

### Fit the data: Using scikit-learn Library

mlr=LinearRegression()  
mlr.fit(X,y)  
coefficients=mlr.coef\_.tolist()  
slope=mlr.intercept\_.tolist()

So the model parameters: slope 0.9248 and coefficients 3.011, and 1.981

### Fit the data: Using Custom Library OLS

First we create our custom NewLinearRegression using the OLS formula above and save this python class as mlreg.py

import numpy as np  
  
  
class NewLinearRegression:  
 def \_\_init\_\_(self) -> None:  
 self.beta = None  
  
 def fit(self, X, y):  
 X = np.concatenate([np.ones((len(X), 1)), X], axis=1)  
 X\_transpose\_X = np.dot(X.transpose(), X)  
 X\_transpose\_X\_inverse = np.linalg.inv(X\_transpose\_X)  
 X\_transpose\_y = np.dot(X.transpose(), y)  
 self.beta = np.dot(X\_transpose\_X\_inverse, X\_transpose\_y)  
  
 def predict(self, X):  
 X = np.concatenate([np.ones((len(X), 1)), X], axis=1)  
 return np.dot(X, self.beta)  
  
 def coeff\_(self):  
 return self.beta[1:].tolist()  
  
 def interceptt\_(self):  
 return self.beta[0].tolist()

Now it’s time to use the new class

from mlreg import NewLinearRegression  
mlr1 = NewLinearRegression()  
mlr1.fit(X,y)  
coefficients1=mlr1.coeff\_()  
slope1=mlr1.interceptt\_()

So the model parameters: slope 0.9248 and coefficients 3.011, and 1.981

### Fit the data: Using Gradient Descent

We create the class

class GDLinearRegression:  
 def \_\_init\_\_(self, learning\_rate=0.01, number\_of\_iteration=1000) -> None:  
 self.learning\_rate = learning\_rate  
 self.number\_of\_iteration = number\_of\_iteration  
 self.weights = None  
 self.bias = None  
  
 def fit(self, X, y):  
 num\_of\_samples, num\_of\_features = X.shape  
 self.weights = np.zeros(num\_of\_features)  
 self.bias = 0  
  
 for \_ in range(self.number\_of\_iteration):  
 y\_predicted = np.dot(X, self.weights) + self.bias  
  
 d\_weights = (1 / num\_of\_samples) \* np.dot(X.T, (y\_predicted - y))  
 d\_bias = (1 / num\_of\_samples) \* np.sum(y\_predicted - y)  
  
 self.weights -= self.learning\_rate \* d\_weights  
 self.bias -= self.learning\_rate \* d\_bias  
  
 def predict(self, X):  
 y\_predicted = np.dot(X, self.weights) + self.bias  
 return y\_predicted  
  
 def coefff\_(self):  
 return self.weights.tolist()  
  
 def intercepttt\_(self):  
 return self.bias

Now we use this similarly as before,

from mlreg import GDLinearRegression  
mlr2= GDLinearRegression(learning\_rate=0.008)  
mlr2.fit(X,y)  
coefficients2=mlr2.coefff\_()  
slope2=mlr2.intercepttt\_()

So the model parameters: slope 0.9248 and coefficients 3.0103, and 1.9802

### Fit the data: Using Stochastic Gradient Descent

First we define the class

class SGDLinearRegression:  
 def \_\_init\_\_(self, learning\_rate=0.01, num\_iterations=1000, batch\_size=1) -> None:  
 self.learning\_rate = learning\_rate  
 self.num\_iterations = num\_iterations  
 self.batch\_size = batch\_size  
 self.theta = None  
 self.mse\_list = None # Initialize mse\_list as an instance attribute  
  
 def \_loss\_function(self, X, y, beta):  
 num\_samples = len(y)  
 y\_predicted = X.dot(beta)  
 mse = (1/num\_samples) \* np.sum(np.square(y\_predicted - y))  
 return mse  
  
 def \_gradient\_function(self, X, y, beta):  
 num\_samples = len(y)  
 y\_predicted = X.dot(beta)  
 grad = (1/num\_samples) \* X.T.dot(y\_predicted - y)  
 return grad  
  
 def fit(self, X, y):  
 # Adding the intercept term (bias) as a column of ones  
 X = np.concatenate([np.ones((len(X), 1)), X], axis=1)  
 num\_features = X.shape[1]  
 self.theta = np.zeros((num\_features, 1))  
  
 self.mse\_list = np.zeros(self.num\_iterations) # Initialize mse\_list  
  
 for i in range(self.num\_iterations):  
 # Randomly select a batch of data points  
 indices = np.random.choice(  
 len(y), size=self.batch\_size, replace=False)  
 X\_i = X[indices]  
 y\_i = y[indices].reshape(-1, 1)  
  
 # Compute the gradient and update the weights  
 gradient = self.\_gradient\_function(X\_i, y\_i, self.theta)  
 self.theta = self.theta - self.learning\_rate \* gradient  
  
 # Calculate loss for the entire dataset (optional)  
 self.mse\_list[i] = self.\_loss\_function(X, y, self.theta)  
  
 return self.theta, self.mse\_list  
  
 def predict(self, X):  
 # Adding the intercept term (bias) as a column of ones  
 X = np.concatenate([np.ones((len(X), 1)), X], axis=1)  
 return X.dot(self.theta)  
  
 def coef\_(self):  
 # Return the coefficients (excluding the intercept term)  
 return self.theta[1:].flatten().tolist()  
  
 def intercept\_(self):  
 # Return the intercept term  
 return self.theta[0].item()  
  
 def mse\_losses(self):  
 # Return the mse\_list  
 return self.mse\_list.tolist()

Now

import matplotlib.pyplot as plt  
from mlreg import SGDLinearRegression  
mlr3=SGDLinearRegression(learning\_rate=0.01, num\_iterations=1000, batch\_size=10)  
theta, \_ = mlr3.fit(X, y)

So the model parameters: slope array([0.93716786]) and coefficients array([3.05190324]), and array([1.99437424])

Up next [knn regression](../../posts/knn/index.qmd)

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