

MA506 Probability and Statistical Inference

Lecture 7: Regression 2

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In [1]: import numpy as np
import matplotlib.pyplot as plt
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1. Extending to a more general cases of Linear Regression

1.1 Instead of 4 samples, we have n samples

Modify the X, Y matrices to incorporate all the samples: $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; \quad X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

And the optimal coefficients $\hat{\beta}$ will have the same expression as before (4) with updated X and Y. Hence still we will have

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

1.2 Instead of $y = \beta_0 + \beta_1 x$ we want :

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \dots + \beta_m x^m$$

Assuming we still have n data points, relative to the base case, now we need to update all matrices involved: X , Y and β :

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; \quad X = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^m \\ 1 & x_2 & x_2^2 & \cdots & x_2^m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^m \end{bmatrix}; \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_m \end{bmatrix}$$

With these new matrices, the optimal coefficients (estimate of β : $\hat{\beta}$) will still have the same expression as (4)

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

1.3 Instead of $y = \beta_0 + \beta_1 x$ we want :
 $y = \beta_0 + \beta_1 \sin(x) + \beta_2 \cos(x)$

Assuming n samples, again updating X , Y and β as follows

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; \quad X = \begin{bmatrix} 1 & \sin(x_1) & \cos(x_1) \\ 1 & \sin(x_2) & \cos(x_2) \\ \vdots & \vdots & \vdots \\ 1 & \sin(x_n) & \cos(x_n) \end{bmatrix}; \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

Like before, with updated X , Y and β , we still have:

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

1.4: Linear regression in multiple dimensions (Multiple Linear Regression)

Suppose we have n samples in d dimensions. Hence each sample has d coordinates. For instance, i^{th} sample is represented as follows

$$(X_i, y_i) = (x_{i1}, x_{i2}, \dots, x_{id}, y_i)$$

Please note that y_i is still 1-dimensional.

Now, suppose we wish to fit a hyperplane of the following form in d dimensions. Hence for a given $X = (x_1, x_2, \dots, x_d)$ it should be able to predict a y value using the following equation

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_d x_d$$

In order to fit this hyperplane, we will again have a new definition of X , Y and β as follows:

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; \quad X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1d} \\ 1 & x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nd} \end{bmatrix}; \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_d \end{bmatrix}$$

And β will again be inferred as:

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

Higher degree polynomials etc can also be incorporated directly into the model as before when doing multiple linear regression

2 Characterizing a linear regression model

2.1 Summarizing discussed forms of linear regression models

With X , Y and β representing covariates, observations and parameters/weights, any regression model that can be expressed in the form:

$$Y = X\beta + \epsilon, \quad \epsilon \sim N(0, \sigma^2 I) \quad (5)$$

is a linear model with an estimate of β : $\hat{\beta} = (X^T X)^{-1} X^T Y$. Assuming n to be the number of samples, here $Y \in \mathbb{R}^n$, $X \in \mathbb{R}^{n \times (p+1)}$, $\beta \in \mathbb{R}^{(p+1)}$, $\sigma^2 \in \mathbb{R}^+$ and I is an n -dimensional identity matrix. Please note that the residual vector: $[e_1, e_2, e_3, e_4]^T$ discussed in the experiments at the beginning of this notebook is just a realization of ϵ in this general model formulation.

Hence, all the models discussed above belong to the general family of Linear Regr with separate definitions for X , Y and β as shown in the below mentioned cases.

Please note X matrix formulated for fitting a regression model is generally referred to :

1. **Case 1:** n 1-dimensional (univariate) samples and fitting a straight line model.

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; \quad X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}; \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

Here $p = 1$.

2. **Case 2:** n 1-dimensional (univariate) samples and fitting

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \dots + \beta_m x^m$$

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; \quad X = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^m \\ 1 & x_2 & x_2^2 & \dots & x_2^m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^m \end{bmatrix}; \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_m \end{bmatrix}$$

Here $p = m$.

3. **Case 3:** n 1-dimensional (univariate) samples and fitting

$$y = \beta_0 + \beta_1 \sin(x) + \beta_2 \cos(x)$$

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; \quad X = \begin{bmatrix} 1 & \sin(x_1) & \cos(x_1) \\ 1 & \sin(x_2) & \cos(x_2) \\ \vdots & \vdots & \vdots \\ 1 & \sin(x_n) & \cos(x_n) \end{bmatrix}; \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

Here $p = 2$.

4. **Case 4:** n d-dimensional (multivariate) samples and fitting

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_d x_d$$

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; \quad X = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1d} \\ 1 & x_{21} & x_{22} & \dots & x_{2d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nd} \end{bmatrix}; \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_d \end{bmatrix}$$

Here $p = d$.

2.2 What makes these regression models linear

Hence, for a regression model to be linear, following conditions should be satisfied:

1. **Linearity**: Y and X should be related linearly. One good way to check it is that the model should have the ability to be expressed as a matrix vector product with coefficients (β) separable from covariate matrix X.
2. **Homoscedasticity**: The variance of residual is the same for any value of X.
3. **Independence**: Observations are independent of each other.
4. **Normality**: For any fixed value of X, Y is normally distributed.

Please note: For the assumed model definition in (5) (mentioned below as well) all 4 requirements for a linear regression model are satisfied:

$$Y = X\beta + \epsilon, \quad \epsilon \sim N(0, \sigma^2 I)$$

1. The product $X\beta$ ensures 1 is satisfied (linearity)
2. Error term ϵ being additive to $X\beta$ with a distribution $N(0, \sigma^2 I)$ guarantees (2), (3) and (4)

2.3 Non-linear regression models

All the models that don't satisfy the linear model specific conditions are a kind of a non-linear regression model. For example Neural Network models. These models don't have closed form expressions for parameters/weights (like $\hat{\beta} = (X^T X)^{-1} X^T Y$ for linear models)

Exercise

1. Generate data from $f(x) = \sin(x) + \log(x)$ for $x \in [0, 10]$
2. Find the weights $\hat{\beta}$ for fitting 4 separate models:
 - $y = \beta_0 + \beta_1 \sin(x)$
 - $y = \beta_0 + \beta_1 \cos(x)$,
 - $y = \beta_0 + \beta_1 \sin(x) + \beta_2 \log(x)$
 - $y = \beta_0 + \beta_1 \cos(x) + \beta_2 \log(x)$
3. Predict $f(x)$ for $x = 5.7$, using the learnt weights $\hat{\beta}$ for each model separately.

In []:

