ISSN PRINT 2319 1775 Online 2320 7876

Research paper UGC CARE Listed (Group -I) Journal Volume 10, Spl Iss 1, 2021

Multiple Linear Regression Examined through Matrix Calculus

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Abstract

Despite the abundance of creative tools available in Applied Mathematics, the fundamental tool that remains paramount to mathematicians is the linear model. This is due to its straightforward and seemingly restrictive attributes, including linearity, constant variance, normality, and independence. Linear models and their associated methodologies stand out as remarkable, adaptable, and potent. Given that the majority of advanced statistical techniques stem from generalizations of linear models, a solid grasp of these models is essential for delving into advanced statistical methods. The core focus of this research article revolves around specific incarnations of the Simple Linear Regression Model, the Multiple Linear Regression Model, and the Least Squares Estimation (LSE) of their parameters, along with the inherent properties of LSE. Furthermore, an inventive proof of the Gauss-Markov theorem has been advanced through the application of Matrix Calculus principles. Additionally, the notion of Best Linear Unbiased Estimation (BLUE) has been elucidated.

1. Introduction

A theoretical framework-equipped model aids in achieving a deeper comprehension of a given phenomenon. It's a mathematical construct designed to generate the observed data[1]. The linear model stands as a foundational element in the training of theoretical and applied mathematicians alike. The scientific method [2]frequently serves as a guided approach in the learning process[3]. Linear statistical models play a pivotal role within these processes, finding extensive utility in the realms of biological, physical, and social sciences, as well as in business and engineering[4]. Although these mathematically constructed models might oversimplify complex real-world issues, they can offer valuable approximations of relationships among observations. Accurate parameter[5] estimators are crucial for enhancing prediction performance. Scientists and engineers[6] employ these estimated models to describe and summarize observed data[7]. In 2017, B. Mahaboob et al. employed Matrix Calculus principles to estimate parameters in a CES production functional model. In 2018, C. Narayana et al. investigated misspecification and predictive accuracy of stochastic linear regression models[8]. Similarly, B. Mahaboob et al. proposed

ISSN PRINT 2319 1775 Online 2320 7876

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computational techniques for least squares and maximum likelihood estimators using Matrix Calculus[9]. In 2019, B. Mahaboob et al. outlined estimation methods for the Cobb-Douglas production functional model[10]. In 2018, Kushbukumari et al. elucidated fundamental concepts of Linear Regression Analysis and[11] demonstrated linear regression calculations in SPSS and Excel. Also in 2018, Shrikant I. Bangdiwala explained [12]methods for fitting simple linear regression models in his article "Regression: Simple Linear." Moreover, in 2017, W. Superta et al. developed a numerical model using nonlinear approaches to estimate thunderstorm activity[13].

2. MULTIPLE LINEAR REGRESSION MODEL

The dependent variable Y is sometimes [14]affected by more than one independent variable. A linear model making association between Y and several predictors can be framed as[15]

$$Y = \alpha_0 + \alpha_1 X_1 + \alpha_2 X_2 + ... + \alpha_i X_i + \epsilon. \tag{3.1}$$

The arbitrary constants α's are called regression coefficients. The random variation in Y which cannot be explained by predictors is provided by the error term ϵ. The model in (3.1) is linear in β's and not necessary in predictors. To estimate β's in (3.1) one can use a sample of 'n'observations on Y and the associated X. For k^th observation the model is

$$Y_k = \alpha_0 + \alpha_1 X_{k1} + \alpha_2 X_{k2} + ... + \alpha_i X_{ki} + \epsilon_k\ . \tag{3.2}$$

3. LEAST SQUARE ESTIMATOR

ISSN PRINT 2319 1775 Online 2320 7876

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For the parameters $\alpha_0, \alpha_1, ...\alpha_i$ one can seek the estimates that minimize

$$(4.1) \quad \sum_{k=1}^{m} \hat{\epsilon_k}^2 = \sum_{k=1}^{m} (Y_k - \hat{Y_k})^2 = \sum_{k=1}^{m} (Y_k - \hat{\alpha_0} - \hat{\alpha_1} X_{k1} - \hat{\alpha_2} X_{k2} - ....\hat{\alpha_i} X_{ki})^2 .$$

To find the values of $\hat{\alpha_i}$ that minimizes (4.1) one can differentiate $\sum_{k=1}^{m} \hat{\epsilon_k}^2$ with respect to each $\hat{\alpha_i}$ and eqaute the results to 0 to get (i+1) equations that are solved for $\hat{\alpha_i}$'s.

This process in compact form with matrix notation is explained below. (4.1) is rewritten as

$$\begin{aligned} \hat{\bar{\epsilon}} \hat{\bar{\epsilon}} &= (\bar{Y} - \bar{X}\hat{\bar{\alpha}})^T (\bar{Y} - \bar{X}\hat{\bar{\alpha}}) \\ \hat{\bar{\epsilon}} \hat{\bar{\epsilon}} &= \bar{Y}^T \bar{Y} - 2\bar{Y}^T \bar{X} \bar{\alpha} + \bar{\alpha}^T \bar{X}^T \bar{X} \bar{\alpha} \\ \frac{\partial \hat{\epsilon}^T \hat{\epsilon}^T}{\partial \bar{\alpha}} &= 0 \implies \bar{0} - \bar{x}^T \bar{Y} + 2\bar{\alpha}^T \bar{Y} + 2\bar{X}^T \bar{X} \hat{\bar{\alpha}} = 0 . \end{aligned}$$

These give normal equations as

$$(4.2) \qquad \bar{X}^T \bar{X} \hat{\bar{\alpha}} = \bar{X}^T \bar{Y} .$$

From (4.2)

$$\bar{X}^T \bar{X} = \begin{bmatrix} m & \sum_k X_{K1} & \dots & \sum_k X_{ki} \\ \sum_k X_{K1} & \sum_k X_{K1}^T & \dots & \sum_k X_{kl} X_{ki} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_k X_{kl} & \sum_k X_{kl} X_{ki} & \dots & \sum_k {X_{ki}}^2 \end{bmatrix}$$

5. Properties of LSE

ISSN PRINT 2319 1775 Online 2320 7876

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(i) If $E(\bar{Y}) = \bar{X}\bar{\alpha}$ then $\hat{\bar{\alpha}}$is an unbiased estimator for $\bar{\alpha}$(shown below)

$$\begin{aligned} E(\hat{\bar{\alpha}}) &= E(\bar{X}^T\bar{X})^{-1}\bar{X}^T\bar{Y}) \\ &= (\bar{X}^T\bar{X})^{-1}\bar{X}^T E(\bar{Y})(\bar{X}^T\bar{X})^{-1}\bar{X}^T\bar{X}\bar{\alpha} = \bar{\alpha} \end{aligned}$$

(ii) If $Cov(\bar{Y} = \sigma^2\bar{I}$the covariance matrix for$\hat{\bar{\alpha}}$ is $\sigma^2(\bar{X}^T\bar{X})^{-1}$(shown below)

$$\begin{aligned} Cov(\hat{\bar{\alpha}}) &= Cov((\bar{X}^T\bar{X}^{-1}\bar{X}^T\bar{Y})) \\ &= (\bar{X}^T\bar{X})^{-1}\bar{X}^T Cov(\bar{Y})[\bar{X}^T\bar{X}^{-1}\bar{X}^T]^T \\ &= (\bar{X}^T\bar{X})^{-1}\bar{X}^T(\sigma^2\bar{I})\bar{X}(\bar{X}^T\bar{X})^{-1} \\ &= \sigma^2()\bar{X}^T\bar{X})^{-1}\bar{X}^T\bar{X}(\bar{X}^T\bar{X})^{-1} \\ &= \sigma^2(\bar{X}^T\bar{X})^{-1}. \end{aligned}$$

Conclusions

Within this research paper, both simple and multiple linear regression models are outlined. The streamlined expression of the multiple linear regression model is introduced through the utilization of Matrix Algebra. The process of Least Squares Estimation (LSE) for regression coefficients is expounded upon employing Matrix Calculus. Additionally, the properties inherent to LSE are established, alongside a fresh proof of the Gauss-Markov Theorem. Looking ahead to future research, these aforementioned concepts can potentially be extended to simple linear regression models. Furthermore, the exploration of additional concepts such as Geometric Least Squares, Maximum Likelihood Estimation (MLE), and Generalized Least Squares could offer valuable avenues of study.

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