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DERLEME /**REVIEW**

SIMPLE LINEAR REGRESSION TECHNIQUES IN MEASUREMENT ERROR MODELS

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ABSTRACT

In simple linear regression, based on OLS (Ordinary Least Squares) technique, there considerate only one error which arises from the dependent variable. In practice there may be some measurement error that may arise from dependent, independent or from both variables. At that point because the assumptions of OLS is not met, the researchers must apply regression techniques that assume the error term may be effected because of the measurements of all variables, either dependent or independent. These kinds of regression techniques are called as “Type II Regression Techniques” in literature.

Under these conditions the aim of this study is to introduce Type II linear regression techniques as a whole which are separately introduced in literature and must be used when there is a measurement error also in the independent variable.

Keywords : Measurement error, Type II linear regression techniques, Method comparison.

ÖLÇÜM HATALI MODELLERDE DOĞRUSAL REGRESYON TEKNİKLERİ

ÖZ

EKK (En Küçük Kareler) temeline dayalı basit doğrusal regresyonda, sadece bağımlı değişkenden kaynaklanan bir hataya yer verilmektedir. Pratikte, bağımlı, bağımsız ya da her iki değişkenden de kaynaklanabilecek ölçüm hataları söz konusu olabilir. Bu noktada EKK varsayımları sağlanmayacağı için araştırmacılar bağımlı ya da bağımsız tüm değişkenlerin ölçümünde meydana gelecek hataları dikkate alan regresyon tekniklerine başvurmalıdır. Bu tür regresyon teknikleri literatürde “Tip II Regresyon Teknikleri” olarak bilinmektedir.

Bu koşullar altında, yapılan bu çalışmanın amacı, bağımsız değişkenin de hata içerdiği durumlarda kullanılması gereken ve literatürde dağınık halde bulunan Tip II doğrusal regresyon tekniklerini bir bütün olarak tanıtmaktır.

Anahtar Kelimeler: Ölçüm hatası, Tip II doğrusal regresyon teknikleri, Metot karşılaştırma.

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1. INTRODUCTION

Linear Measurement error models arise when the independent variable in a regression analysis is measured with error. It is well known that this random measurement error artificially inflates the dispersion of the observations on the independent variable and biased least squares estimates of slope towards zero (Edland, 1996). The least-squares method is frequently used to calculate the slope and intercept of the best line through a set of data points. However, least-squares regression slopes and intercepts may be incorrect if the underlying assumptions of the least-squares model are not met. Two factors in particular that may result in incorrect least-squares regression coefficients are: (a) imprecision in the measurement of the independent (x-axis) variable and (b) inclusion of outliers in the data analysis (Cornbleet and Gochman, 1979). Ordinary Least Squares Regression (OLR) assumes an error-free x variable and a constant analytical imprecision of the y variable (also called "homoscedastic" variance), both of which are seldom met in practice (Stöckl, et al, 1998).

Linear Regression techniques, when there is a measurement error in all variables, are especially used in clinical chemistry, when there is a method comparison problem. "Method Comparison" means there are two or more methods which serve for the same aim and we compare either the new method can be used instead of the current one. Furthermore someone want to measure the agreements of two methods, so one of the alternatives is to use linear regression techniques.

Most of the statistical models used in method comparison studies are designed for normally distributed data. However, some systems in clinical diagnostic are based on counting of certain particles rather than measuring a substance. In some of these cases, particularly in hematology where counting of cell types is of primary importance, the assumption of normal distribution is not always appropriate. Thus, other distributions beside normal distribution need to be considered (Magari 2004).

The comparison of analytical methods using regression analysis began in the fifties when Mandel and Linnig (1957) first applied the joint confidence interval test for the intercept and the slope to chemical problems. However, applying this test to the regression parameters derived from the least squares method assumes that the results in the x-axis (often the reference method) are error-free, or that the errors assigned to the reference method are negligible with respect to those given by the new method (y-axis). This is not always true since the precision of both methods must often be taken into account. These precisions can be considered by using the different existing approaches for calculating regression coefficients and related statistical parameters that consider errors in both axes (Riu and Rius, 1997).

2. MEASUREMENT AND THE MODEL

Measurement is a process made under effects of many factors on the measured variable and measuring process. In the ideal measurement, all the differences by the side of the examined variable are expected to become from the differences between the statistical units (Sümbüloğlu and Sümbüloğlu, 1998). Measurement error is the difference between the true and the measured value of the measured quality (Armağan, 1983, Ercan ve Kan'dan 2006).

The scales x and y may be expressed in the same units. For reasons of convention, it may be important for y to have the same measurement scale as x (Dunn and Roberts, 1999).

Measurement error models can also be used for the nonlinear regression techniques and in the problems that contain more than one independent variable. (Roy, 1994). But the solutions will be more complex in those problems.

A linear relationship between the target values of the two methods is assumed as in [1].

$$Y_i = \alpha + \beta X_i \qquad [1]$$

The measured value is likely to deviate from the target value by some small "random" amount (ε or δ). For a given sample measured by two clinical chemistry methods, the following relations exist (Linnet, 1998):

$$x_i = X_i + \varepsilon_i$$

$$y_i = Y_i + \delta_i$$

The error term that wanted to minimized in Type II regression techniques is the squares of the direct or indirect (by a known angle) distances of the observed values (Xi and Yi, which include some measurement errors) to the regression line which wanted to be estimated.

3. TYPE II LINEAR REGRESSION TECHNIQUES

By the type of the data different statistical techniques can be applied for the model which is collected with some measurement error. If the researcher decides to apply linear regression to these data, then Type II regression techniques which are given below may be used.

If we examine essence, Type II regression techniques also take place in robust techniques. The most important factors to prefer the robust techniques are obtaining unbiased estimates when there is an outlier in data set and when the distribution of the data is far away from normal distribution (Saraçlı, 2008).

3.1 OLS-Bisector Regression Technique

The OLS-Bisector regression Technique simply defines the line that mathematically bisects the OLSYX and the OLSXY lines (Saylor et al., 2006). As Isobe et al. (1990) mentioned, there is not any study in the literature regarding the merits or deficiencies of the OLS-Bisector line.

By OLS-Bisector Technique, the slope can be calculated as in [2], and the calculations of covariance and the variance of the slope are given in [3] and [4].

$$\hat{\beta}_{Bis} = \left(\hat{\beta}_1 + \hat{\beta}_2\right)^{-1}\left[\hat{\beta}_1\hat{\beta}_2 - 1 + \sqrt{\left(1+\hat{\beta}_1^2\right)\left(1+\hat{\beta}_2^2\right)}\right] \quad [2]$$

Here $\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}}$ is the slope of OLS(X|Y) regression and $\hat{\beta}_2 = \frac{S_{yy}}{S_{xy}}$ is the slope of OLS(Y|X) regression.

$$Var\left(\hat{\beta}_{Bis}\right) = \frac{\hat{\beta}_{Bis}^2}{\left(\hat{\beta}_1+\hat{\beta}_2\right)^2\left(1+\hat{\beta}_1^2\right)\left(1+\hat{\beta}_2^2\right)}\left[\left(1+\hat{\beta}_2^2\right)^2 Var\left(\hat{\beta}_1\right) + 2\left(1+\hat{\beta}_1^2\right)\left(1+\hat{\beta}_2^2\right)Cov\left(\hat{\beta}_1,\hat{\beta}_2\right) + \left(1+\hat{\beta}_1^2\right)^2 Var\left(\hat{\beta}_2\right)\right] \quad [3]$$

and

$$Cov\left(\hat{\beta}_1,\hat{\beta}_2\right) = \left(\hat{\beta}_1 S_{xx}^2\right)^{-1}\left\{\sum_{i=1}^{n}\left(x_i-\bar{x}\right)\left(y_i-\bar{y}\right)\left[y_i-\bar{y}-\hat{\beta}_1\left(x_i-\bar{x}\right)\right]\left[y_i-\bar{y}-\hat{\beta}_2\left(x_i-\bar{x}\right)\right]\right\} \quad [4]$$

As a result of bisecting the regression lines which are calculated by OLS technique taking as a depended variable X and Y respectively, OLS-Bisector technique takes into account the measurement errors of all variables and gives a better performance (Saraçlı, 2008).

3.2 Major Axis Regression (Orthogonal) Technique

The Orthogonal regression is geometrically most attractive, being the axis of minimum moment of inertia and being invariant under rotation. However, it can only be used with scale free variables, such as logarithmically transformed variables or ratios of observable variables (Isobe et al., 1990).

Unlike standard regression, the OR line does not depend on which variable is called “independent” and which “dependent.” It always lies between the regression line of y on x and the regression line of x on y (Amman and Ness, 1988)

In Major Axis (Orthogonal) Regression, the error that is aimed to be minimized is shown in Figure 1. (Wolfe, 2007(a)):

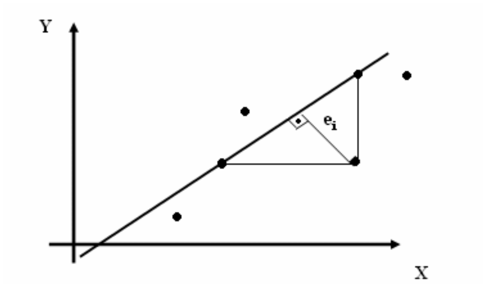

Figure 1. The error that is aimed to be minimized in MA Regression.

The calculation of the slope and the variance of this slope which want to be estimated by this technique are given in [5] and [6].

$$\hat{\beta}_{MA} = \frac{1}{2}\left[\left(\hat{\beta}_2 - \hat{\beta}_1^{-1}\right) + Sign\left(S_{xy}\right)\sqrt{4 + \left(\hat{\beta}_2 - \hat{\beta}_1^{-1}\right)^2}\right] \quad [5]$$

$$Var\left(\hat{\beta}_{MA}\right) = \frac{\hat{\beta}_{MA}^2}{4\hat{\beta}_1^2 + \left(\hat{\beta}_1\hat{\beta}_2 - 1\right)^2}\left[\hat{\beta}_1^{-2}Var\left(\hat{\beta}_1\right) + 2Cov\left(\hat{\beta}_1, \hat{\beta}_2\right) + \hat{\beta}_1^2 Var\left(\hat{\beta}_2\right)\right] \quad [6]$$

In his book, Fuller (1987) does not use the term "Orthogonal Regression" and calls a method of moments estimator. (Carroll and Ruppert 1996). The simplest form of the slope calculation in Fuller's book is as [7]

$$\hat{\beta}_{OR} = \frac{\sigma_y^2 - \sigma_x^2 + \sqrt{\left(\sigma_y^2 - \sigma_x^2\right)^2 + 4\sigma_{xy}^2}}{2\sigma_{xy}^2} \quad [7]$$

3.3 Reduced Major Axis Regression Technique

The reduced major axis regression was proposed to alleviate the scale dependency of orthogonal regression (Isobe et al., 1990).

In Reduced Major Axis Regression, the error that is aimed to be minimized is shown in Figure 2. (Wolfe, 2007(b)).

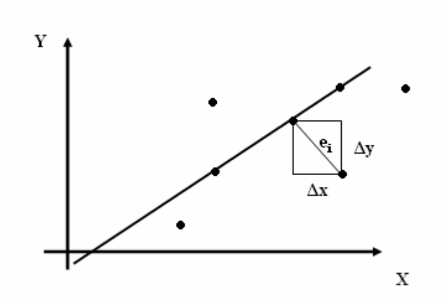

Figure 2. The error that is aimed to be minimized in RMA Regression.

The calculation of the slope and the variance of this slope which want to be estimated by this technique are given in [8] and [9].

$$\hat{\beta}_{RMA} = Sign\left(S_{xy}\right)\left(\hat{\beta}_1\hat{\beta}_2\right)^{1/2} \quad [8]$$

$$Var\left(\hat{\beta}_{RMA}\right) = \frac{1}{4}\left[\frac{\hat{\beta}_1}{\hat{\beta}_2}Var\left(\hat{\beta}_1\right) + 2Cov\left(\hat{\beta}_1, \hat{\beta}_2\right) + \frac{\hat{\beta}_1}{\hat{\beta}_2}Var\left(\hat{\beta}_2\right)\right] \quad [9]$$

3.4 Deming Regression Technique

The Deming method, also called the errors-in-variables model or the functional or structural relationship model in the statistical literature, takes measurement errors for both sets of measurements into account and is therefore more generally applicable than OLR (Linnet, 1998).

In his book, named as "Statistical adjustment of data", Deming (1943) advised to take care the errors of both the independent and the dependent variables and to minimize the common error simultaneously to obtain the best line that fits the data.

Deming approaches the problem by minimizing the sum of the square of the residuals in both the x and y directions simultaneously. This derivation results in the best line to minimize the sum of the squares of the perpendicular distances from the data points to the line (Cornbleet and Gochman, 1979).

To estimate the regression line in Deming regression, the λ value, given in [10], must be calculated first:

$$\lambda = \frac{S_{ex}^2}{S_{ey}^2} \quad [10]$$

Here; S_{ex} and S_{ey} are the error variances of x and y values respectively.

The λ value determines the angle in which to project points onto the line to minimize the sum of squared deviations (Linnet 1998). And in Deming regression, the distance between the observed and predicted values, with this angle is aimed to minimize as error term. When the λ value is equal to 1, this means that the result of Deming regression is equal to the results of orthogonal regression. Because orthogonal regression is a special form of Deming regression in which the variance of error terms are supposed to be equal.

Deming regression calculation assumes Gaussian distribution of errors in both x and y values (Billo, 2001). The error that is aimed to be minimized in Deming regression is shown in Figure 3.

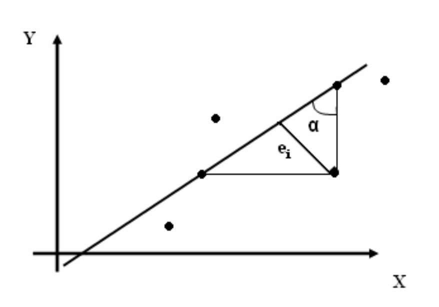

Figure 3. The error that is aimed to be minimized in Deming regression.

The calculation of the slope in Deming regression is given in [11]. The terms u,p, and q are also given in [12]

$$\hat{\beta}_{DEM} = \frac{(\lambda q - u) + \sqrt{(u - \lambda q)^2 + 4\lambda p^2}}{2\lambda p} \quad [11]$$

$$u = \sum (x_i - \bar{x})^2$$

$$q = \sum (y_i - \bar{y})^2$$

$$p = \sum (x_i - \bar{x})(y_i - \bar{y}) \quad [12]$$

For the Deming procedure, general formulas for Standard errors of slope and intercept are complicated and in practice, they are most easily estimated using a computerized resampling principle such as the jackknife method (Linnet, 1999).

The standard error of the slope in Deming regression can be calculated as in [13], [14], [15] and [16] which are based on Jacknife, the resampling technique (Linnet, 1990).

$$b_i = kb - (k-1)b^i \quad [13]$$

Here; b^i is obtained by Jackknife resampling technique.

$$\tilde{b} = \sum_{i=1}^{k} b_i / k \quad [14]$$

$$V_j(\hat{\beta}_{DEM}) = \sum_{i=1}^{k} (b_i - \tilde{b})^2 / (k-1) \quad [15]$$

$$SE(\hat{\beta}_{DEM}) = \sqrt{V_j(b)/k} \quad [16]$$

3.5 Passing-Bablok Regression Technique

Passing and Bablok have proposed a linear regression procedure with no special assumptions regarding the distribution of the data. This nonparametric method is based on ranking the observations so it is computationally intensive. The result is independent of the assignment of the reference method as *X* (the independent variable) and the test method as *Y* (the dependent variable) (Magari, 2002).

The slope and intercept are estimated by a nonparametric principle, which yields resistance towards outliers, and there are no assumptions of Gaussian error distributions Notice, however, that the parametric regression procedures do not presume Gaussian distributions of target values, but only as regards the error distributions. Furthermore, the jackknife principle used for estimation of standard errors for Deming and Weighted Deming procedures is also in principle nonparametric (CBStat, 2008).

As Passing and Bablok (1983) mentioned, the calculation of the slope and the intercept are given in [17], [18] and [19].

$$b_{ij} = \frac{y_i - y_j}{x_i - x_j} \qquad 1 \le i < j \le n \quad [17]$$

$$\hat{\beta}_{PB} = \begin{cases} b_{\left(\frac{N+1}{2}+k\right)} & \text{,if N is odd} \\ \frac{1}{2}\left(b_{\left(\frac{N}{2}+K\right)} + b_{\left(\frac{N}{2}+1+K\right)}\right) & \text{,if N is even.} \end{cases} \quad [18]$$

Here N is the sample size and K is the number of the values of b_{ij} with b_{ij}<-1.

$$a = med\{y_i - bx_i\} \quad [19]$$

The method takes measurement errors for both x and y into account, but the method presumes that the ratio between analytical standard deviations is related to the slope in a fixed manner Otherwise, a biased slope estimate arises. The method is not as efficient as the corresponding parametric procedures, i.e. Deming procedure (CBStat, 2008).

3.6 York Regression Technique

As York (1969) stated in his journal, this regression technique considers the errors in both variables.

The slope in York regression which requires an iterative solution is given in [20], [21], [22], and [24]

$$b = \frac{\sum_{i=1}^{n} W_i \beta_i (y_i - \bar{y})}{\sum_{i=1}^{n} W_i \beta_i (x_i - \bar{x})} \quad [20]$$

Here;

$$W_i = \frac{w(x_i)w(y_i)}{w(x_i) + b^2 w(y_i) - 2br_i\sqrt{w(x_i)w(y_i)}} \quad [21]$$

and

$$\beta_i = W_i \left[\frac{x_i - \bar{x}}{w(y_i)} + \frac{b(y_i - \bar{y})}{w(x_i)} - \left(b(x_i - \bar{x}) + (y_i - \bar{y})\right) \frac{r_i}{\sqrt{w(x_i)w(y_i)}} \right] \quad [22]$$

and

$$\bar{x} = \frac{\sum_{i=1}^{n} W_i x_i}{\sum_{i=1}^{n} W_i} \quad \text{and} \quad \bar{y} = \frac{\sum_{i=1}^{n} W_i y_i}{\sum_{i=1}^{n} W_i} \quad [23]$$

Since W_i and β_i are functions of b ,Eq.[20] must be solved iteratively. Given a set of weights $w(X_i)$ and $w(Y_i)$ and error correlation r_i for each data point, choose an initial guess for b (possibly from either the OLSXY or orthogonal technique). Iterate through the following steps until successive values of b are within a predefined tolerance:

1. Using b , $w(x_i)$, $w(y_i)$ and r_i ,calculate W_i for each data point from [21]

2. Using the observed points (x_i, y_i) and W_i , calculate $\bar{x}$ and $\bar{y}$ from [23]

3. Calculate β_i for each data point from [22]

4. Calculate a new estimate for b from [20] and return to step (1).

5. The intercept, a, is then found from $a = \bar{y} - b\bar{x}$

The York regression technique is thus very straightforward to implement and in our experience seldom requires more than 10 iterations (and usually much less) for convergence. (Saylor et al., 2006)

In simulation studies about York regression, the weights ($w(x_i)$ and $w(y_i)$) and the correlation coefficient r_i, given as above, are taken as 1 and 0 respectively as standard (Saraçlı, 2008).

The variance formula of this slope can be calculated as in [24] (York et al., 2004).

$$\sigma_b^2 = \frac{1}{\sum W_i (x_i - \bar{x})^2} \quad [24]$$

For all the regression techniques given above, the intercept term (except Passing-Bablok regression) can be calculated as in [25]:

$$\hat{\alpha}_j = \bar{y} - \hat{\beta}_j \bar{x} \quad [25]$$

Here as known, $\bar{y}$ and $\bar{x}$ are the means of the yi and xi values respectively.

4. RESULT AND CONCLUSION

By examining the regression techniques either taking account the error term which results from only dependent variable or both variables, regression techniques can be separated to two groups as Type I and Type II regression Techniques. As mentioned above, Type I regression techniques are interested in only the error terms of dependent variables whereas the Type II regession techniques are interested both the error terms of dependent and independent variables. Also in literature Type II techniques are called as “Errors in variables” regression techniques.

When the measurements of both variables include some errors, then Type II regression techniques are necessary to calculate the correct slope and intercept parameters of the regression line. In Type II Regression techniques the measurements of the variables are measured with some error as ε and δ. To decide which Type II regression technique is best for the data set on the hand, the MSE (Mean Squared Error) can guide to the researchers.

Another way to see the agreements of two methods is called as Bland-Altman graph. This technique is also used in method comparison studies but in the restrictions of this study we did not mention this technique. We hope this study will help the researchers when there is a measurement error problem and regression techniques are needed to be used.

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