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On the Equivalence between Orthogonal Regression and Linear Model with Type-II Constraints*

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Dedicated to Lubomír Kubáček on the occasion of his 80th birthday

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Abstract

Orthogonal regression, also known as the total least squares method, regression with errors-in variables or as a calibration problem, analyzes linear relationship between variables. Comparing to the standard regression, both dependent and explanatory variables account for measurement errors. Through this paper we shortly discuss the orthogonal least squares, the least squares and the maximum likelihood methods for estimation of the orthogonal regression line. We also show that all mentioned approaches lead to the same estimates in a special case.

Key words: linear regression model with type-II constraints, orthogonal regression, estimation

2010 Mathematics Subject Classification: 62J05, 62F10

1 Introduction

Orthogonal regression in the simplest form attempts to fit a line that explains the n two-dimensional data points in such way that the sum of the orthogonal squared distances from the data points to the fitted line is minimal. Section 2 is devoted to this statistical problem, where estimators of the unknown regression parameters as well as some of their properties are presented. The standard approach to estimation in orthogonal regression, based on the orthogonal least squares or the maximum likelihood method (e.g. [1, 2, 3, 10, 12]), can cause

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difficulties or even an impossibility of further statistical inference. Orthogonal regression using a linear regression model with type-II constraints [5] gives an opportunity to skip these problems. An iterative algorithm for estimation of orthogonal regression line by linear models is proposed in [4].

The main aim of this paper is to point out that under some conditions the iterative algorithm converges to the same estimates as those obtained by the maximum likelihood method or by the orthogonal least squares method. Details are discussed in Sections 2 and 3.

Finally, in Section 4 the theoretical considerations are applied on a real-data set from anthropology.

2 Orthogonal regression

For the formulation of the orthogonal regression problem (or OR for short) in the simplest form, we need to consider a linear relationship between two variables ν_i and μ_i (given by n observations), i.e.,

$$\nu_i = \beta_1 + \beta_2 \mu_i, \quad i = 1, \ldots, n, \tag{1}$$

where β_1, β_2 are the unknown parameters, namely, β_1 is the intercept and β_2 is the slope of the orthogonal regression line.

Measurements of the points $(\mu_i, \nu_i)'$, $i = 1, \ldots, n$, are corrupted by errors. Thus, we observe $(x_i, y_i)'$ instead of $(\mu_i, \nu_i)'$, where

$$x_i = \mu_i + \varepsilon_{1i}, \qquad y_i = \nu_i + \varepsilon_{2i}. \tag{2}$$

The unobserved variables μ_i and ν_i stand for true values of the explanatory and response variables, respectively, and ε_{1i}, ε_{2i}, $i = 1, \ldots, n$, represent measurement errors of μ_i and ν_i, respectively. Errors are independent random variables with zero mean value and with variances equal to $\mathrm{var}(\varepsilon_{1i}) = \sigma_1^2$ and $\mathrm{var}(\varepsilon_{2i}) = \sigma_2^2$. As a consequence, the OR model is given by both relations (1) and (2). In this paper, we will assume that variances are equal, i.e., $\sigma_1^2 = \sigma_2^2 = \sigma^2$.

In the statistical literature, the functional and structural cases of OR are distinguished. The functional case is considered if μ_i, $i = 1, \ldots, n$, are fixed unknown constants, while for random variables μ_i we consider the structural case of OR. In this paper we will focus on the functional OR [2, 3, 6, 7].

In contrast to the ordinary least squares, OR minimizes the sum of squared distances from the observed points to the regression line, so that the deviations are perpendicular (orthogonal) to the regression line. Hence, the estimator of the line parameters β_1 and β_2 (in the orthogonal regression sense) represents an optimum solution of the minimization problem

$$\min_{\beta_1, \beta_2} \frac{\sum_{i=1}^{n} (y_i - \beta_1 - \beta_2 x_i)^2}{\beta_2^2 + 1}.$$

This minimization method is known as the orthogonal least squares or the total least squares. Standard calculus gives the minimum and we find the estimators [3]

$$\widehat{\beta}_1 = \overline{y} - \widehat{\beta}_2\overline{x}, \tag{3}$$

$$\widehat{\beta}_2 = \frac{s_y^2 - s_x^2 + \sqrt{(s_y^2 - s_x^2)^2 + 4s_{xy}^2}}{2s_{xy}}, \tag{4}$$

where $\overline{x}$, $\overline{y}$ are sample means, s_x^2, s_y^2 are sample variances and s_{xy} is sample covariance. Consequently, under normality, the maximum likelihood method gives the same estimators [1, 3, 10].

We have to point out that the maximum likelihood estimators and the orthogonal least squares solution are the same only in a considered special case, i.e., x_i and y_i are independent normally distributed random variables with the same variance. If the variances σ_1^2 and σ_2^2 are different such that $\sigma_1^2 = \lambda\sigma_2^2$, where $\lambda > 0$ is known, the maximum likelihood estimators are given by the expressions [3]

$$\widehat{\beta}_1 = \overline{y} - \widehat{\beta}_2\overline{x}, \qquad \widehat{\beta}_2 = \frac{\lambda s_y^2 - s_x^2 + \sqrt{(\lambda s_y^2 - s_x^2)^2 + 4\lambda s_{xy}^2}}{2\lambda s_{xy}}.$$

It is shown in [10] that the estimators (3) and (4) are weakly consistent. Conditions for strong consistency can be found in [14, 15]. General results on consistency see, e.g., in [3, 6, 10].

In addition, if we consider that the variance σ^2 is unknown, then its maximum likelihood estimator results in [1, 10]

$$\widehat{\sigma}^2 = \frac{\sum_{i=1}^n \left[\left(y_i - \widehat{\beta}_1 - \widehat{\beta}_2\widehat{\mu}_i\right)^2 + (x_i - \widehat{\mu}_i)^2\right]}{2n}, \tag{5}$$

where the estimator $\widehat{\mu}_i$, $i = 1, \ldots, n$, is of the form

$$\widehat{\mu}_i = \frac{x_i + \widehat{\beta}_2 y_i - \widehat{\beta}_1\widehat{\beta}_2}{1 + \widehat{\beta}_2^2}. \tag{6}$$

The estimator $\widehat{\sigma}^2$ converges in probability to $\sigma^2/2$. This particular inconsistency causes no difficulty, the consistent estimator of σ^2 is simply $2n\widehat{\sigma}^2/(n-2)$. Further, the estimator $\widehat{\mu}_i$ is also inconsistent. Finally, the estimator of ν_i, $i = 1, \ldots, n$, is

$$\widehat{\nu}_i = \widehat{\beta}_1 + \widehat{\beta}_2\widehat{\mu}_i. \tag{7}$$

Hence, we have shown how to obtain the predicted values $(\widehat{\mu}_i, \widehat{\nu}_i)'$ when the observed values are $(x_i, y_i)'$, $i = 1, \ldots, n$.

There exists another possibility how to obtain the estimates of β_1 and β_2, based on singular value decomposition technique. However, this approach is often criticized from the numerical point of view [12].

One of the possible disadvantages of the maximum likelihood estimators, given in this section, are their asymptotic properties; therefore they are not satisfactory when making statistical inference with finite samples. Nevertheless, some approximate procedures can be found in e.g. [8, 9, 10, 13].

3 Orthogonal regression using linear models with type-II constraints

In this section we show that OR can alternatively be handled by linear models with type-II constraints [5], based on the calibration line approach [11, 16]. Suppose that two measurement series on two different objects (substances, quantities), obtained, for example, from two different instruments, are given. Further, let us consider that all measurements are independent with the same variance σ^2. Let us denote by $\mathbf{x} = (x_1, \ldots, x_n)'$ the measurements on the first object, and by $\mathbf{y} = (y_1, \ldots, y_n)'$ the measurements on the second object from the second instrument. Their errorless (true) values are $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_n)'$ and $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_n)'$, respectively. In addition, let these unknown parameters be linearly related.

Indeed, the errorless measurements $(\mu_i, \nu_i)'$ fulfill the relation (1), while the measurements of the observations $(x_i, y_i)'$, $i = 1, \ldots, n$, satisfy (2). The corresponding model can be expressed in the matrix form as

$$\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mu} \\ \boldsymbol{\nu} \end{pmatrix} + \boldsymbol{\varepsilon}, \quad \boldsymbol{\nu} = \beta_1 \mathbf{1}_n + \beta_2 \boldsymbol{\mu}, \quad \operatorname{var}(\boldsymbol{\varepsilon}) = \sigma^2 \mathbf{I}_{2n}, \tag{8}$$

where $\mathbf{1}_n$ stands for vector of n ones. The orthogonal regression line (calibration line) (1) forms nonlinear type-II constraints. Using the Taylor series locally at $\boldsymbol{\mu}^{(0)}, \beta_1^{(0)}$ and $\beta_2^{(0)}$, when the second and higher derivatives are neglected, we can linearize the model (8). The best linear unbiased estimators (BLUE) of $\boldsymbol{\mu}$, $\boldsymbol{\nu}$, β_1 and β_2 in the linearized model and their covariance matrices are derived in [4],

$$\widehat{\boldsymbol{\mu}} = \mathbf{x} + \frac{\beta_2^{(0)}}{\left[\beta_2^{(0)}\right]^2 + 1} \mathbf{M}^{(0)} \left[\mathbf{y} - \boldsymbol{\nu}^{(0)} - \beta_2^{(0)} \left(\mathbf{x} - \boldsymbol{\mu}^{(0)}\right)\right], \tag{9}$$

$$\widehat{\boldsymbol{\nu}} = \mathbf{y} - \frac{1}{\left[\beta_2^{(0)}\right]^2 + 1} \mathbf{M}^{(0)} \left[\mathbf{y} - \boldsymbol{\nu}^{(0)} - \beta_2^{(0)} \left(\mathbf{x} - \boldsymbol{\mu}^{(0)}\right)\right], \tag{10}$$

$$\begin{aligned} \begin{pmatrix} \widehat{\beta}_1 \\ \widehat{\beta}_2 \end{pmatrix} &= \begin{pmatrix} \beta_1^{(0)} \\ \beta_2^{(0)} \end{pmatrix} + \begin{pmatrix} n, & \mathbf{1}'\boldsymbol{\mu}^{(0)} \\ \left[\boldsymbol{\mu}^{(0)}\right]'\mathbf{1}, & \left[\boldsymbol{\mu}^{(0)}\right]'\boldsymbol{\mu}^{(0)} \end{pmatrix}^{-1} \\ &\times \begin{pmatrix} \mathbf{1}'\left[\mathbf{y} - \boldsymbol{\nu}^{(0)} - \beta_2^{(0)}\left(\mathbf{x} - \boldsymbol{\mu}^{(0)}\right)\right] \\ \left[\boldsymbol{\mu}^{(0)}\right]'\left[\mathbf{y} - \boldsymbol{\nu}^{(0)} - \beta_2^{(0)}\left(\mathbf{x} - \boldsymbol{\mu}^{(0)}\right)\right] \end{pmatrix}, \end{aligned} \tag{11}$$

where

$$\mathbf{M}^{(0)} = \mathbf{I}_n - \left(\mathbf{1}, \boldsymbol{\mu}^{(0)}\right) \begin{pmatrix} n, & \mathbf{1}'\boldsymbol{\mu}^{(0)} \\ \left[\boldsymbol{\mu}^{(0)}\right]'\mathbf{1}, & \left[\boldsymbol{\mu}^{(0)}\right]'\boldsymbol{\mu}^{(0)} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{1}' \\ \left[\boldsymbol{\mu}^{(0)}\right]' \end{pmatrix}. \tag{12}$$

One can see that the estimators $\widehat{\boldsymbol{\mu}}$, $\widehat{\boldsymbol{\nu}}$, $\widehat{\beta}_1$ and $\widehat{\beta}_2$ depend on the unknown approximate values $\boldsymbol{\mu}^{(0)}, \boldsymbol{\nu}^{(0)}, \beta_1^{(0)}$ and $\beta_2^{(0)}$, therefore it is necessary to solve them on an iterative manner. The variance σ^2 is usually unknown and can be unbiasedly estimated by [11]

$$\widehat{\sigma}^2 = \frac{(\mathbf{x} - \widehat{\boldsymbol{\mu}})'(\mathbf{x} - \widehat{\boldsymbol{\mu}}) + (\mathbf{y} - \widehat{\boldsymbol{\nu}})'(\mathbf{y} - \widehat{\boldsymbol{\nu}})}{n-2}. \tag{13}$$

In the following, we outline the standard iterative algorithm for estimating the orthogonal regression line, described in four main steps [4]. The first step consists of determining initial values of the intercept β_1 and the slope β_2 of the orthogonal regression line and the errorless recordings $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$. In case a specific prior information on the true values of these parameters occurs, we should take it into account, otherwise the choice should satisfy the relation (1), for example

$$\beta_1^{(0)} = \frac{x_j y_i - x_i y_j}{x_j - x_i}, \; \beta_2^{(0)} = \frac{y_j - y_i}{x_j - x_i}, \tag{14}$$
$$\boldsymbol{\mu}^{(0)} = \mathbf{x}, \; \boldsymbol{\nu}^{(0)} = \beta_1^{(0)}\mathbf{1}_n + \beta_2^{(0)}\boldsymbol{\mu}^{(0)},$$

where $x_i = \min\{x_k : k = 1, \ldots, n\}$, $x_j = \max\{x_k : k = 1, \ldots, n\}$ and y_i, y_j are the corresponding y coordinates. The choice of the initial values does not have any impact on convergence of this algorithm. In the second step, we calculate $\widehat{\beta}_1$, $\widehat{\beta}_2$, $\widehat{\boldsymbol{\mu}}$ and $\widehat{\boldsymbol{\nu}}$ for every data point $(x_i, y_i)'$, $i = 1, \ldots, n$, using the equations (9)-(12). Further, in the the third step we need to update the initial values by the scheme

$$\boldsymbol{\nu}^{(0)} = \widehat{\boldsymbol{\nu}} + (\widehat{\beta}_2 - \beta_2^{(0)})(\widehat{\boldsymbol{\mu}} - \boldsymbol{\mu}^{(0)}), \quad \boldsymbol{\mu}^{(0)} = \widehat{\boldsymbol{\mu}}, \quad \beta_1^{(0)} = \widehat{\beta}_1, \quad \beta_2^{(0)} = \widehat{\beta}_2. \tag{15}$$

We repeat steps 2 and 3 until estimates converge, i.e., until changes in estimates at each iteration are less than some pre-set tolerance.

Estimates obtained from this iterative algorithm converge usually very quickly, and they also preserve the prescribed condition (1). Thus, linear models approach represents an alternative technique for the orthogonal regression; however, the solution is only approximative due to linearization step. On the other hand, this technique enables to provide further statistical inference. This means that under the assumption of normality we can construct e.g. approximative confidence domains or statistical tests.

In the following theorem we will point out the equivalence between the mentioned approaches to orthogonal regression estimation.

Theorem 1 *Let us consider the orthogonal regression model (1) and (2), where x_i and y_i, $i = 1, \ldots n$, are independent random variables with the same variance σ^2. The estimates of the orthogonal regression line coefficients, obtained* *from the iterative algorithm (11), converge to the orthogonal least squares estimates given by the relations (3) and (4). Moreover, under the assumption of normality, the estimates from the iterative algorithm converge to the maximum likelihood estimates.*

Proof The estimators obtained from the iterative algorithm (11) are the BLUEs in the linearized model (8). The nonlinear model (8) can also be expressed as

$$\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mu} \\ \beta_1 \mathbf{1}_n + \beta_2 \boldsymbol{\mu} \end{pmatrix} + \boldsymbol{\varepsilon}, \qquad \mathrm{var}(\boldsymbol{\varepsilon}) = \sigma^2 \mathbf{I}_{2n},$$

or simply as

$$\mathbf{Z} = \mathbf{f}\,(\boldsymbol{\theta}) + \boldsymbol{\varepsilon},$$

where $\mathbf{Z} = (\mathbf{x}', \mathbf{y}')'$, $\boldsymbol{\theta} = (\beta_1, \beta_2, \mu_1, \cdots, \mu_n)'$, $\boldsymbol{\varepsilon} = (\boldsymbol{\varepsilon}_1', \boldsymbol{\varepsilon}_2')'$ and finally $\mathbf{f}\,(\boldsymbol{\theta})$ is a nonlinear function of the unknown parameter $\boldsymbol{\theta}$. Hence, the least squares minimization function is

$$\sum_{i=1}^{2n} (Z_i - f_i(\boldsymbol{\theta}))^2 = \sum_{i=1}^{n} \left[(x_i - \mu_i)^2 + (y_i - \beta_1 - \beta_2 \mu_i)^2 \right]. \tag{16}$$

Since the model is nonlinear, we linearize the function $\mathbf{f}\,(\boldsymbol{\theta})$ by the Taylor series locally at $\boldsymbol{\theta}^{(0)}$, when the second and higher derivatives are neglected. Thus, the resulting linearized model is given by

$$\mathbf{Z} = \mathbf{f}\left(\boldsymbol{\theta}^{(0)}\right) + \boldsymbol{\varphi}^{(0)} \triangle \boldsymbol{\theta} + \boldsymbol{\varepsilon},$$

where

$$\boldsymbol{\varphi}^{(0)} = \left. \frac{\partial \mathbf{f}\,(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}'} \right|_{\boldsymbol{\theta} = \boldsymbol{\theta}^{(0)}} \qquad \text{and} \quad \triangle \boldsymbol{\theta} = \boldsymbol{\theta} - \boldsymbol{\theta}^{(0)}.$$

Now, the BLUE of $\triangle \boldsymbol{\theta}$ can be derived by the least squares method as

$$\widehat{\triangle \boldsymbol{\theta}} = \left(\left[\boldsymbol{\varphi}^{(0)} \right]' \boldsymbol{\varphi}^{(0)} \right)^{-1} \left[\boldsymbol{\varphi}^{(0)} \right]' \left[\mathbf{Z} - \mathbf{f}\left(\boldsymbol{\theta}^{(0)} \right) \right].$$

Hence, $\widehat{\boldsymbol{\theta}} = \widehat{\triangle \boldsymbol{\theta}} + \boldsymbol{\theta}^{(0)}$. If $\widehat{\triangle \boldsymbol{\theta}}^{(k)}$ is calculated in the kth iteration from the iterative algorithm, the values of $\boldsymbol{\theta}^{(0)}$ are determined according to (15) when the estimated values of $\boldsymbol{\theta}$ from the $(k-1)$th iteration are used. Thus, the estimate in the kth iteration is

$$\widehat{\boldsymbol{\theta}}^{(k)} = \widehat{\triangle \boldsymbol{\theta}}^{(k)} + \boldsymbol{\theta}^{(0)}.$$

If the starting point $\boldsymbol{\theta}^{(0)}$ is sufficiently good chosen, then the iterative algorithm converges, i.e., $\widehat{\triangle \boldsymbol{\theta}}^{(k)}$ converges to zero and $\widehat{\boldsymbol{\theta}}^{(k)}$ converges to a point that minimizes (16).

The orthogonal least squares estimators minimize, over all β_1 and β_2, the quantity

$$\sum_{i=1}^{n}\left[(x_i-\hat{\mu}_i)^2+(y_i-\hat{\nu}_i)^2\right]=\sum_{i=1}^{n}\left[(x_i-\hat{\mu}_i)^2+(y_i-\beta_1-\beta_2\hat{\mu}_i)^2\right], \quad (17)$$

where $(\hat{\mu}_i,\hat{\nu}_i)$ given by (6) and (7) is the closest point to an observed point (x_i,y_i) on the orthogonal regression line $\nu_i=\beta_1+\beta_2\mu_i$.

The functions (16) and (17) minimize the same problem and, thus, if the iterative algorithm converges, obtained estimates of the orthogonal regression line coefficients converge to the orthogonal least squares estimates.

The rest of the proof follows from the fact that under normality the maximum likelihood and the orhogonal least squares estimators are the same. □

4 Illustrative example

We demonstrate the above-mentioned theoretical results on a data set from *http://lib.stat.cmu.edu/datasets/bodyfat* (Body Fat data), where 252 men were inspected for 15 anthropological parameters. Here, the chest and hip circumference measurements (in cm) are of interest, see Fig. 1.

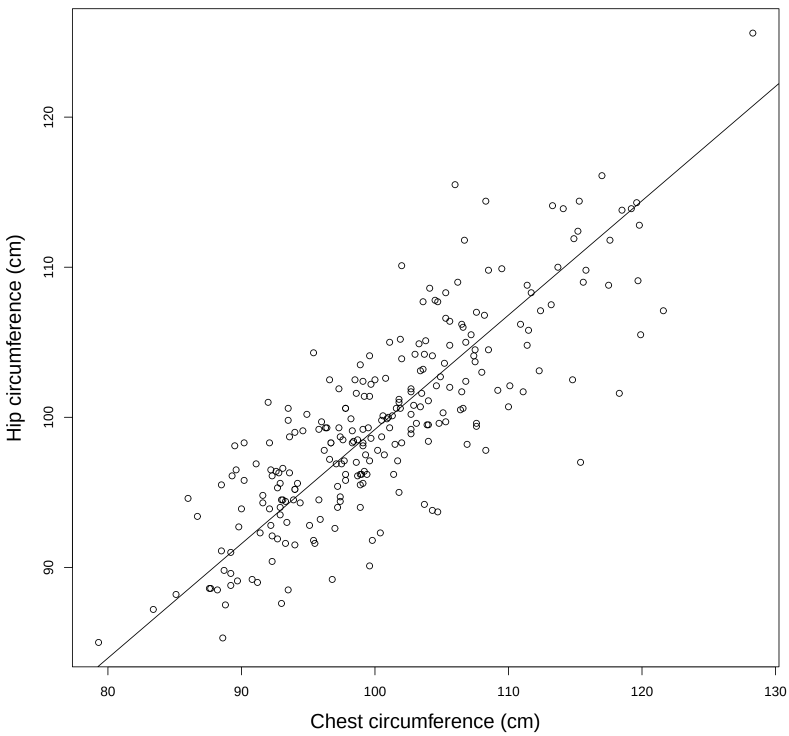

Fig. 1: Body Fat data and the regression line.

Firstly, we computed the regression line using the formulas (3) and (4) for orthogonal regression with results $\widehat{\beta}_1 = 23.0230$ and $\widehat{\beta}_2 = 0.7617$. The results were compared with the iterative algorithm approach. At the beginning, it was necessary to set the initial values, so we proceed on the way suggested in the iterative algorithm and for that purpose we used the relations (14). As a convergence criterion, the Euclidean norm of differences between the estimates of β_1, β_2 from two consecutive steps was taken. Convergence was reached in 17 iterations, with accuracy higher than $\varepsilon = 10^{-9}$ (see Tab. 1 for outputs from chosen iteration steps); the obtained orthogonal regression line was displayed in Fig. 1. Both algorithms really lead to the same results.

Iteration	$\left(\widehat{\beta}_1, \widehat{\beta}_2\right)$
1	$(33.6800979761, 0.655861164078)$
2	$(24.0337941288, 0.751669575358)$
3	$(24.0811858971, 0.751198873823)$
$\vdots$	$\vdots$
15	$(23.0229810998, 0.761709108836)$
16	$(23.0229804890, 0.761709114902)$
17	$(23.0229804886, 0.761709114906)$

Tab. 1: Iteration values of the parameters β_1, β_2 for Body fat data when the initial values are calculated according to (14) as $\beta_1^{(0)} = 19.29428571$ and $\beta_2^{(0)} = 0.8285714286$.

Standard deviations of $\widehat{\beta}_1$, $\widehat{\beta}_2$, which are 3.079 and 0.031, respectively, show high precision of both these estimates of the regression parameters. From Fig. 1 it is noticeable that the growth of chest circumference indicates increasing hip circumference. Concretely, 1 cm growth of the chest circumference causes hip circumference growth in average about 0.762 cm.

5 Conclusions

In the paper a useful alternative for modelling OR by linear models with type-II constraints is proposed. It enables for further approximative statistical inference, even if only small samples are available. Satisfying the requirement of independent random errors with equal variances leads to the equivalence between linear models approach (the least squares method) and the orthogonal least squares method. Moreover, under normality, the equivalence is also fulfilled for the maximum likelihood estimation. If variances of random errors are different, say, σ_1^2, σ_2^2 such that $\sigma_1^2 = \lambda\sigma_2^2$ and $\lambda > 0$ is known, the resulting formulas for the maximum likelihood estimators of the orthogonal regression line parameters will include the ratio of these two different variances, and, thus, the maximum likelihood estimators are different from the orthogonal least squares estimators. Searching for equivalence here would lead to a generalization of covariance structure of the correponding linear model. We leave this problem for future research.

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