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CONSIDERATIONS ON THE VALIDITY AND APPLICABILITY OF THE UEK METHOD*

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Abstract. In Popławski and Kaczmarczyk (2013) a method referred to as UEK was presented and used as a tool in the analysis of sustainable rural development. The purpose of this paper is to demonstrate the methodological inappropriateness of that method. In the linear regression model, the matrix of explanatory variables can have either less than full or full column rank. While all regression parameters are non-estimable in the first case, the well-known and widely used ordinary least squares method can be applied in the second one.

Keywords: linear regression, Moore–Penrose pseudoinverse, UEK method

INTRODUCTION

The formula referred to as UEK was presented for the first time by Kaczmarczyk (2012) in the context of company valuation. Later, it was used as an efficient tool for public debt management (Kawa and Kaczmarczyk, 2012). It was also applied in a quantitative description of sustainable development in the Świętokrzyskie voivodeship (Popławski and Kaczmarczyk, 2013). In Popławski and Kaczmarczyk (2013) the UEK method is used if the matrix of explanatory variables has less than full column rank. To overcome the problem of the resulting singularity of the matrix of coefficients of the system of normal equations, the authors use the Moore–Penrose pseudoinverse (MP pseudoinverse). However, in this way they obtain a biased estimator of non-estimable parameters; therefore, all estimates are useless, and so are all conclusions pertaining to sustainable development of the area under investigation.

This paper will demonstrate that the estimator of linear regression coefficients based on the MP pseudoinverse of the singular matrix of coefficients of the system of normal equations does not have good properties. The Bayesian approach will be employed to show that when the matrix of values of explanatory variables has less than full column rank, it is methodologically invalid to use the UEK in the estimation of all regression coefficients. It is impossible to make inferences about the vector of regression coefficients based only on the information supplied by research data.

In the next part of this paper, the UEK method will be put into the framework of a linear regression model. Then, the properties of the estimator based on the MP pseudoinverse will be discussed. The flaws of the UEK method will be illustrated by the example considered in (Popławski and Kaczmarczyk, 2013) which refers to sustainable rural development in the Świętokrzyskie voivodeship. The paper ends with a brief conclusion.

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The UEK method in the linear regression framework

Let the stochastic version of the model **UE** = **K** discussed in Kawa and Kaczmarczyk (2012) and in Popławski and Kaczmarczyk (2013) be formulated by adding to its left hand side a vector of random disturbances $\boldsymbol{\varepsilon}$, representing the impact of unknown and unobservable factors on the explained variable *K*. The following linear regression model is obtained[1]:

$$\mathbf{K} = \mathbf{UE} + \boldsymbol{\varepsilon} \tag{1}$$

where:

- **K** – is an $n \times 1$ vector of the dependent variable observations
- **U** – is an $n \times m$ matrix of values of explanatory variables
- **E** – is an $m \times 1$ vector of unknown regression coefficients
- $\boldsymbol{\varepsilon} = (\varepsilon_1, \varepsilon_1, ..., \varepsilon_n)'$ is an $n \times 1$ vector of random disturbances.

Moreover, it is assumed that $E(\boldsymbol{\varepsilon}) = 0$, $E(\boldsymbol{\varepsilon\varepsilon}^T) = \sigma^2\mathbf{I}_n$, where $\sigma^2 > 0$.

Popławski and Kaczmarczyk (2013) propose to use the MP pseudoinverse to estimate the unknown parameters of the vector **E**. They obtain the following formula:

$$\hat{\mathbf{E}}^+ = \mathbf{U}^+\mathbf{K} \tag{2}$$

where $\mathbf{U}^+$ is the Moore-Penrose pseudoinverse of the matrix **U**.

Note that if the matrix **U** has full column rank ($r(\mathbf{U}) = m \geq n$), then the matrix $\mathbf{U}^T\mathbf{U}$ is non-singular (i.e. $r(\mathbf{U}^T\mathbf{U}) = m$)[2], and then:

$$\hat{\mathbf{E}}^+ = \mathbf{U}^+\mathbf{K} = (\mathbf{U}^T\mathbf{U})^{-1}\mathbf{U}^T\mathbf{K} \tag{3}$$

and as a consequence, the UEK method coincides with the ordinary least squares (OLS) method. Under the additional assumption that **U** is a non-random matrix, the estimator $\hat{\mathbf{E}}^+$ is the best unbiased linear estimator of the vector **E** (see Goldberger, 1964).

If the matrix **U** has less than full column rank, then the matrix $\mathbf{U}^T\mathbf{U}$ is singular, and therefore:

$$\hat{\mathbf{E}}^+ = (\mathbf{U}^T\mathbf{U})^+\mathbf{U}^T\mathbf{K} \tag{4}$$

[1] The notation is the same as that used by the authors cited.

[2] Because $r(\mathbf{A}^T\mathbf{A}) = r(\mathbf{A})$ for any matrix **A** (see Harville, 2008, p. 79).

Under the assumption that **U** is a non-random matrix, the bias of the estimator $\hat{\mathbf{E}}^+$ is equal to $(\mathbf{U}^+\mathbf{U} - \mathbf{I})\mathbf{E}$ (Pajor, 2017). Thus, when $\mathbf{U}^+\mathbf{U} \neq \mathbf{I}_m$, as assumed in Popławski and Kaczmarczyk (2013) and in Kawa and Kaczmarczyk (2012)[3], the bias of estimator $\hat{\mathbf{E}}^+$ may differ from zero. In other words, if matrix $\mathbf{U}^T\mathbf{U}$ is singular, the MP pseudoinverse does not yield an unbiased estimator of the vector **E**. Apart from this fact, the vector **E** is then not estimable[4] without additional information from outside the dataset. It is impossible to make inferences about the vector of regression coefficients based only on the information supplied by research data. Attention should be therefore focused not on the vector **E** but on the estimable function of **E**. For example, a linear function $\mathbf{q}^T\mathbf{E}$ of parameters in **E** is estimable if and only if $\mathbf{q}^T$ is a linear function of the rows of **U**, i.e. a vector **v** exists such that $\mathbf{q}^T = \mathbf{v}^T\mathbf{U}$ (Searle, 1966; Albert, 1972). Indeed, if $\mathbf{q}^T = \mathbf{v}^T\mathbf{U}$, then $\mathbf{q}^T\hat{\mathbf{E}}^+$ is an unbiased estimator of $\mathbf{q}^T\mathbf{E}$ due to the fact that $\mathbf{U}\hat{\mathbf{E}}^+$ is an unbiased estimator of **UE** (Pajor, 2017): $\mathbf{E}(\mathbf{q}^T\hat{\mathbf{E}}^+) = \mathbf{q}^T\mathbf{E}$. This fact is invariant to which solution of $\mathbf{U}^T\mathbf{UE} = \mathbf{U}^T\mathbf{K}$ is used (Searle, 1966).

The prediction problem

Since $\mathbf{U}\hat{\mathbf{E}}^+$ is an unbiased estimator of **UE**, the estimator $\hat{\mathbf{E}}^+$ can be used in forecasting to find out when the values of explanatory variables used in prediction (contained in a $1 \times m$ vector $\tilde{\mathbf{U}}$) satisfy the following condition: $\tilde{\mathbf{U}} = \mathbf{w}^T\mathbf{U}$ for a given $n \times 1$ vector $\mathbf{w} \in \mathbf{R}^n$.[5] This means that vector $\tilde{\mathbf{U}}$ must be a linear combination of the rows of the matrix **U**. Then the expected value of the prediction error equals zero because:

$$\begin{aligned} E(\tilde{K} - K_{n+1}) &= E(\tilde{\mathbf{U}}\hat{\mathbf{E}}^+ - \tilde{\mathbf{U}}\mathbf{E} - \varepsilon_{n+1}) = \\ &= \tilde{\mathbf{U}}E(\hat{\mathbf{E}}^+ - E) = \tilde{\mathbf{U}}(\mathbf{U}^+\mathbf{U} - \mathbf{I})\mathbf{E} = \\ &= \mathbf{w}^T(\mathbf{UU}^+\mathbf{U} - \mathbf{U})\mathbf{E} = 0 \end{aligned} \tag{5}$$

[3] If the columns of the matrix **U** are linearly independent, then $\mathbf{U}^+\mathbf{U} = \mathbf{I}_m$; and if the rows of the matrix **U** are linearly independent, then $\mathbf{UU}^+ = \mathbf{I}_n$.

[4] A function $f(\mathbf{E})$ is said to be estimable if a vector **z** exists such that $E(\mathbf{z}^T\mathbf{K}) = f(\mathbf{E})$ (Searle, 1966).

[5] In these considerations, the matrices $\tilde{\mathbf{U}}$ and **U** are given. The equation $\tilde{\mathbf{U}} = \mathbf{w}^T\mathbf{U}$ has one or more solutions (for **w**) if and only if $r([\mathbf{U}^T : \tilde{\mathbf{U}}^T]) = r(\mathbf{U}^T)$. If $r([\mathbf{U}^T : \tilde{\mathbf{U}}^T]) = r(\mathbf{U}^T) = n$ then the equation $\tilde{\mathbf{U}} = \mathbf{w}^T\mathbf{U}$ has a unique solution, namely $\mathbf{w}^T = \tilde{\mathbf{U}}\mathbf{U}^+$. If $r([\mathbf{U}^T : \tilde{\mathbf{U}}^T]) < n$ then the equation $\tilde{\mathbf{U}} = \mathbf{w}^T\mathbf{U}$ has an infinite number of solutions (only one of them can be expressed as $\mathbf{w}^T = \tilde{\mathbf{U}}\mathbf{U}^+$, Harville, 2008, p. 144).

where $K_{n+1} = \tilde{\mathbf{U}}\mathbf{E} + \varepsilon_{n+1}$ is the "future" value of the dependent variable; $\tilde{K} = \tilde{\mathbf{U}}\hat{\mathbf{E}}^{+}$ is the predictor of K_{n+1}; ε_{n+1} is the random disturbance such that $E(\varepsilon_{n+1}) = 0$; $E(\varepsilon^2_{n+1}) = \sigma^2$; and $\mathrm{E}(\varepsilon_i\varepsilon_{n+1}) = 0$ for $i = 1, \ldots, n$.

The variance of the prediction error is:

$$\begin{aligned} Var(\tilde{K} - K_{n+1}) &= \sigma^2[\tilde{\mathbf{U}}(\mathbf{U}^T\mathbf{U})^{+}\tilde{\mathbf{U}}^T + \mathbf{I}_1] = \\ &\sigma^2[\mathbf{w}^T\mathbf{U}(\mathbf{U}^T\mathbf{U})^{+}\mathbf{U}^T\mathbf{w} + \mathbf{I}_1] = \\ &\sigma^2\mathbf{I}_1 + \sigma^2\mathbf{w}^T\mathbf{U}\mathbf{U}^{+}\mathbf{w} \end{aligned} \quad (6)$$

It consists of two components: the first one refers to the "future" disturbance, ε_{n+1}, and the second one to the estimation error of **UE** (it is easy to show that $Var(\tilde{\mathbf{U}}\hat{\mathbf{E}}^{+}) = \sigma^2\mathbf{U}\mathbf{U}^{+}$). If the rows of the matrix **U** are linearly independent, then $\mathbf{U}\mathbf{U}^{+} = \mathbf{I}_n$ and, as expected, $\tilde{K} = \mathbf{w}^T\mathbf{K}$. Moreover, $Var(\tilde{\mathbf{U}}\hat{\mathbf{E}}^{+}) = \sigma^2\mathbf{I}_n$, and $Var(\tilde{K} - K_{n+1}) = \sigma^2[\mathbf{w}^T\mathbf{w} + 1]$.

It is clear that the variance of the prediction error depends on σ^2 and increases with the increase in the length of the vector **w**. Unfortunately, in the case of a perfect in-sample fit (i.e. when **K** and $\mathbf{U}\hat{\mathbf{E}}^{+}$ are equal to each other), the parameter σ^2 cannot be evaluated, and consequently the confidence interval cannot be determined for this forecast. Moreover, situations where explanatory variables in the forecast period are linear combinations of the values of explanatory variables within the sample occur very rarely.

Bayesian interpretation of $\hat{\mathbf{E}}^{+}$

Now, the Bayesian approach will be used to analyze the normal multiple regression model when the matrix $\mathbf{U}^T\mathbf{U}$ is singular. This study assumes that the vector of observations (**K**) has a normal distribution with mean **UE** and precision matrix $\tau\mathbf{I}_n$. The density of the vector **K**, with the vector of parameters defined as $\boldsymbol{\theta} = (\tau,\mathbf{E}^T)^T$, is given by the formula:

$$p(\mathbf{K}|\tau,\mathbf{E}) = (2\pi)^{-n/2}\tau^{n/2}\exp(-0.5\tau(\mathbf{K} - \mathbf{UE})^{\mathrm{T}}(\mathbf{K} - \mathbf{UE})) \quad (7)$$

The authors assume that their prior beliefs about the vector of parameters $\boldsymbol{\theta}$ are represented by the normal-gamma distribution[6], that is:

$$p(\mathbf{E},\tau) = p(\mathbf{E}|\tau)p(\tau) = f_{N,m}(\mathbf{E}|\boldsymbol{\mu},\tau^{-1}\mathbf{A}^{-1})\, f_G(\tau|n_0/2, s_0/2) \quad (8)$$

[6] The family of normal-gamma distributions is a conjugate family of joint prior distributions of **E** and τ in the normal linear regression model. If the joint prior distribution of **E** and τ belongs to this family, then the joint posterior distribution of **E** and τ will also belong to the family (Zellner, 1971; Geweke, 2005).

where $f_{N,m}(\cdot|b, B)$ denotes the density of an m-dimensional multivariate normal distribution with mean vector b and covariance matrix B, whereas $f_G(\tau; \alpha, \beta)$ is the density of a gamma distribution with shape parameter α and scale parameter β (with mean α/β). Another assumption is that **A** is a positive-definite matrix (then the matrix $\mathbf{U}^T\mathbf{U} + \mathbf{A}$ is non-singular even though the matrix $\mathbf{U}^T\mathbf{U}$ is singular).

Under the above assumptions, the joint posterior distribution of $\boldsymbol{\theta}$ is also normal-gamma:

$$\begin{aligned} p(\mathbf{E},\tau|\mathbf{K}) &= p(\mathbf{E}|\tau,\mathbf{K})p(\tau|\mathbf{K}) = \\ &= f_{N,m}(\mathbf{E}|\boldsymbol{\mu}_K,\tau^{-1}\mathbf{A}_K^{-1})\, f_G(\tau|n_K/2, s_K/2) \end{aligned} \quad (9)$$

where

$\boldsymbol{\mu}_K = (\mathbf{U}^{\mathrm{T}}\mathbf{U} + \mathbf{A})^{-1}(\mathbf{U}^T\mathbf{K} + \mathbf{A}\boldsymbol{\mu})$,

$\mathbf{A}_K = (\mathbf{U}^{\mathrm{T}}\mathbf{U} + \mathbf{A})$,

$n_K = n + n_0$

$s_K = \mathbf{K}^T\mathbf{K} - \boldsymbol{\mu}_K^T\mathbf{A}_K\boldsymbol{\mu}_K + \boldsymbol{\mu}^T\mathbf{A}\boldsymbol{\mu} + s_0$.

The authors are interested in the inference about the vector **E**. It can easily be shown that the marginal posterior distribution of the vector **E** is a multivariate t-distribution with $n + n_0$ degrees of freedom, location vector μ_K, and precision matrix $\frac{(n + n_0)A_K}{s_K}$. For $n + n_0 > 2$, the posterior mean vector and the posterior covariance matrix exist, and their values are:

$$E(\mathbf{E}|\mathbf{K}) = (\mathbf{U}^T\mathbf{U} + \mathbf{A})^{-1}(\mathbf{U}^T\mathbf{K} + \mathbf{A}\boldsymbol{\mu}) \quad (10)$$

$$V(\mathbf{E}|\mathbf{K}) = \frac{n + n_0}{n + n_0 - 2}\left(\frac{(n + n_0)\mathbf{A}_K}{s_K}\right)^{-1} = \frac{s_K\mathbf{A}_K^{-1}}{n + n_0 - 2} \quad (11)$$

Now, it is assumed that $\mathbf{A} = \delta^2\mathbf{I}_m$ and $\boldsymbol{\mu} = \mathbf{0}$. Then

$$E(\mathbf{E}|\mathbf{K}) = (\mathbf{U}^T\mathbf{U} + \delta^2\mathbf{I}_m)^{-1}\mathbf{U}^T\mathbf{K}.$$

In (Harville, 2008, p. 513), the MP pseudoinverse of a matrix is expressed as a limit. Namely, for any matrix **U**:

$$\mathbf{U}^{+} = \lim_{\delta\to 0}\left(\mathbf{U}^T\mathbf{U} + \delta^2\mathbf{I}_m\right)^{-1}\mathbf{U}^T = \lim_{\delta\to 0}\mathbf{U}^T\left(\mathbf{U}\mathbf{U}^T + \delta^2\mathbf{I}_n\right)^{-1} \quad (12)$$

Thus, if $\delta \to 0$ in the prior distribution of **E**, and consequently, in the posterior, then:

$$\lim_{\delta\to 0}E(\mathbf{E}|\mathbf{K}) = \lim_{\delta\to 0}\left(\mathbf{U}^T\mathbf{U} + \delta^2\mathbf{I}_m\right)^{-1}\mathbf{U}^T\mathbf{K} = \mathbf{U}^{+}\mathbf{K} = \hat{\mathbf{E}}^{+} \quad (13)$$

Thus, given the precision τ, the limit of the posterior mean of the vector **E** equals $\hat{\mathbf{E}}^{+}$. In other words, when the precision of the prior conditional normal distribution for **E** converges to zero (i.e. the prior distribution becomes very spread out), the posterior mean of **E** converges to $\hat{\mathbf{E}}^{+}$. But if an improper prior distribution for **E** is introduced: $p(\mathbf{E}) \propto constant$ (expressing a total ignorance of all elements of **E**), then the posterior distribution of the vector **E** (given τ) will be also improper (Zellner, 1971). Therefore, no inference can be made about **E** without introducing prior information (e.g. represented by a proper prior distribution for **E**). Zellner (1971) shows that in such a case, it is possible to make inferences only about estimable functions of the elements of **E**.

Example: Illustration of the UEK's defects

Let us consider an example of sustainable rural development in the Świętokrzyskie voivodeship, as presented in (Popławski and Kaczmarczyk, 2013). In this case, the dependent variable **K** represents the number of private enterprises per 1,000 working-age population. The 14×18 matrix **U** contains the explanatory variables' values that can influence the number of private enterprises (see Table 1).

In order to illustrate some serious defects of the UEK method when used in practice, two variants will be considered:

- Variant 1: all explanatory variables are expressed in units presented in Table 1 (Variant 1 was considered by Popławski and Kaczmarczyk, 2013, pp. 212–216),
- Variant 2: the explanatory variable u_{11} is expressed in PLN and u_{17} is expressed in 1,000 ha per capita whereas other variables are unchanged.

The estimation results for **E** (based on the MP pseudoinverse) are presented in Table 1. Because the matrix $\mathbf{U}^T\mathbf{U}$ is singular, the set of normal equations has infinitely

Table 1. Explanatory variables and estimates of the vector **E**

	Explanatory variables (u_i)	$\hat{\mathbf{E}}^{+}$ (Variant 1)	$\hat{\mathbf{E}}^{+}$ (Variant 2)
u_1	Population density (persons per square kilometer)	9.414	23.766
u_2	Birthrate (per 1,000 population)	18.268	196.029
u_3	Number of people domiciled per municipality area	353.016	551.314
u_4	Share of pensioners	–385.800	–7 225.683
u_5	Share of population aged up to 55	–7 513.512	–6 938.534
u_6	Population aged 64 and over	459.087	–65 759.421
u_7	Ratio of population aged over 64 to population aged up to 15	367.531	11 428.772
u_8	Coefficient of social burden	2 587.239	3 473.254
u_9	Coefficient of social placement	401.859	–53.407
u_{10}	Number of flats per 1,000 population	2.045	688.767
u_{11}	Own incomes of municipal budgets (PLN thousand) per 1,000 population	2.120	–0.001
u_{12}	Part of municipal incomes which are state budget incomes (PLN per capita)	1.359	–13.831
u_{13}	Number of operators registered in REGON per 1,000 population	38.366	212.284
u_{14}	Economic operators per 1,000 population	–23.100	–156.841
u_{15}	Spatial location coefficient	–3 198.228	–5 565.257
u_{16}	Share of agricultural tax in own municipal incomes	2 105.283	7 566.313
u_{17}	Arable land (ha per capita)	–437.369	–10 767.094
u_{18}	Ratio of public economic operators registered in REGON to the total number of registered operators	–5 312.860	–6 619.372

Source: own elaboration based on Popławski and Kaczmarczyk (2013). The dataset was retrieved from Table 1 in Popławski and Kaczmarczyk (2013), p. 212. In Variant 1, the results differed from those presented in Popławski and Kaczmarczyk (2013), probably due to the accuracy of data used.

many different solutions. The estimator $\hat{\mathbf{E}}^+$ selects only one of them. Estimates obtained with the use of UEK are not reliable because the vector **E** is not estimable. In practice, the invalidity of UEK can be easily illustrated by the fact that changes of measurement unit(s) of explanatory variables may result in changes to estimates of the vector **E**, as shown in Table 1. These changes differ from what was observed in the linear regression model with the non-singular matrix $\mathbf{U}^T\mathbf{U}$ (estimated using the OLS estimator); in that case, if an explanatory variable is divided by a factor, the OLS estimate of the corresponding parameter gets multiplied by this factor. This rule does not hold when the matrix $\mathbf{U}^T\mathbf{U}$ is singular, in which case the MP pseudoinverse is used. To summarize the example under consideration, the estimates of the vector **E** do not provide information about the impact of explanatory variables on the dependent variable. Finally, it must be emphasized that the mean squared estimates of regression coefficients (calculated in Popławski and Kaczmarczyk, 2013, pp. 211 and 216) cannot be treated as the residual variance.

CONCLUSION

The above considerations lead to the conclusion that it is methodologically inappropriate to use the UEK method to estimate the vector of parameters **E** in the linear regression model. This is because when the matrix of values of explanatory variables has less than full column rank, it is impossible to estimate all regression coefficients based only on the available dataset (additional information is needed, e.g. a prior distribution of the vector **E**). As pointed out by Searle (1966), the best linear unbiased estimators (the same for all solutions of normal equations, obtained with the use of a generalized inverse matrix) exist only for certain linear functions of parameters, known as estimable functions. On the other hand, in the case when the matrix of values of explanatory variables has full column rank, the UEK method is equivalent to the ordinary least squares method which can be effectively used only under certain assumptions for explanatory variables and random disturbances.

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