On relationship between regression models and interpretation of multiple regression coefficients

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Abstract

In this paper, we consider the problem of treating linear regression equation coefficients in the case of correlated predictors. It is shown that in general there are no natural ways of interpreting these coefficients similar to the case of single predictor. Nevertheless we suggest linear transformations of predictors, reducing multiple regression to a simple one and retaining the coefficient at variable of interest. The new variable can be treated as the part of the old variable that has no linear statistical dependence on other presented variables.

Keywords: Simple and Multiple Regression; Correlated Predictors; Interpretation of Regression Coefficients.

1 Introduction

Regression analysis is one of the main methods for studying dependency factors in diverse fields of inquiry where use of statistical methods is expedient (see e.g. Draper and Smith (1998)). The efficiency of its application depends on the model and the set of explanatory variables (predictors) chosen. The most popular regression model is described by a linear equation expressing the dependence of the mean value of the variable (response, outcome) to be explained on the set of predictors.

The natural applicability domain of regression analysis is a case of continuous outcome and predictors. In this area, the classical regression analysis theory
provides a thorough description of outcome dependence on explanatory variables considered. Of most interest in the linear model are the coefficients at predictors. For example, in the simplest case of single predictor $X_1$ and dependent variable $Y$ the linear regression equation is given by

$$y = b_0 + b_1 x_1$$

Factor $b_1$ is proportional to the coefficient of correlation between response $Y$ and predictor $X_1$. Furthermore, $b_1$ represents an increase (or a decrease, if $b_1$ is negative) in the mean of $Y$ associated with a 1-unit increase in the value of $X$, $X = x + 1$ versus $X = x$. The sign of $b_1$ indicates the trend in the relationship between $Y$ and $X_1$.

Such thorough information about the relationship between outcome and single explanatory variable makes one wish to treat the coefficients of a multiple regression equation in a similar manner. It is well known, however, that in linear multiple regression models such interpretation of regression coefficients is not correct if there are correlations among predictors (Draper and Smith (1998), Nalimov (1975), Ehrenberg (1975)). Moreover, in some practical cases such interpretation is in conflict with common sense (Varaksin et al. (2004), see below section 4). The unique case where interpretation of multiple regression equation coefficients is meaningful is pairwise statistical independence of predictors. Then multiple regression coefficients coincide with corresponding simple regression coefficients for the outcome on a particular predictor (Draper and Smith (1998)).

Thus, the presence of correlated predictors renders the identification of the biomedical meaning of multiple regression equation coefficients a difficult task. Association among predictors or among predictors and outcome leads to unpredictable changes in regression coefficients and results in a loss of meaning in each particular coefficient.

Nevertheless we cannot confine ourselves to independent (uncorrelated) variables only, as in most applications of regression analysis there are important problems with correlated predictors, e.g. various air pollution rates (see below section 4). Another important example is epidemiological studies (research into disease prevalence and its association with risk factors). Such factors as sex and age are invariably present in epidemiological data, being related to both other independent variables and outcome. These inherent variables which confuse the effect on the response and other predictors are called confounders. Taking into account confounders in data analysis presents a difficult problem that does not have any correct solution as yet.
In a range of biomedical applications of regression analysis, of major interest is some variable $X_1$ which is considered along with accompanying variables $X_2, X_3, ..., X_k$ (confounders). Upon finding a multiple regression equation that depends on all of these predictors one has to treat coefficient $b_1$ standing at the principal predictor, with all other predictors adjusting the action of main variable $X_1$. We shall consider below a way to interpret $b_1$ in terms of simple regression of outcome on a new variable, $X_1^*$. For simplicity, we shall discuss cases of two and three predictors. The general case may be considered in a similar way.

## 2 Regression equation with two predictors

Let us consider continuous variables $Y, X_1, X_2$ and corresponding linear regression equation for outcome $Y$ on predictors $X_1, X_2$

$$y = b_0 + b_1 x_1 + b_2 x_2 \quad (1)$$

As usual, we suppose that coefficients $b_0, b_1, b_2$ and other regression coefficients below have been obtained by the least squares method. We assume that the (linear) dependence of response $Y$ on predictor $X_1$ is significant, so $b_1 \neq 0$. Finally, let the linear regression equation with response $X_1$ and predictor $X_2$ be given by

$$x_1 = c_{120} + c_{12} x_2$$

We define a new variable, $X_1^*$, in which the linear dependence of $X_1$ on $X_2$ is excluded’ as follows

$$X_1^* = X_1 - c_{12} X_2$$

Let us build a simple regression equation describing the mean of outcome $Y$ as a function of new predictor $X_1^*$

$$y = a_{10}^* + a_1^* x_1^* \quad (2)$$

We have pairs of corresponding variables: $X_1$ and $x_1$, $X_1^*$ and $x_1^*$. Obviously, these variables cannot be interchanged; in particular, variables $X_1, X_1^*$ cannot be substituted in equations (1) and (2) instead of $x_1$ and $x_1^*$, respectively. If it were possible, one might transcribe equations (1) and (2) as

$$y = b_0 + b_1 \left( x_1 + \frac{b_2}{b_1} x_2 \right)$$

$$y = a_{10}^* + a_1^* (x_1 - c_{12} x_2)$$
Although these equations are different, they have the same slope, as follows from the following theorem.

**Theorem 1.** In equation (1), coefficient $b_1$ is equal to coefficient $a^*_1$ in equation (2), i.e.

$$b_1 = a^*_1,$$

and it is possible that $\frac{b_2}{b_1} \neq -c_{12}$.

A similar statement holds for coefficients $b_2$ and $a^*_2$, where $a^*_2$ is the coefficient at variable $x^*_2$ in a simple regression equation $y = a^*_{20} + a^*_2 x^*_2$, and a new variable $X^*_2$ is defined from the regression equation $x_2 = c_{210} + c_{21} x_1$ as $X^*_2 = X_2 - c_{21} X_1$.

Formal proof of Theorem 2 is provided in Appendix 1.

Now coefficient $b_1$ of multiple regression equation (1) may be treated as follows. Recall that $b_1$ cannot be interpreted per se. But it is equal to coefficient $a^*_1$ of simple regression model (2). Hence we transform the problem of interpretation of $b_1$ into one of interpretation of a new variable $X^*_1$. It is easy to check that $X^*_1$ and $X_2$ are uncorrelated. So one can say that variable $X^*_1$ is obtained from variable $X_1$ by excluding the part of it that is linearly dependent on it. This does not mean that by constructing variable $X^*_1$ we can split the contributions of $X_1$ and $X_2$ to response $Y$. In fact, there is no way to do this given correlated predictors.

Now consider a more general way to define variable $X^*_1$, namely, let $X^*_1 = X_1 - \gamma X_2$, where $\gamma$ is a real number, and pose the question: how many values may $\gamma$ take for equality (3) to hold? In the case under consideration, we can express the dependence of $a^*_1$ on parameter $\gamma$ in explicit form as follows

$$a^*_1(\gamma) = \frac{\bar{X}_1 Y - \bar{X}_1 \bar{Y} - \gamma (\bar{X}_2 Y - \bar{X}_2 \bar{Y})}{\text{var}(X_1) - 2\gamma \text{cov}(X_1, X_2) + \gamma^2 \text{var}(X_2)},$$

where the bar over a symbol denotes the mean of the variable, $\text{var}$ and $\text{cov}$ stand for variance and covariance, respectively.

**Theorem 2.** Equation $a^*_1(\gamma) = b_1$ has two solutions, videlicet

$$\gamma_1 = c_{12}, \quad \gamma_2 = -\frac{b_2}{b_1}$$

For the proof of this theorem we refer the reader to Appendix 2.

Given the explicit expression for $a^*_1(\gamma)$ in formula (4), we can plot it (see Fig. 1, where artificial data is used with $b_1 = 0.2918$ which is drawn as a horizontal line). There are some general properties in $a^*_1(\gamma)$: it is defined throughout the real axis, has two extrema, and the real axis is an asymptote to it.
3 Regression equation with three predictors

Now consider the case of one outcome $Y$ and three predictors $X_1, X_2, X_3$. The point of interest is predictor $X_1$ the other predictors being confounders. We want to get an interpretation of coefficient $b_1$ at the variable of interest in the multiple regression equation

$$y = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3$$

(5)

We can introduce the regression equation of $X_1$ on covariates $X_2, X_3$:

$$x_1 = c_{0123} + c_{12} x_2 + c_{13} x_3,$$

and define a new variable by the formula

$$X_1^* = X_1 - c_{12} X_2 - c_{13} X_3$$

(6)

As in section 1, we could find a simple regression equation for $Y$ on covariate $X_1^*$

$$y = a_{01}^* + a_1^* x_1^*$$

(7)

Similar to Theorem 2, we have the following statement.

**Theorem 3.** Coefficient $b_1$ of equation (5) is equal to coefficient $a_1^*$ of equation (7), that is

$$b_1 = a_1^*$$

The proof of this theorem is given in Appendix 3.
Going over to a more general case, we can define covariate $X_1^*$ as follows

$$X_1^* = X_1 - \gamma_2 X_2 - \gamma_3 X_3,$$

where $\gamma_2, \gamma_3$ are some real numbers. Then regression coefficient $a_1^*$ becomes a function of two real variables $\gamma_2, \gamma_3$. The shape of surface $z = a_1^*(\gamma_2, \gamma_3)$ is shown in Figure 2 (using simulated data with $b_1 = -2.031$).

As one can see from Fig. 1 and Fig. 2, the character of the dependence of $a_1^*$ on corresponding parameter(s) in both cases is similar. The same is true of the general case.

4 Applications to real data analysis

4.1 Regression with two predictors

Let us consider the use of Theorem 2 for investigating the dependency of incidence on various air pollution toxicants of City St.-Petersburg (Russia). The primary data were published in Scherbo (2002). In the remainder of this section, we assume incidence to be incidence rate in the adult population (i.e. the number of disease cases per 1000 adult population a year) averaged over a 5-year observation period. In the primary data, the rates of incidence were gathered across 19 boroughs of St.-Petersburg. We consider toxicant concentrations as random
variables, i.e. mean toxicant concentration expressed in maximum concentration limit (MCL) terms and averaged over 5-year observation period. Each of these variables takes on 19 values in accordance with the number of boroughs. We denote these covariates by the usual chemical notations: \( CO, NO_2, SO_2, Pb \) etc. (the data consists of 12 pollutants).

The simple linear regression equations of response \( Y \) (incidence) on concentrations of \( CO \) and \( NO_2 \) are given by

\[
Y = 603 + 579 \, CO
\]

\[
Y = 414 + 416 \, NO_2
\]

According to equation (8), incidence increases by 579 cases per 1000 population at an increase in \( CO \) concentration by MCL unit a year. Equation (9) may be interpreted in the same way. In short, both \( CO \) and \( NO_2 \) increase incidence.

There is a tight positive correlation between predictors \( CO \) and \( NO_2 \). Pearson’s correlation coefficient is 0.75, and the regression equation is

\[
CO = -0.131 + 0.576 \, NO_2
\]

This shows that growth in one toxicant is related to growth in another. Hence, one can conjecture that equation (8) does describe an increase in incidence at a simultaneous increase in both pollutants \( (CO \) and \( NO_2) \). A question then arises: could one specify the ‘pure’ influence of each toxicant on incidence, separating the contribution of one toxicant from that of the other?

To extract the contribution of each toxicant to the incidence in the presence of other toxicants, researchers often use a multiple regression equation including all toxicants. Such interpretation is common in some biological and medical applications of regression analysis. We refer to [McNamee (2005)] as atypical exposition. In the case under consideration, we obtain a multiple regression equation

\[
Y = 465 + 390 \, CO + 191 \, NO_2
\]

A lot of authors consider the coefficients of a multiple regression equation obtained by means of the least squares method to be meaningless if there are correlations among predictors ([Draper and Smith (1998), Aivazian et al. (1985), Ehrenberg (1975)])). These coefficients cannot be used to assess separately the dependence of \( Y \) on \( CO \) and \( Y \) on \( NO_2 \). Nevertheless, there are other authors who treat each coefficient of a multiple regression equation as the contribution of an
individual toxicant to the outcome against the background of other toxicants (e.g. McNamee (2005)). Moreover, this contribution has to be refined as compared to (8)–(9). Their supposition is that predictors as if distribute their influence on the outcome in a multiple regression equation so that each predictor describes its influence with the other being in the background. According to this viewpoint, the addition of another toxicant, \( NO_2 \), to \( CO \) and change from (8) to (10) should attenuate the effect of \( CO \) because the corresponding coefficient diminished from 579 to 390. The same conclusion holds for \( NO_2 \) and \( CO \) and equations (9) and (10).

These authors do not provide any substantive explanation for the biomedical meaning of variations in the coefficients in (8)–(9) and (10); nor do they explain the refined contribution of each individual toxicant. Variations in regression coefficients could be explained by going over from simple regressions (8) or (9) to multiple regression (10). Indeed, coefficient \( b_1 = 390 \) in equation (10) is equal to coefficient \( a_{1^*} \) in the simple regression equation

\[
Y = a_{1^*} + a_{1^*} CO^* ,
\]

where covariate \( CO^* \) is defined by

\[
CO^* = CO - 0.576 NO_2 \tag{11}
\]

By (11), predictor \( CO^* \) is obtained from \( CO \) by excluding its part correlated with \( NO_2 \). Then \( b_1 = 390 \) means an increased incidence rate at a growth in \( CO \) concentration excluding the linear statistical dependence of \( CO \) and \( NO_2 \).

One can similarly treat coefficient \( b_2 = 191 \) in (10). It is equal to \( a_{2^*} \) in the simple regression equation

\[
Y = a_{2^*} + a_{2^*} NO_2^* ,
\]

where \( NO_2^* \) is a part of toxicant \( NO_2 \) which contains no linear statistical dependence on \( CO \).

We seem to have obtained a consistent picture: by excluding the (linear) dependence of one toxicant on the other we arrive at a ‘pure’ influence of a particular factor on incidence. Since both factors increase the incidence, and the concentration of each factor increases with growth in the other, one can anticipate that the magnitudes of the coefficients in equation (10) should be less than in (8)–(9). This is exactly so in the case under consideration.
It is not as simple as that though. Let us consider the dependence of incidence \( Y \) on the concentrations of \( CO \) and \( SO_2 \). A simple regression equation of \( Y \) on \( SO_2 \) is given by

\[
Y = 919 + 52 \cdot SO_2
\]

The association between \( CO \) and \( SO_2 \) is very similar to that between \( CO \) and \( NO_2 \). For instance, the correlation coefficient is 0.73 and the regression equation is

\[
CO = 0.272 + 0.316 \cdot SO_2 \tag{12}
\]

The multiple regression equation in the case considered is \( \text{Varaksin et al. (2004)} \)

\[
Y = 634 + 1047 \cdot CO - 278 \cdot SO_2 \tag{13}
\]

Assuming the coefficients of (13) to be refined ones we should treat the magnitude 1047 as a ‘pure’ influence of \( CO \) against the background of \( SO_2 \), and \(-278\) as a ‘pure’ influence of \( SO_2 \) against the background of \( CO \). Obviously, such interpretation of regression coefficients is invalid, since the ‘pure’ influence of toxicant \( SO_2 \) becomes negative. The reason for such misinterpretation is the tight correlation between predictors \( CO \) and \( SO_2 \). One has to take into account this correlation in treating regression coefficients.

The coefficient at \( CO \) in (13) is twice as large as that in (8). By Theorem 2, coefficient \( b_1 = 1047 \) is equal to the slope in

\[
Y = 697 + 1047 \cdot CO^*, \tag{14}
\]

where \( CO^* = CO - 0.316 \cdot SO_2 \). In biomedical terms, we obtain an inexplicable picture: we have reduced the toxic burden on the population by removing one of the two toxicants, but the incidence grows with \( CO \) even more rapidly. In mathematical terms, we can explain this as follows. It is clear from the definition of \( CO^* \) that its range is less than the range of \( CO \). In both cases, the incidence is the same, which implies an increase in coefficient \( b_1 \). Generally, inequality \( b_1 > a_1 \) is impossible if we consider the multiple regression coefficients as refined ones. But if we refer to equality (23), we can see that under \( a_2 \ll a_1 \) and correlation coefficient \( r \) close to 1, inequality \( b_1 > a_1 \) may hold true. The formula (24) also explains the possibility of a negative value for coefficient \( b_2 \).
4.2 Regression with three predictors

Let us consider a regression equation of incidence $Y$ on three predictors $CO, NO_2$ and $SO_2$. By the least square method, we obtain the equation

$$Y = 494 + 857CO + 194NO_2 - 279SO_2$$

Equation (5) becomes

$$CO = -0.108 + 0.386NO_2 + 0.195SO_2$$

The new variable $CO^*$ is defined by (6), and the simple regression equation for $Y$ on this predictor is given by

$$Y = 1076 + 857CO^*$$

We see that $b_1 = a_{1}^*$ as well.

Note that the correlation coefficient of model (12) is $r = 0.74$, and that of model (14) is $r = 0.46$. The latter is less than the coefficient of correlation between incidence $Y$ and $CO (r = 0.58)$.

5 Conclusion

Let there be two regression equations for outcome $Y$

$$y = a_0 + a_1x_1$$

and

$$y = b_0 + b_1x_1 + b_2x_2$$

If predictors $X_1, X_2$ are uncorrelated, then $a_1 = b_1$. Hence, inequality $a_1 \neq b_1$ is caused by the presence of correlation between the predictors. What is the epidemiological meaning of changing coefficient $a_1$ to $b_1$ after adding predictor $X_2$ to the simple regression model? Is the influence of the predictors on the outcome redistributed between them? The answer is definitely ‘no’. Usually, the addition of a second covariate is aimed at taking into account the combined effect of predictors on outcome. But what does ‘take into account’ mean? There are no reasonable explanations of this term.

In view of Theorem 2 we can state that the addition of $X_2$ to regression equation $y = b_0 + b_1x_1$ brings us to regression equation $y = a_{10}^* + a_{1}^*x_1^*$. The new variable $X_1^*$ contains no linear statistical dependence on $X_2$. A similar interpretation holds for the case of three variables as well as for the general one.
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Appendix 1

Proof of the Theorem

Let us first prove a technical statement, being of significance in its own right. Let there be a set of predictors $X_1, X_2, ..., X_k$ and let $Y_0$ be an outcome. The values of $p$ observations over predictors and the outcome combine into matrices $X$ and $Y$

$$X = \begin{pmatrix}
1 & X_{11} & \cdots & X_{1k} \\
1 & X_{12} & \cdots & X_{12} \\
\vdots & \vdots & \ddots & \vdots \\
1 & X_{1p} & \cdots & X_{kp}
\end{pmatrix}, \quad Y = \begin{pmatrix}
Y_1 \\
Y_2 \\
\vdots \\
Y_p
\end{pmatrix}$$

The first column contains unities so that we have the same formulae for calculating $b_0$ in the same way as other $b_i$. Let $B$ denote the column of coefficients $b_0, b_1, b_2, \ldots, b_k$. To find a linear regression equation for response $Y$ from predictors $X_1, X_2, \ldots, X_k$, we have to minimize the mean square residual of $Y$ and $X B$ i.e.

$$\min_B (Y - X B)(Y - X B)^T$$

where the $T$ denotes matrix transposition. The problem (15) has a unique solution under the usual least squares method assumptions, e.g. if the matrix $X^T X$ is invertible (see e.g. Draper and Smith [1998] Chapter 5). Such assumption will be needed throughout Appendix 1.

Let $\Gamma$ denote a nonsingular square matrix of order $k$

$$\Gamma = \begin{pmatrix}
\gamma_{11} & \gamma_{12} & \cdots & \gamma_{1k} \\
\gamma_{12} & \cdots & \gamma_{12} \\
\vdots & \vdots & \ddots & \vdots \\
\gamma_{k1} & \gamma_{k2} & \cdots & \gamma_{kk}
\end{pmatrix}$$

and let $C$ be a matrix of order $(k + 1) \times (k + 1)$.
\[
C = \begin{pmatrix}
1 & 0 & 0 & \ldots & 0 \\
0 & \gamma_{11} & \gamma_{12} & \ldots & \gamma_{1k} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \gamma_{k1} & \gamma_{k2} & \ldots & \gamma_{kk}
\end{pmatrix}
= \begin{pmatrix}
1 & 0 \\
0 & \Gamma
\end{pmatrix}
\]

Let us introduce a vector, \( X_0 = (1, X_1, X_2, \ldots, X_k) \), and consider linear transformation of variables \( X_1, X_2, \ldots, X_k \) by the matrix \( C \)

\[
X^*_0 = X_0 C
\]  

Thus, the new variables \( X^*_0 = (1, X^*_1, X^*_2, \ldots, X^*_k) \) obtained from variables \( X_0 = (1, X_1, X_2, \ldots, X_k) \) by means of linear transformation are given by

\[
X^*_i = \sum_{j=1}^{k} \gamma_{ij} X_j
\]

Finally, we denote by \( X^* \) a matrix constructed from \( X^*_0 \) in the same way as \( X \) from \( X_0 \), and \( B^* \) stands for the column of coefficients \( b^*_0, b^*_1, \ldots, b^*_k \).

**Proposition 1.** Let multiple regression equation of outcome \( Y_0 \) on predictors \( X_1, X_2, \ldots, X_k \) be

\[
y = \sum_{i=0}^{k} b_i x_i
\]

Then coefficients \( b^*_0, b^*_1, \ldots, b^*_k \) of the multiple regression equation for \( Y_0 \) on predictors \( X^*_1, X^*_2, \ldots, X^*_k \)

\[
y = \sum_{k=0}^{n} b^*_k x^*_k
\]

can be found from the matrix equality

\[
B^* = C^{-1} B
\]

It is easy to check that under condition \((16)\) we have

\[
X^* = X C
\]  

To find a regression equation relative to new variables \( X^*_i \) we need to solve the minimization problem
Given equality (17), we have
\[(Y - X^* B^*)(Y - X^* B^*)^T = (Y - X C B^*)(Y - X C B^*)^T\]

Hence we obtain \(C B^* = B\), since the minimization problem (15) has a unique solution. It is obvious from its definition that matrix \(C\) is invertible and
\[C^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & \Gamma^{-1} \end{pmatrix}\]

This brings us to the end of the proof of the Proposition.

**Proof** To prove Theorem 2 consider the case of two predictors \(X_1, X_2\), and matrix \(C\) is equal to
\[C = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -c_{12} & 1 \end{pmatrix}\]

Then \(X_1^* = X_1 - c_{12} X_2\) and \(X_2^* = X_2\). Applying the Proposition to matrix \(C\), we obtain
\[B^* = \begin{pmatrix} b_0^* \\ b_1^* \\ b_2^* \end{pmatrix} = C^{-1} B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & c_{12} & 1 \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} b_0 \\ b_1 \\ b_2 + c_{12} b_1 \end{pmatrix}\]

It can be easily seen that \(X_1^*\) and \(X_2\) are uncorrelated (correlation coefficient is equal to zero). Therefore, coefficients \(b_1^*, b_2^*\) of the multiple regression equation for outcome \(Y\) on predictors \(X_1^*, X_2\)
\[y = b_0^* + b_1^* x_1^* + b_2^* x_2\]
are equal to the corresponding coefficients of the simple regression equations for \(Y\) on predictors \(X_1^*\) and \(X_2\), respectively
\[y = a_{01}^* + a_1^* x_1^*, \quad y = a_{02} + a_2 x_2\]
\[b_1^* = a_1^*, \quad b_2^* = a_2\]

Using (18), we obtain \(b_1^* = b_1\), and combining this with (19) we obtain \(b_1 = a_1^*\), which finishes the proof.
Appendix 2

Proof of the Theorem 2

Let us consider linear transformation of variable $X_1$

$$X_1^* = X_1 - \gamma X_2$$

(20)

Then in the regression equation

$$y = a_{10}^* + a_{1}^* x_1^*$$

(21)

coefficient $a_1^*$ becomes a function of parameter $\gamma$. Its explicit expression is given by

$$a_1^*(\gamma) = \frac{X_1 Y - X_1 Y - \gamma (X_2 Y - X_2 Y)}{\text{var}(X_1) - 2\gamma \text{cov}(X_1, X_2) + \gamma^2 \text{var}(X_2)},$$

(22)

**Proof** (of Theorem 2) Recall the following regression equations for outcome $Y$ on predictors $X_1, X_2$ (jointly and separately)

$$
y = b_0 + b_1 x_1 + b_2 x_2
$$

$$
y = a_{01} + a_1 x_1
$$

$$
y = a_{02} + a_2 x_2
$$

and we introduce matrices

$$A = (a_1, a_2), \quad B = (b_1, b_2), \quad C = \begin{pmatrix} 1 & c_{12} \\ c_{21} & 1 \end{pmatrix},$$

where $c_{ij}$ are regression coefficients from the equations

$$x_1 = c_{012} + c_{12} x_2$$

$$x_2 = c_{021} + c_{21} x_1$$

According to the theorem Panov and Varaksin (2010), we have equality $A = B \cdot C$. Now, suppose that $C$ is an invertible matrix (the opposite case is discussed below in the Remark 5). Then

$$B = A \cdot C^{-1}$$

Thus we obtain the following representation of regression coefficients $b_1, b_2$ ($r$ denotes the correlation coefficient between $X_1, X_2$)
We get the roots of the equation \( \sigma \) where

\[
\begin{align*}
b_1 &= \frac{a_1 - a_2 c_{21}}{1 - c_{12} c_{21}} = \frac{a_1 - a_2 c_{21}}{1 - r^2} \\
b_2 &= \frac{a_2 - a_1 c_{12}}{1 - c_{12} c_{21}} = \frac{a_2 - a_1 c_{12}}{1 - r^2}
\end{align*}
\]  

From (23)–(24), it follows

\[
\begin{align*}
a_1 - a_2 c_{21} &= b_1 (1 - r^2), \quad a_2 - a_1 c_{12} = b_2 (1 - r^2) \\
b_1 c_{12} &= a_2 - b_2, \quad b_2 c_{21} = a_1 - b_1 \\
c_{12} &= \frac{a_2 - b_2}{b_1} = \frac{a_2 - b_2}{b_1}, \quad c_{21} = \frac{a_1}{b_2} - \frac{b_1}{b_2} = \frac{a_1 - b_1}{b_2} \\
r^2 &= c_{12} c_{21} = \frac{a_1 a_2}{b_1 b_2} - \frac{a_1}{b_1} - \frac{a_2}{b_2} + 1, \quad 1 - r^2 = 1 - \frac{a_1}{b_1} + \frac{a_2}{b_2} - \frac{a_1 a_2}{b_1 b_2}
\end{align*}
\]

If we equate the right hand side of (23) to the right hand side of (22), we obtain the roots of the equation \( a_1^* (\gamma) = b_1 \) (after some simplification)

\[
\gamma_{1,2} = \frac{1}{2 (a_1 - a_2 c_{21}) \text{var} (X_2) - 2 \text{cov} (X_1, X_2) (a_1 - a_2 c_{21}) - a_2 \text{var} (X_2) (1 - c_{12} c_{21})} \pm \frac{1}{\sqrt{4 (-a_2 + a_1 c_{12}) c_{21} \text{var} (X_1) \text{var} (X_2) (-a_1 + a_2 c_{21}) + (-2 a_1 \text{cov} (X_1, X_2) + a_2 (2 c_{21} \text{cov} (X_1, X_2) + \text{var} (X_2) (1 - c_{12} c_{21})))^2}}
\]

Applying (25), we get

\[
\gamma_{1,2} = \frac{1}{2 \text{var} (X_2) b_1 (1 - r^2) - 2 r \sigma (X_1) \sigma (X_2) b_1 (1 - r^2) - a_2 \text{var} (X_2) (1 - r^2) \pm \frac{1}{\sqrt{4 b_1 b_2 c_{21} (1 - r^2)^2 \text{var} (X_1) \text{var} (X_2) + (-2 a_1 r \sigma (X_1) \sigma (X_2) + a_2 (2 c_{21} r \sigma (X_1) \sigma (X_2) + \text{var} (X_2) (1 - r^2)))^2}}
\]

where \( \sigma (X_i) = \sqrt{\text{var} (X_i)} \).

Next, we expand the second summand in the radicand and factor out the \(-2 r \sigma (X_1) \sigma (X_2)\). After that, \( a_1 - a_2 c_{21} \) is substituted by \( b_1 (1 - r^2) \) (see (25)). We get

\[
\gamma_{1,2} = \frac{1}{2 \text{var} (X_2) b_1 (1 - r^2)} \left[ (1 - r^2) (2 r \sigma (X_1) \sigma (X_2) b_1 - a_2 \text{var} (X_2)) \right] \pm \sqrt{4 b_1 b_2 c_{21} (1 - r^2)^2 \text{var} (X_1) \text{var} (X_2) + (-2 r \sigma (X_1) \sigma (X_2) b_1 (1 - r^2) + a_2 \text{var} (X_2) (1 - r^2))^2}
\]
or
\[
\gamma_{1,2} = \frac{1}{2b_1} \left[ 2rb_1 \frac{\sigma(X_1)}{\sigma(X_2)} - a_2 \pm \sqrt{4b_1 b_2 c_{21} \text{var}(X_1) + \left( 2rb_1 \frac{\sigma(X_1)}{\sigma(X_2)} - a_2 \right)^2} \right]
\]

Applying (25) again, we obtain the required equalities
\[
\gamma_{1,2} = \frac{1}{2b_1} \left[ 2b_1 c_{12} - a_2 \pm \sqrt{4b_1 b_2 c_{12} + (2b_1 c_{12} - a_2)^2} \right] =
\]
\[
c_{12} - \frac{a_2}{b_1} \pm \sqrt{\left( \frac{a_2}{b_1} - c_{12} \right) c_{12} + \left( c_{12} - \frac{a_2}{2b_1} \right)^2} =
\]
\[
c_{12} - \frac{a_2}{b_1} \pm \sqrt{\frac{a_2}{b_1} c_{12} - c_{12}^2 + c_{12}^2 - \frac{a_2}{b_1} c_{12} + \left( \frac{a_2}{2b_1} \right)^2} = c_{12} - \frac{a_2}{2b_1} \pm \frac{a_2}{2b_1}
\]

That is
\[
\gamma_1 = c_{12}, \quad \gamma_2 = c_{12} - \frac{a_2}{b_1}
\]
or
\[
\gamma_1 = c_{12}, \quad \gamma_2 = \frac{b_2}{b_1}
\]

Remark If correlation matrix C is singular, then \( r^2 = 1 \), i.e. predictors \( X_1, X_2 \) are proportional. In this case, the problem of finding a multiple regression equation on variables \( X_1, X_2 \) cannot be posed, since it leads to an inconsistent system of linear equations.

Appendix 3

Proof of the Theorem 3

The method of proving Theorem 3 as considered in this Appendix contains the main ideas of the proof of the general statement.

Let the linear multiple regression equation for outcome \( Y \) on predictors \( X_1, X_2, X_3 \) be
\[
y = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3
\]

We introduce new variable \( X_1^* \) by
\[
X_1^* = X_1 - \gamma_2 X_2 - \gamma_3 X_3,
\]
where \( \gamma_2, \gamma_3 \) are some constants. So we perform linear transformation of predictors by the matrix

\[
C = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & -\gamma_2 & 1 & 0 \\
0 & -\gamma_3 & 0 & 1
\end{pmatrix}, \quad \det (C) = 1
\]

The inverse matrix \( C^{-1} \) is equal to

\[
C^{-1} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & \gamma_2 & 1 & 0 \\
0 & \gamma_3 & 0 & 1
\end{pmatrix}
\]

Hence the coefficients of the regression equation for \( Y \) on \( X_1, X_2, X_3 \) and that on \( X_1^*, X_2^* = X_2, X_3^* = X_3 \) are connected by (see Appendix 1)

\[
\begin{pmatrix}
b_0^* \\
b_1^* \\
b_2^* \\
b_3^*
\end{pmatrix} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & \gamma_2 & 1 & 0 \\
0 & \gamma_3 & 0 & 1
\end{pmatrix} \cdot \begin{pmatrix}
b_0 \\
b_1 \\
b_2 \\
b_3
\end{pmatrix} = \begin{pmatrix}
b_0 \\
b_1 \\
\gamma_2 b_1 + b_2 \\
\gamma_3 b_1 + b_3
\end{pmatrix}
\]

In particular, for arbitrary \( \gamma_2, \gamma_3 \) coefficients \( b_1 \) and \( b_1^* \) are equal. From now on we assume \( \gamma_2 = c_{12}, \gamma_3 = c_{13} \).

Let us consider a simple regression equation for \( Y \) on \( X_1^* \)

\[
y = a_{01}^* + a_1^* x_1^*
\]

We have divided the proof of Theorem 3 into a sequence of lemmas.

**Lemma 1.** The multiple correlation coefficient of variable \( X_1^* \) on predictors \( X_2, X_3 \) is equal to zero.

**Proof** Let \( \rho_{1,23}^* \) be the multiple correlation coefficient of \( X_1^* \) on variables \( X_2, X_3 \). By its definition

\[
\left( \rho_{1,(23)}^* \right)^2 = 1 - \frac{|\text{Corr}|}{C_{11}},
\]

where \( |\text{Corr}| \) is the determinant of the correlation matrix of variables \( X_1^*, X_2, X_3 \), and \( C_{11} \) is the cofactor of the (1,1) entry of the matrix \( \text{Corr} \). Therefore
\[
|Corr| = \begin{vmatrix}
1 & r_{12} & r_{13} \\
r_{21} & 1 & r_{23} \\
r_{31} & r_{32} & 1
\end{vmatrix},
C_{11} = \begin{vmatrix}
1 & r_{23} \\
r_{32} & 1
\end{vmatrix},
\]

Similar to the case of two predictors, one can see that \(r_{12} = r_{21} = r_{13} = r_{31} = 0\). Hence
\[
|Corr| = \begin{vmatrix}
1 & 0 & 0 \\
0 & 1 & r_{23} \\
0 & r_{32} & 1
\end{vmatrix} = C_{11} = \begin{vmatrix}
1 & r_{23} \\
r_{32} & 1
\end{vmatrix},
\]
i.e. \(\rho_{1;23}^* = 0\).

**Lemma 2.** Let us have multiple regression equations for outcome \(Y\) on variables \(X_1^*, X_2\)
\[
y = b'_0 + b'_1 x_1^* + b'_2 x_2
\]  
(27)
and that on variables \(X_1^*, X_3\)
\[
y = b''_0 + b''_1 x_1^* + b''_3 x_3
\]
Also, consider simple regression equations for outcome \(Y\) on predictors \(X_2\) and \(X_3\) respectively
\[
y = a_{02} + a_2 x_2 \\
y = a_{03} + a_3 x_3
\]
Then
\[
b'_2 = a_2, b'_3 = a_3
\]
Besides,
\[
b'_1 = b''_1 = a_1^*,
\]  
(28)
where \(a_1^*\) is the regression coefficient from equation (2).

Proof. As it is mentioned above, covariates \(X_1^*, X_2\) are uncorrelated as well as \(X_1^*, X_3\). Hence \(b'_2 = a_2, b'_3 = a_3\). The last equality (28) is implied by Theorem 2.

**Lemma 3.** Let there be a multiple regression equation for variable \(X_3, X_1^*, X_2\)
\[ x_3 = \alpha_{0312} + \alpha_{31}^* x_1^* + \alpha_{32} x_2 \]  

(29)

Then

\[ \alpha_{31}^* = 0 \]

For the multiple regression equation of \( X_2 \) on predictors \( X_1^*, X_3 \)

\[ x_2 = \alpha_{0213} + \alpha_{21}^* x_1^* + \alpha_{23} x_3 \]

we have

\[ \alpha_{21}^* = 0 \]

**Proof** We obtain it by a tedious calculation. By the least squares method, coefficient \( \alpha_{31}^* \) can be obtained from a system of linear equations. The numerator of the expression for \( \alpha_{31}^* \) is the determinant

\[
\begin{vmatrix}
X_1 - c_{12} X_2 - c_{13} X_3 & X_3 & X_3 & X_2 \\
X_2 & X_1 X_3 - c_{12} X_2 X_3 - c_{13} X_3^2 & X_2 X_3 & X_2 X_3 \\
X_3 & X_2 X_3 & X_3^2 & X_2^2 \\
X_3 & X_2 X_3 & X_3^2 & X_2^2 \\
\end{vmatrix} = (30)
\]

From corresponding systems of linear equations we obtain

\[
c_{12} = \frac{1}{X_3} \begin{vmatrix}
1 & X_1 & X_3 & X_3 \\
X_2 & X_1 X_3 & X_2 X_3 & X_2 X_3 \\
X_3 & X_2 X_3 & X_3^2 & X_2^2 \\
X_3 & X_2 X_3 & X_3^2 & X_2^2 \\
\end{vmatrix}, \quad c_{13} = \frac{1}{X_3} \begin{vmatrix}
1 & X_2 & X_1 & X_1 \\
X_3 & X_2 X_3 & X_1 X_2 & X_1 X_2 \\
X_3 & X_2 X_3 & X_3^2 & X_2^2 \\
X_3 & X_2 X_3 & X_3^2 & X_2^2 \\
\end{vmatrix}
\]

After substituting these into (30) and making necessary simplifications we thus obtain \( \alpha_{31}^* = 0 \).

The second equality is proved in just the same way.

**Proof of Theorem 3** By (26) we have \( b_1 = b_1^* \). Lemma 5 shows that \( b_1' = b_1'' = a_1^* (c_{12}, c_{13}) \). In what follows we need an appropriate generalization of the theorem Panov and Varaksin (2010). It is provided below in Appendix 4. Applying it, we get

\[
b_1' = b_1^* + b_3^* \alpha_{31}^* \]  

(31)

This proves Theorem 3, since \( \alpha_{31}^* = 0 \) by lemma 5.
Appendix 4

A theorem on relationship among regression coefficients

What follows is a statement of the theorem used in Appendix 3.

**Theorem (Panov)** Let there be an outcome $Y$ and a set of predictors $X_1, X_2, \ldots, X_k$. Consider a multiple regression equation for the outcome on the set of predictors

$$y = b_0 + \sum_{i=1}^{k} b_i x_i$$  \hspace{1cm} (32)

From the set of predictors $X_1, X_2, \ldots, X_k$, we extract a subset $\{X_{i_1}, X_{i_2}, \ldots, X_{i_m}\}$ and introduce regression equations for each predictor on the subset of predictors extracted

$$x_i = c_i + \sum_{j=1}^{m} c_{i,i_j} x_{i_j}$$  \hspace{1cm} (33)

We suppose that $c_i = 0, c_{i,i_j} = \delta_{i,i_j}$ for $i \in \{i_1, i_2, ..., i_m\}$.

Finally, let there be a multiple regression equation for outcome $Y$ on the set of predictors $\{X_{i_1}, X_{i_2}, \ldots, X_{i_k}\}$

$$y = a_0 + \sum_{j=1}^{k} a_{i_j} x_{i_j}$$  \hspace{1cm} (34)

Then

$$a_{i_j} = \sum_{i=1}^{k} b_i c_{i,i_j}$$  \hspace{1cm} (35)

This theorem has been used in Appendix 3 as follows. The set of all predictors is $\{X_1^*, X_2, X_3\}$, the extracted set of predictors is $\{X_1^*, X_2\}, i_1 = 1, i_2 = 2$. Then (32) becomes the equation (see 26)

$$y = b_0^* + b_1^* x_1^* + b_2^* x_2 + b_3^* x_3$$

The (33) transforms into (29), and

$$c_{11} = 1, c_{12} = 0, c_{21} = 0, c_{22} = 1, c_{31} = a_{31}, c_{32} = a_{32}$$  \hspace{1cm} (36)

The (34) is equation (27), and
Thus (35) becomes (for $a_1 = b'_1$)
\[
b'_1 = b'^*_1 c_{11} + b'^*_2 c_{21} + b'^*_3 c_{31}
\]
Applying (36), we obtain (31)
\[
b'_1 = b'^*_1 + b'^*_3 \alpha'^*_3
\]

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