ON THE CONSTITUENT ITEMS OF THE REDUCTION AND THE REMAINDER IN THE METHOD OF LEAST SQUARES

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1. Consider a set of variates y_i, $(i = 1, 2, \cdots, n)$, which are normally and independently distributed with variance 1. Let also a matrix (x_{ik}) with $i = 1, 2, \cdots, n; k = 1, 2, \cdots, s$ and rank s be given. Find $b_1, \cdots, b_s$ in terms of y_i so that

$$\psi^2 = \sum_i (y_i - \sum_k x_{ik} b_k)^2$$

is a minimum. This minimum value shall be denoted by $\psi^2_{\min}$.

It is known (see e.g. R. A. Fisher, "Applications of Student's distribution", *Metron* Vol. 5, Part 3 (1925)) that $\psi^2_{\min}$ varies as does χ^2 with $n - s$ degrees of freedom and that it is possible to express $\psi^2_{\min}$ as the sum of $n - s$ squares of linear functions of the y_i. In the following lines $\sum_i y_i^2$ will be expressed as the sum of n squares of such functions which are independent and of variance 1. The sum of the first s squares will equal $\sum_i y_i^2 - \psi^2_{\min}$ and therefore the remaining $n - s$ squares equal $\psi^2_{\min}$.

Thus a simple way will be found of writing down explicitly the linear functions, whose existence only was proved by Professor Fisher in *Metron.*

2. We first calculate $\psi^2_{\min}$.

$\frac{\partial \psi^2}{\partial b_l} = 0$, for $l = 1, 2, \cdots, s$, gives the normal equations

$$\sum_{i=1}^{n} x_{il} y_i = \sum_{i=1}^{n} \sum_{k=1}^{s} x_{il} x_{ik} b_k, \tag{1}$$

which can be written

$$\sum_{i=1}^{n} x_{il} y_i = \sum_{k=1}^{s} X_{lk} b_k \tag{2}$$

with

$$X_{lk} = \sum_{i=1}^{n} x_{il} x_{ik}.$$

It follows from (1) that

$$\psi^2_{\min} = \sum_{i=1}^{n} y_i^2 - \sum_{i=1}^{n} \sum_{l=1}^{s} \sum_{k=1}^{s} x_{il} x_{ik} b_l b_k = \sum_{i=1}^{n} y_i^2 - \sum_{l=1}^{s} \sum_{k=1}^{s} X_{lk} b_l b_k, \tag{A}$$

where the b are solutions of (1).

3. A second expression for $\psi^2_{\min}$ can be found as follows: Introducing

$$c_i = \sum_{k=1}^{s} x_{ik} b_k$$

we obtain from (1)

$$\sum_{i=1}^{n} x_{il} c_i = \sum_{i=1}^{n} x_{il} y_i , \qquad (l = 1, 2, \cdots s). \tag{3}$$

Now if z_{iu}, $(u = s + 1, \cdots n)$, are any $n - s$ independent solutions of

$$\sum_{i=1}^{n} z_{iu} x_{il} = 0, \qquad (l = 1, 2, \cdots, s),$$

then the c_i satisfy also

$$\sum_{i=1}^{n} z_{iu} c_i = 0, \qquad (u = s + 1, \cdots n). \tag{4}$$

Let such a set of z_{iu} be chosen. Then (3) will be solved by

$$c_i = y_i - \sum_{v=s+1}^{n} \lambda_v z_{iv} \tag{5}$$

with λ_v as indefinite factors and these c_i satisfy (4), if

$$\sum_{i=1}^{n} z_{iu} y_i = \sum_{v=s+1}^{n} \sum_{i=1}^{n} z_{iu} z_{iv} \lambda_v , \qquad (u = s + 1, \cdots n), \quad \text{or} \quad \sum_{i=1}^{n} z_{iu} y_i = \sum_{v=s+1}^{n} Z_{uv} \lambda_v \tag{6}$$

with

$$Z_{uv} = \sum_{i=1}^{n} z_{iu} z_{iv} .$$

Because of (2) the equation (A) can be transformed into

$$\psi^2_{\min} = \sum_{i=1}^{n} y_i^2 - \sum_{l=1}^{s} \sum_{i=1}^{n} x_{il} y_i b_l = \sum_{i=1}^{n} y_i^2 - \sum_{i=1}^{n} y_i c_i = \sum_{i=1}^{n} \sum_{v=s+1}^{n} \lambda_v z_{iv} y_i$$

which is, because of (6)

$$\psi^2_{\min} = \sum_{u=s+1}^{n} \sum_{v=s+1}^{n} Z_{uv} \lambda_u \lambda_v , \tag{B}$$

where the λ are solutions of (6).

The comparison of (A) and (B) gives

$$\sum_{i=1}^{n} y_i^2 = \sum_{l=1}^{s} \sum_{k=1}^{s} X_{lk} b_l b_k + \sum_{u=s+1}^{n} \sum_{v=s+1}^{n} Z_{uv} \lambda_u \lambda_v$$

where the first form on the r.h.s. shows the reduction of $\sum_{i=1}^{n} y_i^2$ by the method of least squares and the second form constitutes the remainder.

4. These two forms must now be expressed in terms of the y_i.

We introduce the notations

$$X^{(1)} = X_{11}, \qquad X^{(2)} = \begin{vmatrix} X_{11} X_{12} \\ X_{21} X_{22} \end{vmatrix}, \qquad \cdots X^{(s)} = \begin{vmatrix} X_{11} & \cdots & X_{1s} \\ \cdots & \cdots & \cdots \\ X_{s1} & \cdots & X_{ss} \end{vmatrix}$$

and

$$Z^{(s+1)} = Z_{s+1,s+1}, \qquad Z^{(s+2)} = \begin{vmatrix} Z_{s+1\,s+1} Z_{s+1\,s+2} \\ Z_{s+2\,s+1} Z_{s+2\,s+2} \end{vmatrix} \quad \text{etc.}$$

It is well known (and can easily be verified) that

$$\sum_{l=1}^{s} \sum_{k=1}^{s} X_{lk} b_l b_k = \frac{1}{X^{(1)}} (X_{11} b_1 + \cdots + X_{1s} b_s)^2$$
$$+ \frac{1}{X^{(1)} X^{(2)}} \left(\begin{vmatrix} X_{11} X_{12} \\ X_{21} X_{22} \end{vmatrix} b_2 + \cdots + \begin{vmatrix} X_{11} X_{1s} \\ X_{21} X_{2s} \end{vmatrix} b_s \right)^2$$
$$+ \cdots + \frac{1}{X^{(s-1)} X^{(s)}} X^{(s)2} b_s^2$$

which may be written

$$\frac{1}{X^{(1)}} \left(\sum_{k=1}^{s} X_{1k} b_k \right)^2 + \frac{1}{X^{(1)} X^{(2)}} \begin{vmatrix} X_{11} & \sum_{k=1}^{s} X_{1k} b_k \\ X_{21} & \sum_{k=1}^{s} X_{2k} b_k \end{vmatrix}^2$$
$$+ \cdots + \frac{1}{X^{(s-1)} X^{(s)}} \begin{vmatrix} X_{11} X_{12} & \cdots & \sum_{k=1}^{s} X_{1k} b_k \\ \cdots & \cdots & \cdots \\ X_{s1} X_{s2} & \cdots & \sum_{k=1}^{s} X_{sk} b_k \end{vmatrix}^2 .$$

Using (2), this can be expressed in terms of the y_i instead of b_k as follows:

$$\frac{1}{X^{(1)}} \left(\sum_{i=1}^{n} x_{i1} y_i \right)^2 + \frac{1}{X^{(1)} X^{(2)}} \begin{vmatrix} X_{11} & \sum_{i=1}^{n} x_{i1} y_i \\ X_{21} & \sum_{i=1}^{n} x_{i2} y_i \end{vmatrix}^2$$

(7)

$$+ \cdots + \frac{1}{X^{(s+1)} X^{(s)}} \begin{vmatrix} X_{11} X_{12} & \cdots & \sum_{i=1}^{n} x_{i1} y_i \\ \cdots & \cdots & \cdots \\ X_{s1} X_{s2} & \cdots & \sum_{i=1}^{n} x_{is} y_i \end{vmatrix}^2 .$$

Similarly by (6) the second form can be transformed into

$$(8)\ \psi^2_{\min} = \frac{1}{Z^{(s+1)}}\left(\sum_{i=1}^{n} z_{i_{s+1}} y_i\right)^2 + \cdots + \frac{1}{Z^{(n-1)}Z^{(n)}} \begin{vmatrix} Z_{s+1\,s+1} Z_{s+1\,s+2} \cdots \sum_{i=1}^{n} z_{is+1} y_i \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ Z_{ns+1}\ Z_{ns+2}\ \cdots \sum_{i=1}^{n} z_{in}\, y_i \end{vmatrix}^2.$$

The rank of (x_{ik}) is s, so that the order of the suffices can always be chosen so as to make the above denominators different from zero.

Thus both the reduction and the remainder have been expressed by sums of squares, whose numbers correspond to the "degrees of freedom" s and $n - s$ respectively.

5. It remains to be shown that the linear functions of the y_i appearing in each form are mutually orthogonal and that in every one of them the sums of the squares of the coefficients are unity.

Now if we call the n linear forms which occur above $\sum_{j=1}^{n} a_{ij} y_j$, $(i = 1, 2, \cdots, n)$, then our proof implies that

$$\sum_{i=1}^{n} y_i^2 = \sum_{i=1}^{n}\left[\sum_{j=1}^{n} a_{ij} y_j\right]^2 = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} a_{ij} a_{ik} y_j y_k .$$

This is an identity for any y_i, hence we must have

$$\sum_{i=1}^{n} a_{ij}\, a_{ik} = 1 \quad \text{if} \quad j = k, \quad \text{and}$$

$$= 0 \quad \text{if} \quad j \neq k.$$

We have thus shown that the matrix (a_{ij}) is orthogonal and it follows that

$$\sum_{i=1}^{n} a_{ji}\, a_{ki} = 1 \quad \text{if} \quad j = k \quad \text{and}$$

$$= 0 \quad \text{if} \quad j \neq k.$$

6. In practical applications the x_{ik} will be given and if the expression (7) or (8) is to be written down we must first solve the set of equations

$$\sum_{i=1}^{n} z_{iu}\, x_{il} = 0, \qquad (l = 1, 2, \cdots, s).$$

We may assume that

$$\begin{vmatrix} x_{11} & \cdots & x_{s1} \\ \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots \\ x_{1s} & \cdots & x_{ss} \end{vmatrix} \neq 0.$$

There exist, of course, an infinity of solutions. A very simple one can be found if the matrix (x_{ik}) is completed into a square matrix by adding 1 in the diagonal places and 0 elsewhere. We obtain

$$\begin{vmatrix} x_{11} & \cdots & x_{s1} & x_{s+1\,1} & \cdots & x_{ns} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{1s} & \cdots & x_{ss} & x_{s+1\,s} & \cdots & x_{ns} \\ 0 & \cdots & 0 & 1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & 0 & \cdots & 1 \end{vmatrix} \neq 0.$$

The minors of the terms of any of the $s + 1$th, $\cdots$ nth line give one of $n - s$ independent sets of solutions for the z_{iu}.

If, e.g. $s = 1$, then the z_{iu} are

$$\begin{matrix} -x_{21} & x_{11} & 0 & 0 & \cdots \\ -x_{31} & 0 & x_{11} & 0 & \cdots \\ -x_{41} & 0 & 0 & x_{11} & \cdots \end{matrix}$$

etc.

and the Z are

$$\begin{matrix} x_{11}^2 + x_{21}^2, & x_{21}x_{31}, & x_{21}x_{41} \\ x_{21}x_{31}, & x_{11}^2 + x_{31}^2, & x_{31}x_{41} \\ x_{21}x_{41}, & x_{31}x_{41}, & x_{11}^2 + x_{41}^2 \end{matrix}$$

etc.

Hence, for $s = 1$, $n = 2$,

$$\psi_{\min}^2 = \sum_{i=1}^{n} y_i^2 - \frac{1}{x_{11}^2 + x_{21}^2}(x_{11}y_1 + x_{21}y_2)^2 = \frac{1}{x_{11}^2 + x_{21}^2}(-x_{21}y_1 + x_{11}y_2)^2$$

and for $s = 1$, $n = 3$

$$\psi_{\min}^2 = \sum_{i=1}^{n} y_i^2 - \frac{(x_{11}y_1 + x_{21}y_2 + x_{31}y_3)^2}{x_{11}^2 + x_{21}^2 + x_{31}^2}$$

$$= \frac{1}{x_{11}^2 + x_{21}^2}(-x_{21}y_1 + x_{11}y_2)^2 + \frac{\begin{vmatrix} x_{11}^2 + x_{21}^2 & -x_{21}y_1 + x_{11}y_2 \\ x_{21}x_{31} & -x_{31}y_1 + x_{11}y_3 \end{vmatrix}^2}{(x_{11}^2 + x_{21}^2)\begin{vmatrix} x_{11}^2 + x_{21}^2 & x_{21}x_{31} \\ x_{21}x_{31} & x_{11}^2 + x_{31}^2 \end{vmatrix}}.$$

If, however, $s = 2$, $n = 3$, then easy calculations lead to

$$\psi^2_{\min} = \sum_{i=1}^{n} y_i^2 - \frac{(x_{11}y_1 + x_{21}y_2 + x_{31}y_3)^2}{x_{11}^2 + x_{21}^2 + x_{31}^2}$$

$$- \frac{\begin{vmatrix} x_{11}^2 + x_{21}^2 + x_{31}^2 & x_{11}y_1 + x_{21}y_2 + x_{31}y_3 \\ x_{11}x_{12} + x_{21}x_{22} + x_{31}x_{32} & x_{12}y_1 + x_{22}y_2 + x_{32}y_3 \end{vmatrix}}{(x_{11}^2 + x_{21}^2 + x_{31}^2 \begin{vmatrix} x_{11}^2 + x_{21}^2 + x_{31}^2 & x_{11}x_{12} + x_{21}x_{22} + x_{31}x_{32} \\ x_{12}x_{11} + x_{22}x_{21} + x_{32}x_{31} & x_{12}^2 + x_{22}^2 + x_{32}^2 \end{vmatrix}}$$

$$= \left(\begin{vmatrix} x_{21} x_{31} \\ x_{22} x_{32} \end{vmatrix} y_1 + \begin{vmatrix} x_{31} x_{11} \\ x_{32} x_{12} \end{vmatrix} y_2 + \begin{vmatrix} x_{11} x_{21} \\ x_{12} x_{22} \end{vmatrix} y_3 \right)^2$$

$$\div \left(\begin{vmatrix} x_{21} x_{31} \\ x_{22} x_{32} \end{vmatrix}^2 + \begin{vmatrix} x_{31} x_{11} \\ x_{32} x_{12} \end{vmatrix}^2 + \begin{vmatrix} x_{11} x_{21} \\ x_{12} x_{22} \end{vmatrix}^2 \right).$$

As a specialized case consider $s = 1$, and $x_{11} = x_{21} = \cdots = x_{n1} = 1$. Then the Z are

$$\begin{matrix} 2 & 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & 2 & 1 & 1 & \cdots & 1 & 1 \\ \cdots & & & & & & \\ 1 & 1 & 1 & 1 & \cdots & 2 & 1 \\ 1 & 1 & 1 & 1 & \cdots & 1 & 2 \end{matrix}$$

and

$$\psi^2_{\min} = \sum_{i=1}^{m} y_i^2 = \frac{1}{n}\left(\sum_{i=1}^{n} y_i\right)^2 = \sum_{i=1}^{n}\left(y_i - \frac{\sum_{i=1}^{n} y_i}{n}\right)^2.$$

The sum of squares into which $\psi^2_{\min}$ can be transformed is then found to be

$$\frac{1}{2}(-y_1 + y_2)^2 + \frac{1}{2\cdot 3}(-y_1 - y_2 + 2y_3)^2 + \frac{1}{3\cdot 4}(-y_1 - y_2 - y_3 + 3y_4)^2 + \cdots .$$ [1]

[1] This is the result contained in a paper by J. O. Irwin, "Independence of the constituent items in the analysis of variance" *Suppl. Roy. Stat. Soc. Jour.* Vol. 1 (1934).