## **Theory underlying** *pulver*

A general linear regression model is given as

$$
y = X\beta + \epsilon, \ \epsilon \sim N(0, \sigma^2 I).
$$

Here  $y^T = (y_1, y_2, ..., y_n)$  is an  $n \times 1$  vector, the dependent variable. X represents the  $n \times$  $(p + 1)$  covariate matrix with corresponding  $\beta^T = (\beta_0, \beta_1, ..., \beta_p)$  a  $(p + 1) \times 1$  vector of unknown regression coefficients. The  $n \times 1$  vector  $\epsilon$  serves as error term has variance  $\sigma^2$ , and  $\epsilon_1$ , ...,  $\epsilon_n$  are independent and identical distributed (i.i.d.).

Let 
$$
X = \begin{pmatrix} 1 & x_1 & z_1 & w_1 = x_1 \cdot z_2 \\ 1 & x_2 & z_2 & w_2 = x_2 \cdot z_2 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & z_n & w_n = x_n \cdot z_n \end{pmatrix}
$$
, and the unknown regression coefficients

 $\beta^T = (\beta_0 \quad \beta_1 \quad \beta_2 \quad \beta_3)$ . The then above general linear model reduces to the following linear regression model

$$
y = \beta_0 + \beta_1 x + \beta_2 z + \beta_3 w + \epsilon, \epsilon \sim N(0, \sigma^2),
$$

with  $\epsilon_1, ..., \epsilon_n$  being independent and identical distributed (*i. i. d.*).

We want to test the null-hypothesis that  $\beta_3 = 0$  against the alternative hypothesis that  $\beta_3 \neq 0$ , where  $\beta_3$  is the regression coefficient of w. In order to eliminate the intercept  $\beta_0$ , we center all variables, such that  $\sum_i y_i = \sum_i x_i = \sum_i z_i = \sum_i w_i = 0$ , to obtain the following simplified regression model:

$$
y = \beta_1 x + \beta_2 z + \beta_3 w + \epsilon, \qquad \epsilon \sim N(0, \sigma^2) \text{ i.i.d.}
$$

(For simplicity, we retain the notations from above for the simplified model (for variable names  $y$ , x, z, and  $w$  for the centered variables, regression coefficients, error term))

The vectors x, z and w span a subspace S of  $\mathbb{R}^n$ . The ordinary least-squares (OLS) estimates of  $\hat{\beta}$  are found by minimizing the residual sum of squares over  $y - X\beta$ :

$$
\hat{\beta} = \arg\min_{\beta} \ (y - X\beta)^T (y - X\beta).
$$

Geometrically, this means that  $\hat{\beta}_1, \hat{\beta}_2,$  and  $\hat{\beta}_3$  must be selected such that

$$
y' = \hat{\beta}_1 x + \hat{\beta}_2 z + \hat{\beta}_3 w \tag{1}
$$

is the orthogonal projection of y onto S, the subspace spanned by  $w$ ,  $x$ , and z. It can be shown that if x, y, and z form an orthogonal basis of S, the coefficients of the orthogonal projection  $y'$ of  $\nu$  onto  $S$  are given by

$$
\hat{\beta}_1 = \frac{\langle y, x \rangle}{\langle x, x \rangle} , \hat{\beta}_2 = \frac{\langle y, z \rangle}{\langle z, z \rangle} , \hat{\beta}_3 = \frac{\langle y, w \rangle}{\langle w, w \rangle} [1].
$$

Unlike the usual formula for computing OLS coefficient estimates  $(\hat{\beta} = (X^T X)^{-1} X^T y)$ , this formula does not involve an expensive matrix inversion, but instead is easy and fast to compute.

In general,  $w, x$ , and  $z$  do not form an orthogonal basis, so we proceed as follows.

- 1. Create an orthogonal basis  $v_1$ ,  $v_2$ , and  $v_3$  for S based on x, z, and w, respectively.
- 2. Compute  $y'$ , the orthogonal projection of  $y$  onto  $S$ , using the orthogonal basis created in step 1.
- 3. Deduce the estimate of the regression coefficient for  $w$  from the regression coefficients for  $y'$ .
- 4. Compute the Student's *t*-test statistic to test  $\beta_3 = 0$  as a function of the correlation coefficient r between y' and  $\beta_3 \nu_3$ .

### **1. Create an orthogonal basis for S**

Let

 $v_1 = x$ ,

$$
v_2 = z - proj(z, v_1), \text{and}
$$

$$
v_3 = w - proj(w, v_1) - proj(w, v_2),
$$

where

$$
proj(a,b) = \frac{\langle a,b \rangle}{\langle b,b \rangle}b
$$

is the orthogonal projection of a onto b. The vectors  $v_1$ ,  $v_2$  and  $v_3$  form an orthogonal basis of S. By construction, we clearly observe that  $v_1$  is dependent on x only,  $v_2$  is dependent on z and x and  $v_3$  depends on x, z, and w.

### **2. Orthogonally project y onto S**

The orthogonal projection  $y'$  of  $y$  onto  $S$  has the form

$$
y' = \beta_1' v_1 + \beta_2' v_2 + \beta_3' v_3 \tag{2}
$$

where

$$
\beta'_i = \frac{\langle y, v_i \rangle}{\langle v_i, v_i \rangle} \quad (i = 1, 2, 3),
$$

with  $||a|| = \sqrt{\langle a, a \rangle}$ ,

and  $\langle a, b \rangle = \sum a_i b_i$  $\boldsymbol{n}$  $i=1$ being the inner product of vectors a and b in  $\mathbb{R}^n$ .

#### **3. Deduce the estimate of w's regression coefficient**

We want to estimate the regression coefficient  $\beta_3$  of the vector w given in Equation 1 using Equation 2. The vector w occurs in  $v_3$  but not in  $v_1$  or  $v_2$ . This allows us to write y' as

$$
y' = \beta_1' v_1 + \beta_2' v_2 + \beta_3' v_3
$$
  
\n
$$
= \beta_1' v_1 + \beta_2' v_2 + \beta_3' (w - \text{proj}(w, v_1) - \text{proj}(w, v_2))
$$
  
\n
$$
= \beta_1' v_1 + \beta_2' v_2 + \beta_3' w - \beta_3' \text{proj}(w, v_1) - \beta_3' \text{proj}(w, v_2)
$$
  
\n
$$
= \beta_3' w + \beta_1' v_1 + \beta_2' v_2 - \beta_3' \text{proj}(w, v_1) - \beta_3' \text{proj}(w, v_2)
$$
  
\n
$$
= \beta_3' w + \beta_1' v_1 + \beta_2' v_2 - \underbrace{\beta_3' \frac{\langle w, v_1 \rangle}{\langle v_1, v_1 \rangle}}_{scalar} v_1 - \underbrace{\beta_3' \frac{\langle w, v_2 \rangle}{\langle v_2, v_2 \rangle}}_{scalar} v_2
$$
  
\n
$$
= \beta_3' w + c \left( \underbrace{v_1}_{c(x)}, \underbrace{v_2}_{c(x,z)} \right)
$$
  
\n
$$
= \beta_3' w + c(x, z)
$$

where  $c(...)$  represents a linear combination of x or x and z, accordingly. This allows us to identify  $\beta_3$ , and we estimate the regression coefficient of w in Equation (1):

$$
\beta_3 = \beta_3' = \frac{\langle y, v_3 \rangle}{\langle v_3, v_3 \rangle}.
$$

# **4.** Compute the Student's *t*-test statistic to test  $\beta_3 = 0$  as a function of the correlation **coefficient** *r* between  $y'$  and  $\beta_3$   $v_3$ .

We want to show that the Student's *t*-test statistic usually used to test for  $\beta_3 = 0$  in a linear regression model, with  $t \geq t^*$  for significant threshold  $t^*$  can be computed using the Pearson's correlation coefficient r. The Pearson's correlation coefficient r between  $y'$  and  $v_3$ (both centered) is computed as follows:

$$
r = \frac{\sum_{i=1}^{N} y_i'^2 v_{3i}}{\|y'\| \|v_3\|} = \frac{\sum_{i=1}^{N} y_i'^2 v_{3i}}{\sqrt{\sum_{i=1}^{N} y_i'^2} \sqrt{\sum_{i=1}^{N} v_{3i}^2}}.
$$

It then has to hold that  $r \geq t^* \cdot \sqrt{\frac{1}{n!}}$  $\frac{1}{DF + t^{*2}}$  if we want to reject the null-hypotesis.

The fact that  $v_1, v_2$ , and  $v_3$  are orthogonal means that  $\beta_3$  is actually the OLS estimate of the regression coefficient  $r$  in the simple linear regression

$$
y' = \beta_3 \ v_3 + \epsilon, \ \epsilon \sim N(0, \sigma^2) \ i.i.d \tag{3}
$$

The Student's *t* –statistic to test for coefficient  $\beta_3 = 0$  is given by

$$
t = \frac{\beta_3}{se(\beta_3)}
$$

and it has a Student's t distribution with  $DF = n - 4$  degrees of freedom. Subtracting 4 results from the number of regression coefficients in the initial model and the estimated variance of  $\epsilon$ :  $\hat{\beta}_1$ ,  $\hat{\beta}_2$ ,  $\hat{\beta}_3$ ,  $s^2$ .

From the theory of simple linear regression, we know the following relationships (e.g., see Snedecor and Cochran 1967 [2], chapter 7.3, p. 175 ff.):

a) 
$$
\beta_3 = r \frac{se(y)}{se(v_3)}
$$
  
\nb)  $se(\beta_3) = s / \sqrt{\sum_{i=1}^n v_3_i^2}$   
\nc)  $s^2 = \frac{1 - r^2}{DF} \sum_{i=1}^N y_i'^2$   
\nd)  $se(a) = \sqrt{\frac{1}{n-1} \sum_{i=1}^n a_i^2}$ , with vector  $a$  in  $\mathbb{R}^n$  and  $\sum_i a_i = 0$ ,

where  $\beta_3$  is the OLS estimate of Equation 3; se(y) and se( $v_3$ ) are the sample estimates of the standard deviations of y and  $v_3$ , respectively; se( $\beta_3$ ) is the estimate of the standard deviation of  $\beta_3$ ;  $s^2$  is the OLS estimate of  $\sigma^2$ , the variance of the error term  $\epsilon$ ; r is the Pearson's correlation coefficient of y and  $v_3$ ; and DF is the degree of freedom.

After plugging Equations a–d into the formula for the Student's *t*, we obtain the following:

$$
t = \frac{\beta_3}{se(\beta_3)}
$$
  
\n
$$
= \frac{r \frac{se(y')}{se(v_3)}}{\sqrt{\sum_{i=1}^{N} v_{3i}^2}}
$$
  
\n
$$
= \frac{r se(y') \sqrt{\sum_{i=1}^{N} v_{3i}^2}}{se(v_3) \sqrt{\frac{(1-r^2)}{DF} \sum_{i=1}^{N} y_i'^2}}
$$
  
\n
$$
= \frac{r \sqrt{DF}}{\sqrt{(1-r^2)}} \cdot \frac{se(y') \sqrt{\sum_{i=1}^{n} v_{3i}^2}}{se(v_3) \sqrt{\sum_{i=1}^{n} y_i'^2}}
$$
  
\n
$$
= \frac{r \sqrt{DF}}{\sqrt{(1-r^2)}} \cdot \frac{\sqrt{\frac{1}{n-1} \sum_{i=1}^{n} y_i'^2} \sqrt{\sum_{i=1}^{n} v_{3i}^2}}{\sqrt{\frac{1}{n-1} \sum_{i=1}^{n} v_{3i}^2} \sqrt{\sum_{i=1}^{n} y_i'^2}}
$$
  
\n
$$
= \frac{r \sqrt{DF}}{\sqrt{(1-r^2)}}
$$

- 1. Saville D, Wood GR, Statistical methods: The geometric approach. Springer Science & Business Media; 2012.
- 2. Snedecor, G. and W. Cochran, Statistical methods. 6th ed. Ames Iowa: University Press; 1967. p. 349-352.