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 ϵ serves as error term has variance σ^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

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

with $\epsilon_1, \dots, \epsilon_n$ 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 β_3 is the regression coefficient of w. In order to eliminate the intercept β_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:

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

(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

$$y' = \hat{\beta}_1 x + \hat{\beta}_2 z + \hat{\beta}_3 w$$
 (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 y 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 $\beta_3 v_3$.

1. Create an orthogonal basis for S

Let

 $v_1 = x$,

$$v_2 = z - proj(z, v_1)$$
, 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

$$y' = \beta'_1 v_1 + \beta'_2 v_2 + \beta'_3 v_3$$
(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 $\langle a, b \rangle = \sum_{i=1}^{n} a_i b_i$ 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 β_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

$$y' = \beta_1' v_1 + \beta_2' v_2 + \beta_3' v_3$$

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

where c(...) represents a linear combination of x or x and z, accordingly. This allows us to identify β_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 $t \ge t^*$ 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:

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

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

The fact that v_1, v_2 , and v_3 are orthogonal means that β_3 is actually the OLS estimate of the regression coefficient *r* in the simple linear regression

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

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 ϵ : $\hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_3, s^2$.

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)
$$\beta_3 = r \frac{se(y')}{se(v_3)}$$

b) $se(\beta_3) = s / \sqrt{\sum_{i=1}^n v_{3_i}^2}$
c) $s^2 = \frac{1 - r^2}{DF} \sum_{i=1}^N y_i'^2$
d) $se(a) = \sqrt{\frac{1}{n-1} \sum_{i=1}^n a_i^2}$, with vector a in \mathbb{R}^n and $\sum_i a_i = 0$,

where β_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 β_3 ; s^2 is the OLS estimate of σ^2 , the variance of the error term ϵ ; 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:

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

- 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.