16 Lecture 16 Feb 24

Last time

- Confidence intervals for SLR
- Multiple linear regression

Today

- Multiple correlation
- Lab review

A multiple linear regression (MLR) model w/ p independent variables

Let p independent variables be denoted by x_1, \ldots, x_p .

- Observed values of p independent variables for i^{th} subject from sample denoted by x_{i1}, \ldots, x_{ip}
- response variable for i^{th} subject denoted by Y_i
- For i = 1, ..., n, MLR model for Y_i :

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} + \epsilon_i$$

• As in SLR, $\epsilon_1, \ldots, \epsilon_n \stackrel{iid}{\sim} N(0, \sigma^2)$

Least squares estimates of regression parameters minimize SS[E]:

$$SS[E] = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{i1} - \dots - \beta_p x_{ip})^2$$

$$\hat{\sigma}^2 = \frac{SS[E]}{n-p-1}$$

Interpretations of regression parameters:

- σ^2 is unknown <u>error variance</u> parameter
- $\beta_0, \beta_1, \dots, \beta_p$ are p+1 unknown regression parameters:
 - $-\beta_0$: average response when $x_1 = x_2 = \cdots = x_p = 0$
 - $-\beta_i$ is called a <u>partial slope</u> for x_i . Represents mean change in y per unit increase in x_i with all other independent variables held fixed.

Matrix formulation of MLR

Let a vector for p observed independent variables for individual i be defined by

$$x_{i\cdot} = (1, x_{i1}, x_{i2}, \dots, x_{ip}).$$

The MLR model for Y_1, \ldots, Y_n is given by

$$Y_{1} = \beta_{0} + \beta_{1}X_{11} + \beta_{2}X_{12} + \dots + \beta_{p}X_{1p} + \epsilon_{1}$$

$$Y_{2} = \beta_{0} + \beta_{1}X_{21} + \beta_{2}X_{22} + \dots + \beta_{p}X_{2p} + \epsilon_{2}$$

$$\vdots = \vdots$$

$$Y_{n} = \beta_{0} + \beta_{1}X_{n1} + \beta_{2}X_{n2} + \dots + \beta_{p}X_{np} + \epsilon_{n}$$

This system of n equations can be expressed using matrices:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where

- Y denotes a response vector of size $n \times 1$
- X denotes a design matrix of size $n \times (p+1)$
- β denotes a vector of regression parameters of size $(p+1) \times 1$
- ϵ denotes an error vector of size $n \times 1$

Here, the error vector ϵ is assumed to follow a multivariate normal distribution with variance-covariance matrix $\sigma^2 \mathbf{I}_n$. For individual i,

$$y_i = \mathbf{x}_{i \cdot} \boldsymbol{\beta} + \epsilon_i.$$

Some simplified expressions: (a is a known $p \times 1$ vector)

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}$$

$$\mathbf{Var} \left(\hat{\boldsymbol{\beta}} \right) = \sigma^2 (\mathbf{X}^T \mathbf{X})^{-1}$$

$$= \mathbf{\Sigma}$$

$$\widehat{\mathrm{Var}} (\hat{\boldsymbol{\beta}}) = MS[E] (\mathbf{X}^T \mathbf{X})^{-1}$$

$$= \widehat{\mathbf{\Sigma}}$$

$$\widehat{\mathrm{Var}} (\mathbf{a}^T \hat{\boldsymbol{\beta}}) = \mathbf{a}^T \widehat{\mathbf{\Sigma}} \mathbf{a}$$

Question: what are the dimensions of each of these quantities?

- $(\mathbf{X}^T\mathbf{X})^{-1}$ may be verbalized as "x transposed x inverse"
- $\widehat{\Sigma}$ is the estimated variance-covariance matrix for the estimate of the regression parameter vector $\widehat{\beta}$

• X is assumed to be of full rank.

Some more simplified expressions:

$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$$

$$= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

$$= \mathbf{H}\mathbf{Y}$$

$$\hat{\boldsymbol{\epsilon}} = \mathbf{Y} - \hat{\mathbf{Y}}$$

$$= \mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}$$

$$= (\mathbf{I} - \mathbf{H})\mathbf{Y}$$

- $\hat{\mathbf{Y}}$ is called the vector of <u>fitted</u> or predicted values
- $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ is called the <u>hat matrix</u>
- $\hat{\epsilon}$ is the vector of <u>residuals</u>

For the Duncan's data example on income, education and prestige, with p=2 independent variables and n=45 observations,

$$\mathbf{X} = \begin{bmatrix} 1 & 62 & 86 \\ 1 & 72 & 76 \\ \vdots & \vdots & \vdots \\ 1 & 8 & 32 \end{bmatrix}$$

and

$$\mathbf{X}^{T}\mathbf{X} = \begin{bmatrix} 45 & 1884 & 2365 \\ 1884 & 105148 & 122197 \\ 2365 & 122197 & 163265 \end{bmatrix}$$

$$(\mathbf{X}^{T}\mathbf{X})^{-1} = \begin{bmatrix} 0.10211 & -0.00085 & -0.00084 \\ -0.00085 & 0.00008 & -0.00005 \\ -0.00084 & -0.00005 & 0.00005 \end{bmatrix}$$

$$(\mathbf{X}^{T}\mathbf{X})^{-1}\mathbf{X}^{T}\mathbf{Y} = \begin{bmatrix} -6.0646629 \\ 0.5987328 \\ 0.5458339 \end{bmatrix} = ?$$

$$SS[E] = \boldsymbol{\epsilon}^{T}\boldsymbol{\epsilon} = (\mathbf{Y} - \hat{\mathbf{Y}})^{T}(\mathbf{Y} - \hat{\mathbf{Y}}) = 7506.7$$

$$MS[E] = \frac{SS[E]}{df} = \frac{7506.7}{45 - 2 - 1} = 178.73$$

$$\hat{\boldsymbol{\Sigma}} = MS[E](\mathbf{X}^{T}\mathbf{X})^{-1} = \begin{bmatrix} 18.249481 & -0.151845008 & -0.150706025 \\ -0.151845 & 0.014320275 & -0.008518551 \\ -0.150706 & -0.008518551 & 0.009653582 \end{bmatrix}$$

Multiple correlation, JF 5.2.3

The sums of squares in multiple regression are defined in the same manner as in SLR:

$$TSS = \sum (Y_i - \bar{Y})^2$$

$$RegSS = \sum (\hat{Y}_i - \bar{Y})^2$$

$$RSS = \sum (Y_i - \hat{Y}_i)^2 = \sum \hat{\epsilon}_i^2$$

Not surprisingly, we have a similar analysis of variance for the regression:

$$TSS = RegSS + RSS$$

The squared multiple correlation R^2 , representing the proportion of variation in the response variable captured by the regression, is defined in terms of the sums of squares:

$$R^2 = \frac{RegSS}{TSS} = 1 - \frac{RSS}{TSS}.$$

Because there are several slope coefficients, potentially with different signs, the *multiple* correlation coefficient is, by convention, the positive square root of R^2 . The multiple correlation is also interpretable as the simple correlation between the fitted and observed Y values, i.e. $r_{\hat{Y}Y}$.

Adjusted- R^2

Because the multiple correlation can only rise, never decline, when explanatory variables are added to the regression equation (HW1), investigators sometimes penalize the value of R^2 by a "correction" for degrees of freedom. The corrected (or "adjusted") R^2 is defined as:

$$R_{adj}^{2} = 1 - \frac{\frac{RSS}{n-p-1}}{\frac{TSS}{n-1}}$$
$$= 1 - \left[\frac{(1-R^{2})(n-1)}{n-p-1} \right]$$

Confidence intervals

Confidence intervals and hypothesis tests for individual coefficients closely follow the pattern of simple-regression analysis:

- 1. substitute an estimate of the error variance (MSE) for the unknown σ^2 into the variance term of $\hat{\beta}_i$
- 2. find the estimated standard error of a slope coefficient $\widehat{SE}(\hat{\beta}_i)$
- 3. $t = \frac{\hat{\beta}_i \beta_i}{\widehat{SE}(\hat{\beta}_i)}$ follows a t-distribution with degrees of freedom as associated with SSE.

Therefore, we can construct the $100(1-\alpha)\%$ confidence interval for a single slope parameter by (why?):

$$\hat{\beta}_i \pm t(n-p-1,\alpha/2)\widehat{SE}(\hat{\beta}_i)$$

Hand-waving proof:

Hypothesis tests

We first test the null hypothesis that all population regression slopes are 0:

$$H_0: \beta_1 = \beta_2 = \dots = \beta_p = 0$$

The test statistics,

$$F = \frac{RegSS/p}{RSS/(n-p-1)}$$

follows an F-distribution with p and n-p-1 degrees of freedom.

We can also test a null hypothesis about a *subset* of the regression slopes, e.g.,

$$H_0: \beta_1 = \beta_2 = \dots = \beta_q = 0.$$

Or more generally, test the null hypothesis

$$H_0: \beta_{q_1} = \beta_{q_2} = \dots = \beta_{q_k} = 0$$

where $0 \le q_1 < q_2 < \cdots < q_k \le p$ is a subset of k indices. To get the F-statistic for this case, we generally perform the following steps:

- 1. Fit the full ("unconstrained") model, in other words, model that provides context for H_0 . Record SSR_{full} and the associated df_{full}
- 2. Fit the reduced ("constrained") model, in other words, full model constrained by H_0 . Record SSR_{red} and the associated df_{red}
- 3. Calculate the F-statistic by

$$F = \frac{[SSR_{red} - SSR_{full}]/(df_{red} - df_{full})}{SSR_{full}/df_{full}}$$

4. Find p-value (the probability of observing an F-statistic that is at least as high as the value that we obtained) by consulting an F-distribution with numerator $df(ndf) = df_{red} - df_{full}$ and denominator $df(ddf) = df_{full}$. Notation: $F_{ndf,ddf}$, see Figure 16.1.

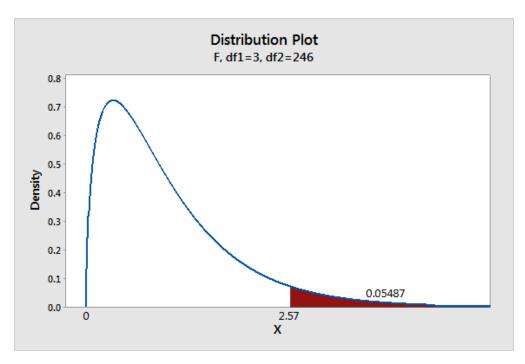


Figure 16.1: An example for p-value for F-statistic value 2.57 with an $F_{3,246}$ distribution