13 Lecture 13: Feb 23

Last time

- Lab 2 review
- Multiple linear regression

Today

- HW1 review next week
- HW2 posted, due March 4th
- Inference of MLR
- more review on probability

Matrix formulation of MLR

Let a $(1 \times (p+1))$ 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:

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

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

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

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

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

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

- ullet $\hat{\mathbf{Y}}$ 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 residuals

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

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

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

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

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

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

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

Multiple correlation, JF 5.2.3

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

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

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

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

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 $0 \le q_1 < q_2 < \dots < q_k \le p$ 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 13.1.



Figure 13.1: An example for p-value for F-statistic value 2.57 with an $F_{3,246}$ distribution

A little more background review

Reference:

- Statistical Inference, 2nd Edition, by George Casella & Roger L. Berger
- Review of Probability Theory by Arian Maleki and Tom Do

Chi-square, t-, and F-Distributions

Let $Z_1, Z_2, \ldots, Z_k \stackrel{iid}{\sim} N(0, 1)$, then $X^2 \equiv Z_1^2 + Z_2^2 + \cdots + Z_k^2 \sim \chi_k^2$ (with k degrees of freedom). If $X \sim \chi_k^2$

$$\mathbf{E}(X) = k$$

$$\mathbf{Var}(X) = 2k.$$

Student's t versus χ^2

If $X_1, \ldots, X_n \stackrel{iid}{\sim} N(\mu, \sigma^2)$, then

$$\frac{\bar{X} - \mu}{\sigma / \sqrt{n}} \sim N(0, 1).$$

When σ is unknown,

$$\frac{\bar{X} - \mu}{\hat{\sigma}/\sqrt{n}} \sim t_{n-1}$$
, where $\hat{\sigma} = \sqrt{\frac{\sum (X_i - \bar{X})^2}{n-1}}$.

Note that

$$\begin{split} \frac{\bar{X} - \mu}{\hat{\sigma}/\sqrt{n}} &= \frac{\bar{X} - \mu}{\sigma/\sqrt{n}} \cdot \frac{1}{\frac{\hat{\sigma}}{\sigma}} \\ &= Z \cdot \frac{1}{\sqrt{\frac{\sum (X_i - \bar{X})^2}{(n-1)\sigma^2}}} \\ &= \frac{Z}{\sqrt{\frac{X_{n-1}^2}{n-1}}} \end{split}$$

F versus χ^2

$$F_{ndf,ddf} \equiv \frac{\chi_{ndf}^2/ndf}{\chi_{ddf}^2/ddf}$$

t versus F

$$t_k = \frac{Z}{\sqrt{\chi_k^2/k}}$$
$$= \frac{\sqrt{\chi_1^2/1}}{\sqrt{\chi_k^2/k}}$$
$$= \sqrt{F_{1,k}}$$

or, in other words, $t_k^2 = F_{1,k}$

Random vectors and matrices

The cdf for random vector

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} \text{ is } F_{\mathbf{Y}}(\mathbf{y}) = \Pr(Y_1 \leqslant y_1, Y_2 \leqslant y_2, \dots, Y_n \leqslant y_n)$$

If a joint pdf exists, then $f_{\mathbf{Y}}(\mathbf{y}) = f_{\mathbf{Y}}(y_1, \dots, y_n)$ and

$$F_{\mathbf{Y}}(\mathbf{y}) = \int_{-\infty}^{y_1} \int_{-\infty}^{y_2} \dots \int_{-\infty}^{y_n} f_{\mathbf{Y}}(\mathbf{t}) d\mathbf{t}$$

Moments

$$\mathbf{E}\left(\mathbf{Y}\right) = \boldsymbol{\mu}_{\mathbf{Y}} = \begin{bmatrix} E(Y_1) \\ E(Y_2) \\ \vdots \\ E(Y_n) \end{bmatrix} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{bmatrix}$$

$$\mathbf{Var}\left(\mathbf{Y}\right) = \mathbf{E}\left((\mathbf{Y} - \boldsymbol{\mu}_{\mathbf{Y}})(\mathbf{Y} - \boldsymbol{\mu}_{\mathbf{Y}})^T\right)$$

$$= \mathbf{E}\left(\begin{bmatrix} (Y_1 - \mu_1)^2 & (Y_1 - \mu_1)(Y_2 - \mu_2) & \dots \\ (Y_2 - \mu_2)(Y_1 - \mu_1) & (Y_2 - \mu_2)^2 & \dots \\ \dots & \end{bmatrix}\right)$$

$$= \mathbf{E}\left([(Y_i - \mu_i)(Y_j - \mu_j), i = 1, 2, \dots, n, j = 1, 2, \dots, n]\right)$$

$$= (\sigma_{ij})_{i=1, 2, \dots, n; j=1, 2, \dots, n}$$

where $\sigma_{ij} = Cov(Y_i, Y_j)$

Linear functions

Let $\mathbf{X} \in \mathbb{R}^{k \times 1}$, $\mathbf{Y} \in \mathbb{R}^{n \times 1}$ and $\mathbf{A} \in \mathbb{R}^{k \times 1}$, $\mathbf{B} \in \mathbb{R}^{k \times n}$ be non-random, then

$$\begin{aligned} \mathbf{X} &= \mathbf{A} + \mathbf{B} \mathbf{Y} \\ \mathbf{E} \left(\mathbf{X} \right) &= \mathbf{A} + \mathbf{B} \mathbf{E} \left(\mathbf{Y} \right) \\ \mathbf{Var} \left(\mathbf{X} \right) &= \mathbf{B} \mathbf{Var} \left(\mathbf{Y} \right) \mathbf{B}^{T} \end{aligned}$$

Sums of random vectors

$$\begin{aligned} & \mathbf{X} &= \mathbf{Y} + \mathbf{Z} \\ & \mathbf{E}\left(\mathbf{X}\right) &= \mathbf{E}\left(\mathbf{Y}\right) + \mathbf{E}\left(\mathbf{Z}\right) = \mathbf{E}\left(\mathbf{Y} + \mathbf{Z}\right) \end{aligned}$$

Note that there is no independence assumed above.

$$\mathbf{Var}\left(\mathbf{X}\right) = \mathbf{Var}\left(\mathbf{Y} + \mathbf{Z}\right) = \mathbf{Var}\left(\mathbf{Y}\right) + \mathbf{Var}\left(\mathbf{Z}\right) + Cov(\mathbf{Y}, \mathbf{Z}) + Cov(\mathbf{Z}, \mathbf{Y})$$

If \mathbf{Y}, \mathbf{Z} are uncorrelated, then $\mathbf{Var}(\mathbf{X}) = \mathbf{Var}(\mathbf{Y}) + \mathbf{Var}(\mathbf{Z})$